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PROVISIONAL

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

and

INTERNATIONAL UNION OF BIOCHEMISTRY

JOINT COMMISSION ON BIOCHEMICAL NOMENCLATURE*

CONFORMATIONAL NOMENCLATURE FOR FIVE- AND SIX-MEMBERED RING FORMS OF MONOSACCHARIDES AND THEIR DERIVATIVES

Comments on these recommendations are welcome and should be set within 8 months from October 1981 to the Secretary of the Commission:

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UK

Comments from the viewpoint of languages other than English are especially encouraged. These may have special significance regarding the publication in various countries of translations of the nomenclature eventually approved by IUPAC.

*Membership of the Commission for 1979-81 is as follows:

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PROVISIONAL

IUPAC-IUB Joint Commission on Biochemical Nomenclature (JCBN)

Conformational Nomenclature for Five-and Six-Membered Ring Forms of Monosaccharides and Their Derivatives

Information on the conformation of carbohydrates is steadily increasing and there is a need for integrated recommendations on the conformational nomenclature of the most common ring-forms. The present set of recommendations is based upon a report of a subcommittee[1].

1. The approximate conformation of a five or six-membered ring form of a carbohydrate may be indicated by an italic, capital letter, designating the type of ring shape, and numerals, distinguishing between the variants of each (e.g. $^4C_1$). The conformational descriptor follows the name of the monosaccharide, e.g. D-glucose-$^4C_1$.

2. The letter is the appropriate one of the following:

Six-Membered Rings. *C* (for chair), *B* (for boat), *S* (for skew) (i.e., the form midway between two boats in the cycle of flexible forms), and *H* (for half-chair).

Five-Membered Rings. *E* (for envelope) and *T* (for twist).

Note. The various shapes are illustrated in examples (*1*)–(*16*) and in Fig. 1. These representations are idealized, minor divergences being neglected. Some of the forms shown may occur only transitorily rather than as preferred conformations.

3. The numerals are the locants of the ring-atoms that lie outside a reference plane defined under section 4. The locants of ring-atoms that lie on the side of the reference plane from which the numbering appears clockwise (this is the 'upper' side of the plane of a furanoid or pyranoid Haworth formula written in the normal manner) are written as superscripts and precede the letter; those of the ring-atoms that lie on the other side of the reference plane are written as subscripts and follow the letter.

In furanoid and pyranoid rings, the ring oxygen or other ring heteroatom, e.g. sulfur, is denoted by its element symbol (e.g. O, S). Compounds that are *meso* and can be numbered in either of two ways are regarded as belonging to the D series for the purpose of defining the direction of numbering.

4. The reference plane for each ring shape is chosen as follows (Note: some of the coplanarity relations implied in these rules are strictly true only for ideal rings having 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 aldopyranoses: $^4C_1$ 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 aldopyranoses: $^{1,4}B$, $B_{1,4}$, $^{2,5}B$, $B_{2,5}$, $^{0,3}B$ and $B_{0,3}$.

Skews. Each skew form has two potential reference planes, containing three adjacent atoms and the remaining non-adjacent atom. The reference plane is

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This is a document of the IUPAC-IUB Commission on Biochemical Nomenclature (JCBN) whose members are P. Karlson (chairman), H. B. F. Dixon, Y. Jeannin, C. Liébecq (as chairman of the IUB Committee of Editors of Biochemical Journals), B. Lindberg, K. L. Loening, G. P. Moss, and S. F. Velick. Comments may be sent to any member of the commission or to its secretary: H. B. F. Dixon, University Department of Biochemistry, Tennis Court Road, Cambridge, England, CB2 1QW. A preliminary version was published in *J. Chem. Soc. Chem. Commun.* 505–508 (1973). JCBN thanks the expert panel listed below, and also J. C. P. Schwarz who originally drafted the document, for their work and subsequent advice, and thanks the other members of the Nomenclature Committee of IUB (H. Bielka, W. B. Jakoby, B. Keil, and E. C. Webb) for consultation.

[1] Members: L. C. Cross, the late E. Hardegger, O. Hoffmann-Ostenhof, D. Horton, K. L. Loening, D. J. Manners, W. G. Overend, H. Paulsen (chairman), and R. S. Tipson.

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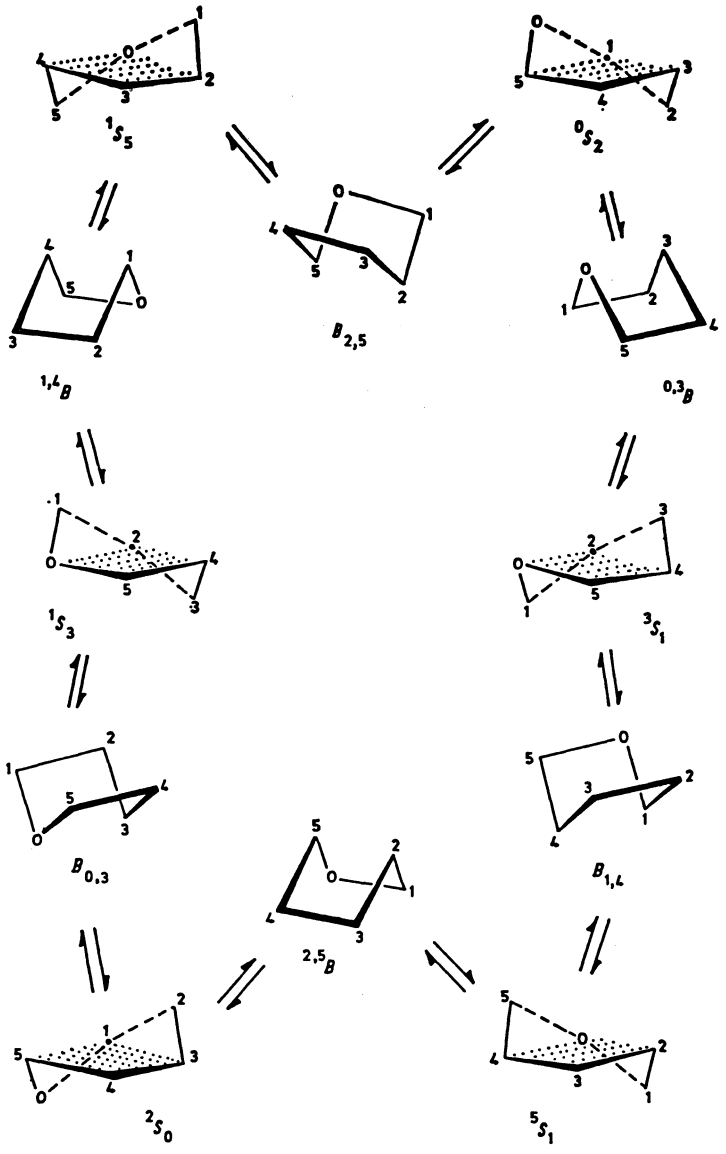


Fig. 1. *The flexible boat-skew cycle for aldopyranoses*

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 [example (*8*) and Fig. 1]. Possible conformations for aldopyranoses $^1S_3$, $^3S_1$, $^1S_5$, $^5S_1$, $^0S_2$ and $^2S_0$.(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 Fig. 1.)

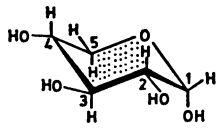
Half-Chairs. The reference plane is defined by the four adjacent coplanar atoms [example (*9*)]. Possible conformations for aldopyranoses: $^0H_1$, $^1H_0$, $^1H_2$, $^2H_1$, $^2H_3$, $^3H_2$, $^3H_4$, $^4H_3$, $^4H_5$, $^5H_4$, $^5H_0$, and $^0H_5$.

Five-Membered Rings

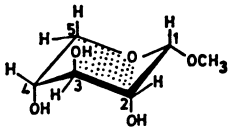
Envelopes. The reference plane is defined by the four adjacent coplanar atoms [examples (*10*), (*12*), and (*15*)]. Possible conformations for aldofuranoses: ^1E, E_1, ^2E, E_2, ^3E, E_3, ^4E, E_4, ^0E, and E_0.

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 (*11*) and (*12*)]. Possible conformations for aldofuranoses: $^0T_1$, $^1T_0$, $^1T_2$, $^2T_1$, $^2T_3$, $^3T_2$, $^3T_4$, $^4T_3$, $^4T_0$, and $^0T_4$.

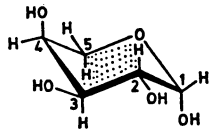
Examples



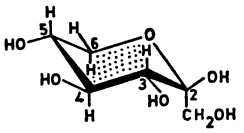
α-D-Xylopyranose-$^4C_1$
(*1*)



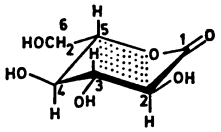
Methyl α-D-xylopyranoside-$^1C_4$
(*2*)



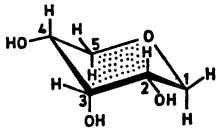
β-L-Arabinopyranose-$^4C_1$
(*3*)



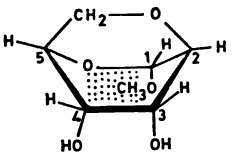
β-D-*xylo*-Hexulopyranose-$^5C_2$
(*4*)



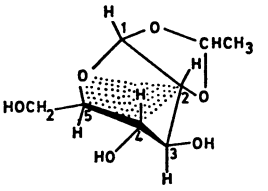
L-Glucono-1,5-lactone-$^1C_4$
(*5*)



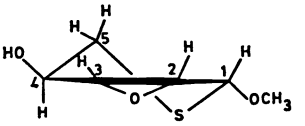
1,5-Anhydroribitol-$^4C_1$
(*6*)



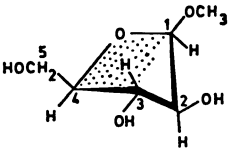
Methyl 2,6-anhydro-α-D-altropyranoside-$^{2,5}B$
(*7*)



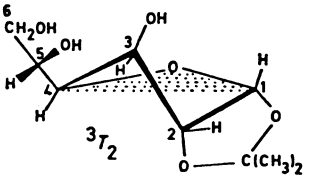
1,2-*O*-Ethylidene-α-D-glucopyranose-$^1S_3$
(*8*)



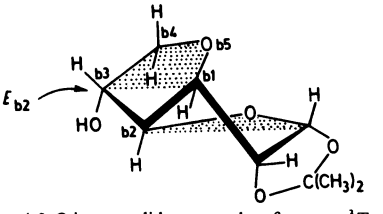
Methyl 2,3-anhydro-5-thio-β-L-lyxopyranoside-^5H_S
(*9*)



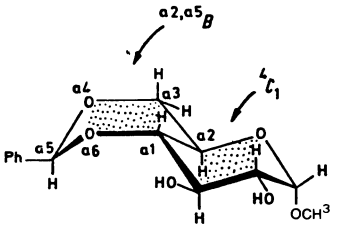
Methyl β-D-arabinofuranoside-E_2
(*10*)



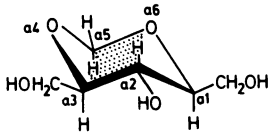
1,2-*O*-Isopropylidene-β-L-idofuranose-$^3T_2$
(*11*)



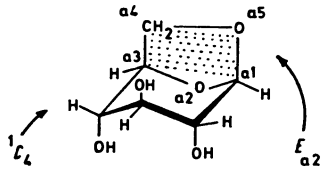
3,6-Anhydro-1,2-*O*-isopropylidene-α-D-glucofuranose-$^3T_2$
(*12*)



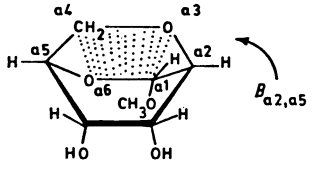
Methyl 4,6-*O*-(*S*)-benzylidene-α-D-glucopyranoside-$^4C_1$ (having the unusual configuration at the benzylidene carbon atom)
(*13*)



2,4-*O*-Methyleneribitol-$^{a4}C_{a1}$
(*14*)



1,6-Anhydro-β-D-glucopyranose-$^1C_4$
(*15*)



Methyl 2,6-anhydro-α-D-altropyranoside-$^{2,5}B$
(*16*)

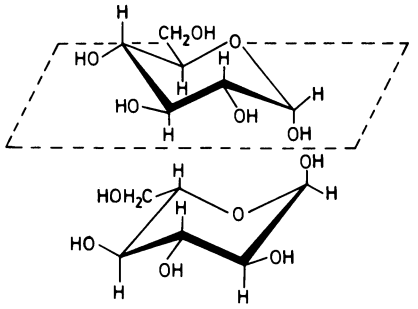


Fig. 2. *Mirror images.* α-D-Glucopyranose-$^4C_1$ (above) and α-L-glucopyranose-$^1C_4$ (below). Mirror plane in dashed lines

The ring atoms forming the reference planes in some typical conformations are given in the Table.

5. Because the conformational symbols for enantiomers are different (e.g. Fig. 2), it is important to state in the context whether the D or L form is under consideration. Enantiomers have the same reference plane, and it should be noted that the mirror image of α-D-glucose-$^4C_1$ is α-L-glucose-$^1C_4$ (Fig. 2). The conformation of a racemic compound should be given by using the appropriate notation for each enantiomer, e.g. DL-glucose-$^4C_1$(D), $^1C_4$(L).

6. In a ring other than a parent-sugar pyranoid or furanoid ring, the ring-carbon atom that bears the lowest number according to conventional carbohydrate nomenclature may be designated a1, the remaining ring atoms, including any heteroatoms, being numbered consecutively a2, a3, and so on, beginning with the relevant portion of the parent carbohydrate chain or ring that is part of the ring in question [examples (*12*)–(*16*)]. 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, and so on.

Acknowledgements. The illustrations have been kindly provided by The Royal Society of Chemistry or reproduced, with permission, from Schwarz, J. C. P. (1973) *J. Chem. Soc. Chem. Commun.* 505–508.

Type of sugar	Conformation	Atoms of reference plane	Above plane	Below plane	Notation	Example
Aldopyranose	chair	C-2, C-3, C-5, O-5	C-4	C-1	$^4C_1$	(*1*)
Aldopyranose	chair	C-2, C-3, C-5, O-5	C-1	C-4	$^1C_4$	(*2*)
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	$B_{1,4}$	not shown
Aldopyranose	skew	C-2, C-4, C-5, O-5	C-1	C-3	$^1S_3$	(*8*)
Aldopyranose	skew	C-1, C-3, C-4, C-5	C-2	O-5	^2S_O	not shown
Aldopyranose	half-chair	C-1, C-2, C-3, C-4	C-5	S-5	^5H_S	(*9*)
Aldopyranose	half-chair	O-5, C-1, C-2, C-3	C-4	C-5	$^4H_5$	not shown
Aldofuranose	envelope	O-4, C-1, C-3, C-4	–	C-2	E_2	(*10*)
Aldofuranose	envelope	C-1, C-2, C-4, O-4	C-3	–	^3E	not shown
Aldofuranose	twist	C-1, O-4, C-4	C-3	C-2	$^3T_2$	(*11*)
Aldofuranose	twist	C-3, C-4, O-4	C-2	C-1	$^2T_1$	not shown