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PROVISIONAL

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

and

INTERNATIONAL UNION OF BIOCHEMISTRY

JOINT COMMISSION ON BIOCHEMICAL NOMENCLATURE*

NOMENCLATURE OF BRANCHED-CHAIN MONOSACCHARIDES

Comments on these recommendations are welcome and should be sent within 8 months from January 1982 to the Secretary of the Commission

Dr. H. B. F. DIXON
Department of Biochemistry
University of Cambridge
Tennis Court Road
Cambridge CB2 1QW
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 was as follows:

Chairman: P. KARLSON (FRG); *Secretary*: H. B. F. DIXON (UK); *Members*: B. L. HORECKER (USA); Y. JEANNIN (France); C. LIÉBECQ (Belgium - as Chairman of IUB Committee of Editors of Biochemical Journals); B. LINDBERG (Sweden); K. L. LOENING (USA); G. P. MOSS ((UK); J. REEDIJK (Netherlands); S. F. VELICK (USA): J. F. G. VLIEGENTHART (Netherlands)

Additional contributors to the formulation of these recommendations:

Nomenclature Committee of IUB (those additional to JCBN): H. BIELKA (GDR); W. B. JAKOBY (USA): B. KEIL (France); E. C. WEBB (Australia)

Expert Panel: H. PAULSEN (Convener, FRG); L. C. CROSS (UK): late E. HARDEGGER (Switzerland); O. HOFFMANN-OSTENHOF (Austria); D. HORTON (USA); K. L. LOENING (USA); D. J. MANNERS (UK); W. G. OVEREND (UK); R. S. TIPSON (USA).

IUPAC-IUB Joint Commission on Biochemical Nomenclature (JCBN)

Nomenclature of Branched-Chain Monosaccharides

Recommendations 1980

The naming of acyclic forms is described, and the first part of this is the rules for choosing which is the parent chain. This leads to naming the parent monosaccharide, including the naming of the *C*-substituent that forms the branch. Stereochemical conventions have to be extended to specify configuration: the two substituents at one carbon on the parent chain are put in order of priority; that of higher priority is considered to replace hydroxyl and that of lower priority to replace hydrogen in assigning a name to the parent monosaccharide. Equivalent groups and terminal substitution are dealt with separately. Cyclic forms are then described. Many examples are given.

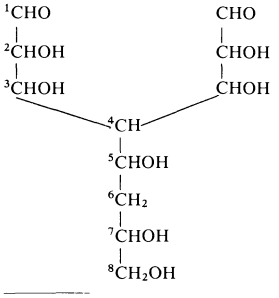
1. NAMING THE ACYCLIC FORM

1.1. *Basis of the Name*

A branched-chain monosaccharide will be named as a derivative of a parent unbranched monosaccharide, expressed in its acyclic form.

1.2. *Choice of Parent Chain*

The parent chain will be the all-carbon unbranched chain having one or more potential carbonyl groups and containing the greatest number of monosaccharide carbon units. If any choice remains, preference will be given to the chain containing the greatest number of carbon atoms. Example:

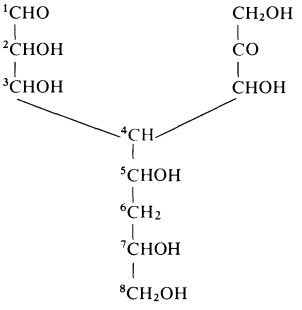


Document of the IUB-IUPAC Joint Commission on Biochemical Nomenclature (JCBN). Its members are: P. Karlson (chairman), H. B. F. Dixon, B. L. Horecker, Y. Jeannin, C. Liébecq (as chairman of the IUB Committee of Editors of Biochemical Journals), B. Lindberg, K. L. Loening, and G. P. Moss. Comments and suggestions for future revisions of these recommendations may be sent to its secretary, H. B. F. Dixon, University Department of Biochemistry, Tennis Court Road, Cambridge, England, CB2 1QW, or any member. JCBN thanks the expert panel of H. Paulsen (convener), L. C. Cross, E. Hardegger, O. Hoffmann-Ostenhof, D. Horton, K. L. Loening, D. J. Manners, W. G. Overend, and R. R. Tipson for drafting these proposals, its predecessor, CBN, for setting up the pannel, and other members of the Nomenclature Committee of IUB (H. Bielka, W. B. Jakoby, B. Keil, and E. C. Webb) for consultation.

The parent is the numbered octose, not the alternative heptodialdose.

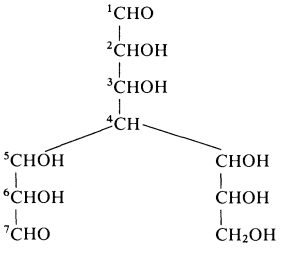
If choice remains after the application of the above rule, that choice will be made according to the following order of preference, treated in the order given.

a) An aldose has preference over a ketose. Example:



The parent is the numbered octose, not the alternative 2-octulose.

b) The maximum number of (potential) carbonyl groups. Example:



The numbered dialdose has preference over the alternatives.

Reproduced from *Eur. J. Biochem.*, Vol.119, pp.5-8 (1981)
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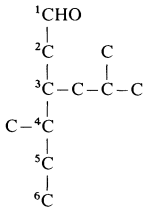
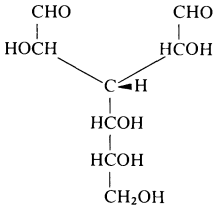
c) The branch point(s) will have the lowest locants possible. Example:

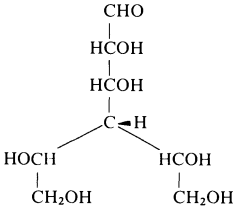


The parent is the vertical numbered chain, not the alternative turning right at 3, because the locants of the branches are 3,4, instead of 3,5.

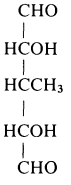
d) The priority of rule Carb-2 (here and elsewhere see [1]). Examples:



3-Deoxy-3-*C*-(L-*glycero*-
-1-hydroxy-2-oxoethyl)-D-*altro*-
-hexose (not D-*glycero*-, D-*gluco*-
by Rule Carb-2a)



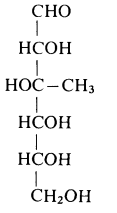
4-Deoxy-4-*C*-(L-*glycero*-
-1,2-dihydroxyethyl)-D-*gulo*-
-hexose (not D-*glycero*-, L-*talo*-
by Rule Carb-2a)



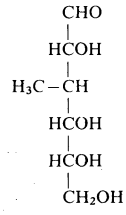
3-Deoxy-3-methyl-*ribo*-
-pentodialdose. N.B. Considered as
the D-form for defining the
direction of numbering
(Rule Carb-2b)

1.3. *Naming of Parent Monosaccharide*

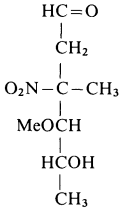
Unless the two substituents at the branch point of the parent chain are equivalent, or one of them is equivalent to an attached portion of the parent chain (see 1.4), it is necessary to distinguish between these two substituents in order to specify the stereochemistry of the branch point. The priority of the two substituents (including hydrogen if present) at the branch point is determined by the procedure (based largely on atomic number) used in the sequence rules (see Appendix 2 in [3]). The configuration symbol is then derived from Rule Carb-8 using the substituent having the higher priority in place of the corresponding hydroxyl group (cf. Rule Carb-14 for amino sugars and Rule Carb-36 for sulfur and selenium analogues). Examples:



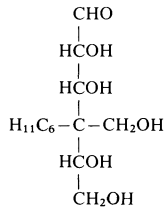
3-*C*-Methyl-D-glucose (oxygen
has priority over carbon)



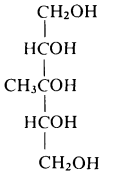
3-Deoxy-3-*C*-methyl-D-*gluco*-
-hexose (carbon has priority over
hydrogen)



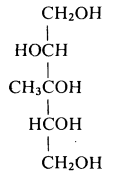
2,3,6-Trideoxy-3-*C*-methyl-
-4-*O*-methyl-3-*C*-nitro-D-*lyxo*-
-hexose (nitrogen has priority over
carbon)



4-*C*-Cyclohexyl-4-deoxy-
-4-*C*-(hydroxymethyl)-D-*allo*-
-hexose (oxygen has priority over
carbon [C-2'])



3-*C*-Methyl-ribitol

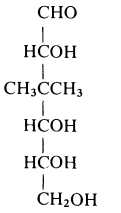


3-*C*-Methyl-D-arabinitol

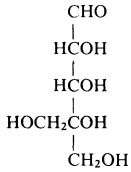
Note. The first example is named from D-glucose because it is a substituted D-glucose; the second is named from D-*gluco*-hexose because by loss of oxygen it has ceased to be a substituted glucose although it has the D-*gluco* configuration.

1.4. *Naming of Parent Monosaccharides that Have Two Equivalent Groups*

If the two substituents at the branch point of the parent chain are equivalent, or if one of them is equivalent to an attached portion of the parent chain, then the parent monosaccharide must be named according to Rule Carb-14 for unsubstituted deoxymonosaccharides. Examples:



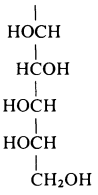
3-Deoxy-3,3-di-*C*-methyl-
-D-*ribo*-hexose



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

1.5. *The Branches*

Each branch will be named either systematically or trivially as an alkyl or substituted alkyl radical, etc., replacing a *C*-hydrogen atom of the parent unbranched-chain monosaccharide. Within the branch the configurations around asymmetric centres will be indicated by use of configurational prefixes (Rules Carb-8 and Carb-9). If the first atom of the branch is chiral, the main chain counts as group X in applying Rule Carb-8. Example:



L-*gluco*-1,2,3,4,5-Pentahydroxypentyl
or
L-*gluco*-Pentitol-yl

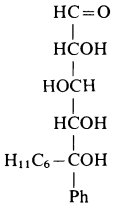
1.6. *Numbering*

The parent unbranched-chain monosaccharide will be numbered according to Rule Carb-4; i.e. in an aldose, the carbon atom of the (potential) carbonyl group is atom number one; in a ketose it has the lower number possible.

The carbon atoms of each branch will be numbered by Arabic numerals starting at the carbon atom attached to the main chain (see Nomenclature of Organic Chemistry, A-2-9).

2. TERMINAL SUBSTITUTION

If the terminal carbon atom of a monosaccharide is asymmetric as a result of the presence of two carbon substituents that cannot be regarded as belonging to the sugar chain, the stereochemistry at the new asymmetric centre will be indicated by use of the Sequence Rule (*R* or *S*) (see also Rules Carb-34 and Carb-35). Example:



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

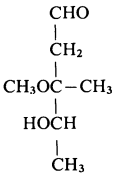
3. NAMING OF CYCLIC FORMS

In contrast with Rule Carb-20, the name of a cyclic form of a branched-chain monosaccharide will be based on that of the systematic name of the acyclic form wherein the two carbohydrate atoms between which cyclization has taken place are both considered to be part of the main chain. The cyclic form is then defined by the use of conventional cyrbohydrate configurational nomenclature.

4. GENERAL EXAMPLES

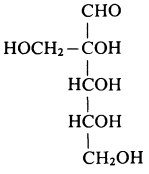
Acyclic Forms

Cladinose



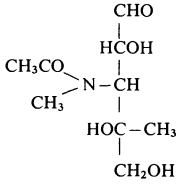
2,6-Dideoxy-3-*C*-methyl-3-*O*-methyl-L-*ribo*-hexose

Hamamelose



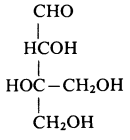
2-*C*-(Hydroxymethyl)-D-ribose

N-Acetylgarosamine



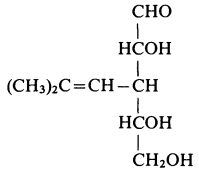
3-Deoxy-4-*C*-methyl-3-*C*-(*N*-methyl-acetamido)-L-arabinose
Note: This compound is regarded as an arabinose rather than an *arabino*-pentose because the replacement of oxygen by nitrogen (or other heteroatom) still leaves it considered as an arabinose derivative

D-Apiose

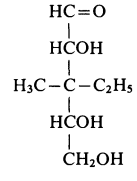


3-*C*-(Hydroxymethyl)-D-*glycero*-tetrose

Other



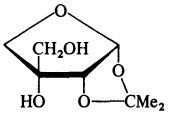
3-Deoxy-3-*C*-(2-methyl-1-propenyl)-D-*xylo*-pentose



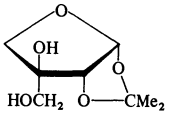
3-Deoxy-3-*C*-ethyl-3-*C*-methyl-D-*ribo*-pentose

Cyclic Forms

From D-apiose

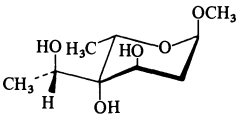


3-*C*-(Hydroxymethyl)-1,2-*O*-isopropylidene-α-D-*erythro*-tetrofuranose



3-*C*-(Hydroxymethyl)-1,2-*O*-isopropylidene-β-L-*threo*-tetrofuranose

Other



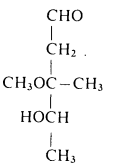
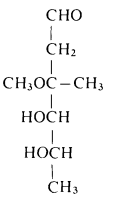
Methyl 2,6-dideoxy-4-*C*-(L-*glycero*-1-hydroxyethyl)-α-L-*xylo*-hexopyranoside

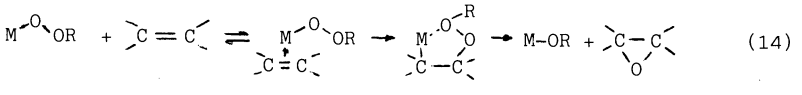
REFERENCES

1. IUPAC Commission on the Nomenclature of Organic Chemistry and IUPAC-IUB Commission on Biochemical Nomenclature, Tentative rules for carbohydrate nomenclature, part 1, 1969, *Biochemistry*, *10*, 3985–4004 and 4995 (1971), *Biochim. Biophys. Acta*, *244*, 223–302 (1971), *Eur. J. Biochem. 21*, 455–476 (1971) and *25*, 4 (1972) and *J. Biol. Chem. 247*, 613–635 (1972). See also pages *174–195* in [2].
2. International Union of Biochemistry (1978) *Biochemical Nomenclature and Related Documents*, The Biochemical Society, London.
3. IUPAC Commission on Nomenclature of Organic Chemistry, Rules for the nomenclature of organic chemistry, section E, stereochemistry (recommendations 1974) *Pure Appl. Chem. 45*, 11–30 (1976). See also pages *1–18* in [2] and section E in [4].
4. International Union of Pure and Applied Chemistry (1979) *Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H*, Pergamon Press, Oxford.

Pure & Appl. Chem., Vol.54, No.12, p.2785, 1982.
Pergamon Press Ltd. Printed in Great Britain.

ERRATA

Volume, Issue and Year	Page no. and location	Correction
49, 5 (1977)	671-673	In the "Recommended Reference Materials for the Realization of Physicochemical Properties - Section: Absorbance and Wavelength" infrared absorption bands were suggested as reference for wavenumber calibration. More recent revised data have been published by IUPAC in a book entitled Tables of Wavenumbers for the Calibration of Infrared Spectrometers compiled by A.R.H. COLE (Pergamon Press, Oxford, 1977). Wavenumbers appearing in sections II/8, II/9, II/10 and II/11 of Recommendations on Reference Materials should be replaced by the values published by COLE.
54, 1 (1982)	208, Abstract, line 2	for 'dexcy' read 'deoxy'
	209, column 2, 3rd name	for 1,1,2,2-Tetrahydro read 1,1,2,2-Tetradehydro
	210, column 1, 4th name	for 6,7,7,8-Tetrahydro read 6,7,7,8-Tetradehydro
	214, column 2, structure for Cladinose	for  read 
54, 3 (1982)	681, Abstract, line 3	for TiO_2 1892±30 read TiO_2 1843±15 (in air)
		for ZnO_2 2710±25 read ZnO_2 2710±35
54, 8 (1982)	1455, Table 1 (i) column $-\Delta H_h^o$ for Hg^{2+}	for 1940 read 1845
	(ii) footnote a to Table 1	add ΔH_h^o of Hg^{2+} has been misprinted in Ref. 19
	1457, Table 2 column 1, last item	for $BP\bar{h}_4$ read BPh_4^-
	1459, Table 3 column 1, 12th item	for $Hg(\ell)/Hg^{2+}$ read $Hg(\ell)/Hg_2^{2+}$
54, 10 (1982)	1859, Eq.(14)	correct version is as follows:



(14)

4'