## PROVISIONAL

# INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

and

# INTERNATIONAL UNION OF BIOCHEMISTRY

## JOINT COMMISSION ON BIOCHEMICAL NOMENCLATURE\*

# NOMENCLATURE OF UNSATURATED MONOSACCHARIDES

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

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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:

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IUPAC-IUB Joint Commission on Biochemical Nomenclature (JCBN) Nomenclature of Unsaturated Monosaccharides Recommendations 1980

Recommendation are given for naming unsaturated monosaccharides. Double bonds are indicated with the infix 'en' and its use is described. Triple bonds and cumulative double bonds require 'dexcy' prefixes to convert sugars into derivatives on which the operator 'dehydro' can indicate double and triple bonds.

These recommendations relate 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 or organic nomenclature [1].

#### 1. DOUBLE BONDS

Monosaccharide derivatives having a double bond between two contiguous carbon atoms of the backbone chain shall be named by inserting, into the name for the corresponding fully saturated derivative, the infix 'x-en'. The infix shall be placed directly after the stem name that designates the chain length of the sugar. The locant x is the position number or the lower-numbered carbon atom involved in the double bond. Steric relations at a double bond will be designated, if necessary, by the affixes (Z)- and (E)-preceding the whole name.

#### Notes

a) 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 will not be used or modified as a class name for monosaccharide derivatives having a double bond in any other position.

b) Following the principle of first naming the saturated derivative, compounds having a >C=CR-O- group as

Document of the IUPAC-IUB Joint Commission on Biochemical Nomenclature (JCBN) whose 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 may be sent to the secretary of JCBN, H. B. F. Dixon, University Department of Biochemistry, Tennis Court Road, Cambridge, England, CB2 1QW, or to any member. JCBN thanks an expert panel consisting of L. C. Cross, E. Hardegger, O. Hoffmann-Ostenhof, D. Horton, K. L. Loening, D. J. Manners, W.G. Overend, H. Paulsen (convener) and R. S. Tipson for preparing the document, and other members of the Nomenclature Committee of IUB (H. Bielka, W. B. Jakoby, B. Keil, and E. C. Webb) for consultation. part of a ring system are named as unsaturated derivatives of anhydro alditols if R is hydrogen or carbon; if R is halogen, chalcogen, or nitrogen-family element, the resulting name is that of a glycenose or glycenosyl derivative.

c) When necssary for euphony, the infix 'eno' may be used.

d) The steric designators (Z)- and (E)- (see [2]) 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 the (Z)- form.

#### 2. TRIPLE BONDS

#### OR CUMULATIVE DOUBLE BONDS

Monosaccharide derivatives having a triple bond or cumulative double bonds in the backbone chain shall be named on the basis of the corresponding fully saturated sugar by using the appropriate number of dehydro and deoxy prefixes (see Note). The prefixes shall be placed in alphabetical order before the stem name.

Alternatively, these compounds may be assigned systematic names in line with the IUPAC rules of organic nomenclature.

#### Note

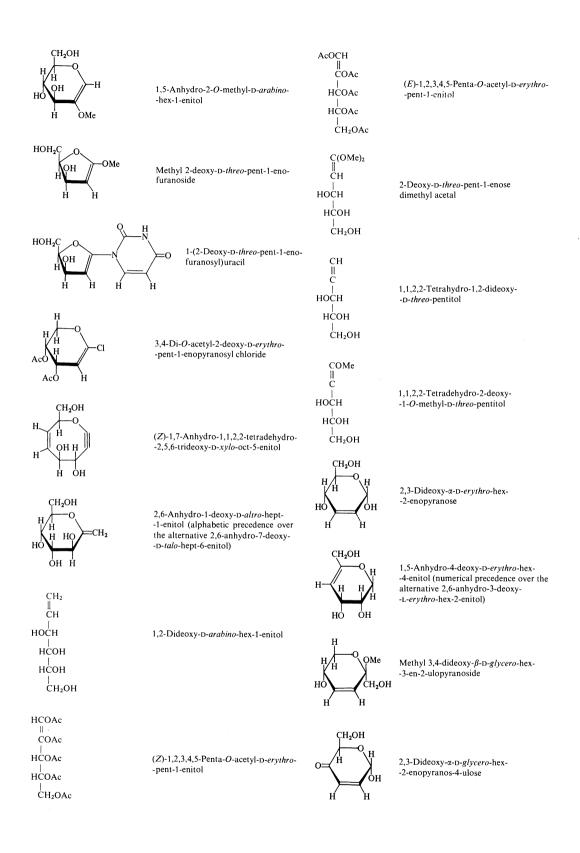
Since these compounds contain in the backbone chain carbon atoms with neither H nor OH on them, and since, on the other hand, the carbohydrate suffixes, such as -itol, imply an oxygen attached to every carbon atom (see [4]) parent compounds such as pentynitol or 2,3-pentadienitol cannot exist.

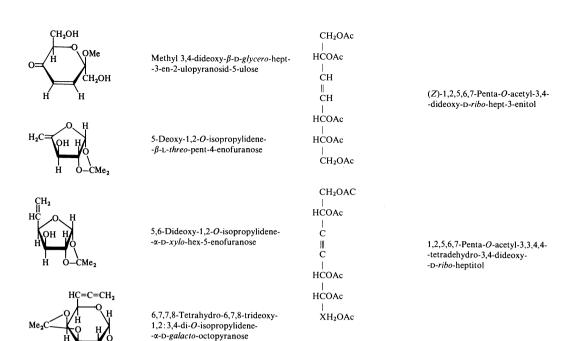
EXAMPLES



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

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OAc

CH. -0 6-O-Acetyl-5,5,6,6-tetradehydro-5-deoxy--α-D-xylo-hexofuranose

5,5,6,6-Tetradehydro-5,6,8-trideoxy-

-1,2-O-isopropylidene-a-D-xylo-

-octo-1,4-furanos-7-ulose

## REFERENCES

- 1. International Union of Pure and Applied Chemistry (1979) Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H, Pergamon Press, Oxford,
- 2. IUPAC Commission on Nomenclature of Organic Chemistry, Rules IOPAC Commission on Nomenciature of organic Chemistry, Rules for the nomenclature of organic chemistry, section E, stereo-chemistry (recommendations 1974) Pure Appl. Chem. 45, 11-30 (1976). See also section E in [1] and pages 1-18 in [3].
  International Union of Biochemistry (1978) Biochemical Nomen-clature and Related Documents, The Biochemical Society, London.
- 4. 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), J. Biol. Chem. 247, 613-635 (1972). See also pages 174-195 in [3].

## ERRATA

Volume, Issue and Year	Page no. and location	Correction
<u>49</u> , 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 <u>Tables of Wavenumbers for the</u> <u>Calibration of Infrared Spectrometers</u> compiled by <u>A.R.H. COLE (Pergamon Press, Oxford, 1977). Wave-</u> numbers 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.
<u>54</u> , 1 (1982)	208, Abstract, line 2	<u>for</u> 'dexcy' <u>read</u> 'deoxy'
	209, column 2, 3rd name	for 1,1,2,2-Tetrahydro read 1,1,2,2-Tetradehydro
	210, column l, 4th name	for 6,7,7,8-Tetrahydro read 6,7,7,8-Tetradehydro
	214, column 2, structure for Cladinose	$\begin{array}{ccc} CHO & CHO \\ I \\ CH_2 \\ CH_2 \\ \hline \\ CH_3OC - CH_3 \\ HOCH \\ HOCH \\ I \\ CH_3 \\ CH$
<u>54</u> , 3 (1982)	681, Abstract, line 3	<u>for</u> TiO <sub>2</sub> 1892±30 <u>read</u> TiO <sub>2</sub> 1843±15 (in air) <u>for</u> ZnO <sub>2</sub> 2710±25 <u>read</u> ZnO <sub>2</sub> 2710±35
<u>54</u> , 8 (1982)	1455, Table 1 (i) column -∆H <sup>0</sup> for Hg <sup>2+</sup> h (ii) footnote a to Table 1	for 1940 read 1845 add $\Delta H_{\rm h}^{\rm O}$ of Hg <sup>2+</sup> has been misprinted in Ref. 19
	1457, Table 2 column 1, last item	$for BP_{4}$ read $BPh_{4}$
	1459, Table 3 column 1, l2th item	for $Hg(\ell)/Hg^{2+}$ read $Hg(\ell)/Hg_2^{2+}$
<u>54</u> , 10 (1982)	1859, Eq.(14)	correct version is as follows:
	M <sup>-0</sup> OR +	$C = C = C = M^{-0} OR \rightarrow M^{-0} OR \rightarrow M^{-0} OR + C - C $ (14)
		4'