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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

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