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A Logical Relationship Between the Names and Structures of Aldoses and Ketoses Using Extended Binary and Decimal Numbers

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Abstract

In this study, we introduce a very simple and highly practical method for naming aldoses and ketoses—both in their Fischer projection forms and in their cyclic structures—by using binary and decimal number systems. With the help of this method, the Fischer projection of any monosaccharide can be easily converted into its cyclic or Haworth form, and the cyclic structure can also be changed back to the Fischer form without difficulty. This approach also makes it possible to determine the R and S configuration of any chiral carbon using a binary number pattern, removing the need to assign priorities to the attached groups through the traditional Cahn–Ingold–Prelog rules. Additionally, using this numerical method, one can quickly draw the mirror image (enantiomer) of any monosaccharide based on its given name or structure. Overall, this technique provides a faster and more systematic way to name, understand, and represent different sugar molecules.

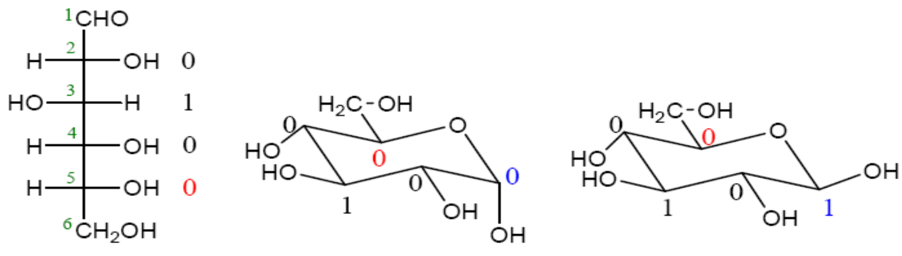
Keywords- Aldose, Ketose, Binary number, Decimal number, Fischer form

Introduction

Many students have difficulty naming and drawing structure of aldoses and ketoses in chain and cyclic forms, because trivial names as well as other naming methods do not represent their structure. In order to solve such a problem, several papers have suggested bar-codes [1-6], and binary and decimal numbers, though in some cases it has led to more complications [7-10]. For example, a recently published paper for naming and drawing structures of aldohexoses is based on the special arrangement of trivial names of aldohexose, using the Fiesers' mnemonic aid "all altruists gladly make gum in gallon tanks" to memorize it and then, proceed to assign numbers 0-7 to the trivial names of D-series of these monosacharides [11]. However, if one reminds that in any system of nomenclature (as IUPAC nomenclature) there must be a logical relationship between structure and name based on clear and unambiguous conventions, he/she will find that the above decimal numbers (stereonumbers), as well as their corresponding binary numbers, have no logical connection with the structure of monosaccharides discussed. Therefore, in order to establish such a logical connection between the name and structure of any monosaccharide, we propose here the extended binary and decimal numbers. With such a naming system, it is easily possible to distinguish D and L isomers, interconvert Fischer projections and their corresponding cyclic forms, and finally, rapidly assign configuration descriptors (R or S) to each chiral center. It will also facilitate teaching process and help students learn and improve certain skills, as well as increase their academic success and knowledge retention without any confusion.

DISCUSSION

For any carbohydrate, as suggested by McGinn and Wheatley, a hydroxyl group to the right and the left of its Fischer projection is designated as 0 and 1, respectively [10]. For example, the binary number for compound 1 is 0100. In such a binary number, the rightmost and the leftmost places correspond to the orientation of the hydroxyl group at the last and the first chiral center of Fischer projection, respectively. A very important point is that the rightmost place of such a binary number determines whether it is a *D* or an *L* carbohydrate; that is, 0 (an even number) stands for *D* and 1 (an odd number) stands for L. It goes without saying that when a binary number is converted to its corresponding stereonumber, it will also be an even or an odd number. Therefore, an even number (whether binary or decimal) is always representative of a *D* carbohydrate. In other words, the necessary and sufficient condition for a carbohydrate to be a *D* isomer is that its stereonumber and/or binary number be an even number. The corollary of this statement is that the stereonumber for an *L* isomer will be always an odd number. With this background, herein we suggest to use the stereonumber of a monosaccharide such as in its IUPAC nomenclature. Hence, compound 1 (*D*-glucose) should be named as *4_aldohexose*. The underline symbol prevents any confusion with the numbers used to define locations in IUPAC nomenclature. With the formation of pyranose ring, an additional chiral center is created that leads to the two stereoisomers; α and β anomers (colored in blue in Scheme 1). If this additional chiral center is designated as 0 or 1 (for α or β anomers respectively), then one can name the α-anomer as 4_*aldohexopyranose* and β-anomer as 20_*aldohexopyranose* (Scheme 1).

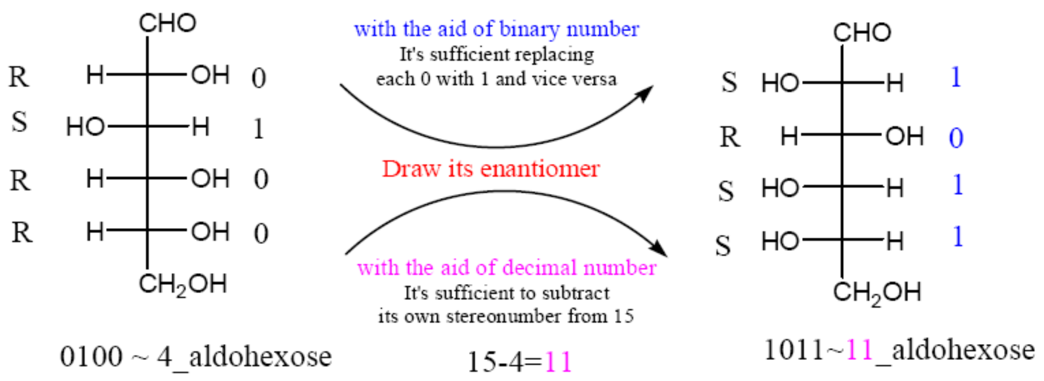


1 | α-anomer | β-anomer

	1	α-anomer	β-anomer
Binary number	0100	00100	10100
Stereonumber	4	4	20
Name	4_aldohexose	4_aldohexopyranose	20_aldohexopyranose

Scheme 1. Nomenclature of Fischer and pyranose forms of *D*-glucose by stereonumber

With our proposed system of nomenclature, one can also derive the binary number for the enantiomer of a given carbohydrate by just replacing each 0 with 1 and vice versa. For example, 0110 is converted to 1001. Here, it seems that 0 and 1 are mirror images of each other! This important point prompted us to call binary numbers 0110 and 1001 enantionumbers. It is evident that the sum of any two n bit enantionumbers is a new n bit binary number composed of only ones, in which n is the number of chiral centers. This sum, for the chain and ring forms of aldohexoses (with 4 chiral centers) is therefore, 1111 and 11111 respectively. As the corresponding stereonumbers of 1111 and 11111 are 15 and 31, to obtain the stereonumber for the enantiomer of any aldohexose, it is sufficient to subtract its own stereonumber from 15 (for the chain form) or 31 (for the ring form). Take for example 4_aldohexose, the enantiomer of which will be 11_aldohexose (see Scheme 2).



Scheme 2. How to draw an enantiomer with the aid of binary and decimal numbers for D-glucose

Table 1 represents all Fischer and pyranose forms of aldohexoses with their corresponding binary and decimal numbers. As seen, the stereonumbers of D-aldohexoses with 4 chiral centers are all even numbers from 0 to14 (for any carbohydrate with n chiral centers, all even numbers from 0 to 2^n-2):

0_Aldohexose	2_Aldohexose	4_Aldohexose	6_Aldohexose
8_Aldohexose	10_Aldohexose	12_Aldohexose	14_Aldohexose

Table – 1 : Binary and Decimal Numbers of D and L (both Fischer and Pyranose Forms) of Aldohexoses

Entry	Aldohexoses	Fischer form				Pyranose form							
		Binary number		Decimal number		Binary number				Decimal number			
		D	*L*	*D*	*L*	α		β		α		β	
						D	*L*	*D*	*L*	*D*	*L*	*D*	L
1	allose	0000	1111	0	15	00000	11111	10000	01111	0	31	16	15
2	gulose	0010	1101	2	15-2=13	00010	11101	10010	01101	2	31-2=29	18	31-18=13
3	glucose	0100	1011	4	15-4=11	00100	11011	10100	01011	4	31-4=27	20	31-20=11
4	galactose	0110	1001	6	15-6=9	00110	11001	10110	01001	6	31-6=25	22	31-22=9
5	altrose	1000	0111	8	15-8=7	01000	10111	11000	00111	8	31-8=13	24	31-24=7
6	idose	1010	0101	10	15-10=5	01010	10101	11010	00101	10	31-10=21	26	31-26=5
7	mannose	1100	0011	12	15-12=3	01100	10011	11100	00011	12	31-12=19	28	31-28=3
8	talose	1110	0001	14	15-14=1	01110	10001	11110	00001	14	31-14=17	30	31-30=1

And in the case of *L*-aldohexoses with 4 chiral centers, stereonumbers are all odd numbers from 1 to 15 (for any carbohydrate with n chiral centers, all odd numbers from 1 to 2^n-1):

1_Aldohexose	3_Aldohexose	5_Aldohexose	7_Aldohexose
9_Aldohexose	11_Aldohexose	13_Aldohexose	15_Aldohexose

An important point to be noted is that in the literature, assigning the configuration descriptors (*R* and *S*) to the chiral centers has been ignored or not logically explained. However, with this new horizon, one can easily find the *R* and *S* descriptors with the aid of a given binary number, without directly being engaged in priority of bonded groups. A closer inspection revealed that in Fischer projection of carbohydrates, 0 and 1 are exactly equivalent to the configuration descriptors *R* and *S*, respectively. Note that the reverse is true for the anomeric carbon of the pyranose ring, simply due to the lower priority of its -OH group with respect to the ring oxygen.

Furthermore, one can easily draw the pyranose forms of any carbohydrate knowing just the binary number of its Fischer or ring form. For instance, in the case of carbohydrate 1, the binary numbers of its pyranose rings are 10100 and 00100. In this context, it is sufficient to note that:

1. The rightmost place defines the stereochemistry of the carbon bearing the -CH_2OH group (0 stands for *D* or *R* and 1 stands for *L* or *S*).
2. When the rightmost and the next to the rightmost places make 00 or 11, the corresponding vicinal groups (-CH_2OH and -OH) are trans to each other. For 01 and 10, the corresponding substituents will be *cis*.

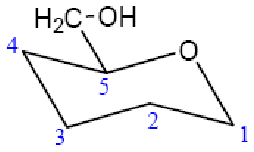
3. For any other two adjacent places, reverse of the above statement is true; i.e., for 00 or 11 the groups are cis and for 10 or 01 they are trans (Fig. 1).

Fig. – 1 : *Cis/trans* relationship between adjacent places of binary numbers

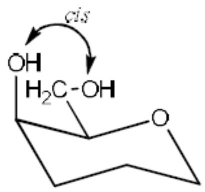
Following what discussed one will get the pictorial representation of the cis/trans relationship for 10100 and 00100 binary numbers:

Given the points discussed so far, let us draw 10110 step by step:

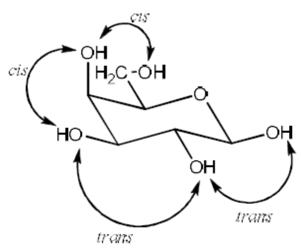
1. Draw the chair form of the pyranose ring by placing -CH_2OH group at equatorial position, which guarantees the *R* (or *D*) configuration of carbon #5.



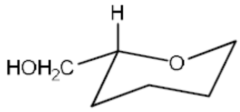
2. Now draw the vicinal -OH to -CH_2OH at axial position (this will guarantee the cis relationship of these groups).



3. Following such a reasoning for other -OH groups, you will obtain:



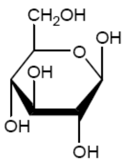
Note 1: To draw the pyranose ring of *L*-aldohexoses, it suffices to start with the following structure.



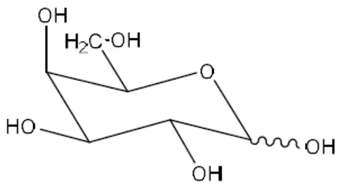
Note 2: To draw the Haworth forms of pyranose rings, it is just sufficient to sketch the following structures and proceed thereupon. Starting with -CH_2OH group, one can easily find the *cis/trans* relationship of all vicinal substituents (see Fig. 1).

D isomer *L* isomer

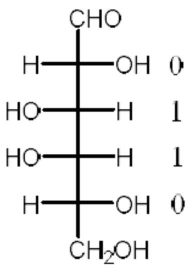
The Haworth form of 10100 is as shown below:



Note 3: To draw the Fischer projection of a given pyranose ring such as,



It is sufficient to first derive its corresponding binary number by ignoring the anomeric carbon. For D-aldohexose, as seen above, the rightmost place of its binary number is 0 (the carbon attached to the CH_2OH group). Starting with -CH_2OH group, one can easily find the cis/trans relationship of all vicinal substituents (see Fig. 1) and arrive at the four bit number 0110 for the corresponding Fischer projection. And that is all!



The key points stated are also applicable to ketoses. Table 2 represents binary and decimal numbers for the Fischer form of ketohexoses.

Table – 2 : Binary and Decimal Number of D and L Fischer Forms of Ketohexoses

Entry	Ketohexose *D* and *L*	Fischer form			
		Binary number		Decimal number	
		D	*L*	*D*	*L*
1	Psicose	000	111	0	7
2	Sorbose	010	101	2	7 - 2 = 5
3	Fructose	100	011	4	7 - 4 = 3
4	Tagatose	110	001	6	7 - 6 = 1

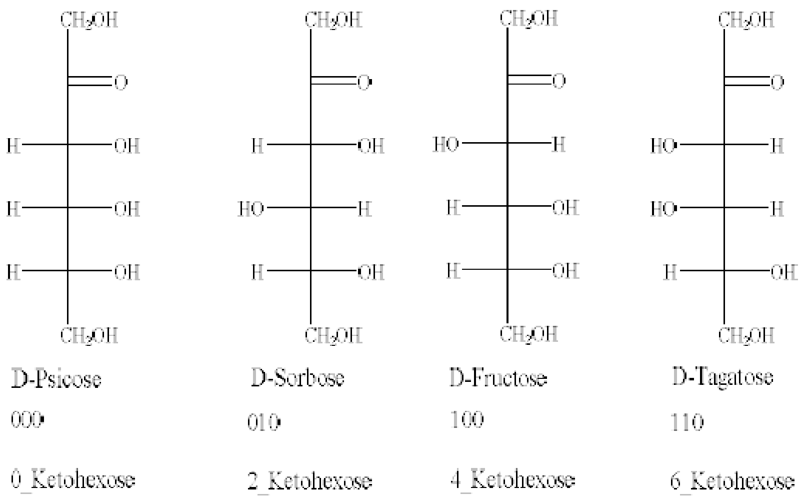
As shown, for *D*-ketohexoses with 3 chiral centers, stereonumbers are all even numbers from 0 to 6:

0_ketohexose 2_ketohexose 4_ketohexose 6_ketohexose

And in the case of *L*-ketohexoses with 3 chiral centers, stereonumbers are all odd numbers from 1 to 7:

1_ketohexose 3_ketohexose 5_ketohexose 7_ketohexose

Example



CONCLUSION

In this study, we showed that binary and decimal numbers of monosaccharides (aldoses and ketoses) are exact manifestation of their structure and naming. It is just sufficient to understand and learn the logic behind this system of nomenclature to see that it is very easy to name aldoses and ketoses (both chain and cyclic forms) and draw corresponding structures from their names. Hence,

* Any given even and odd binary and decimal number is an indication of a *D* and *L* aldohexose respectively;

* Each 0 and 1 in a binary number stands for *R* and *S* configuration of a given chiral center respectively (note that the reverse is true for the anomeric carbon of the ring form).

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