

# APPLICATION OF STEREO NUMBERS IN SUGAR CHEMISTRY\*

S. NEELAKANTAN

Department of Chemistry, Madurai University, Madurai-2

**M**OST students of organic chemistry comprehend the fact that there are sixteen ( $2^4$ ) stereoisomers possible for an aldohexose containing four asymmetric carbon atoms and that they can be represented by eight pairs of enantiomers each of which is composed of one D- and its corresponding L-isomer. However, students are not familiar with quick naming of these eight pairs of isomers. As an aid for remembering the names of the eight D-aldohexoses in relation to their stereochemistry, Fieser and Fieser<sup>1</sup> have suggested the following mnemonic: "*All altruists gladly make gum in gallon tanks*". The use of this mnemonic finds a place also in a book on carbohydrates.<sup>2</sup> Corresponding to the portions italicised in the above mnemonic, the names of the aldohexoses are allose, altrose, glucose,

is written  $-\text{CH}_2\text{OH}$ . Then for C-5 (the last asymmetric carbon atom), the OH group is written to the right of the vertical chain of the projection formula for all the eight arrangements. For C-4, the OH group is represented to the right for the first four formulæ and to the left for the rest four. For C-3, the OH group is written to the right for the first two, then to the left for the next two, again to the right for the subsequent two and finally to the left for the last two formulæ. The configuration of C-2 is indicated in such a way that the first formula has the OH to the right, the second to the left, the third to the right and so on. The result is as indicated in Chart I. From this representation, the configurations of the eight L-aldohexoses also follow (see Chart I).

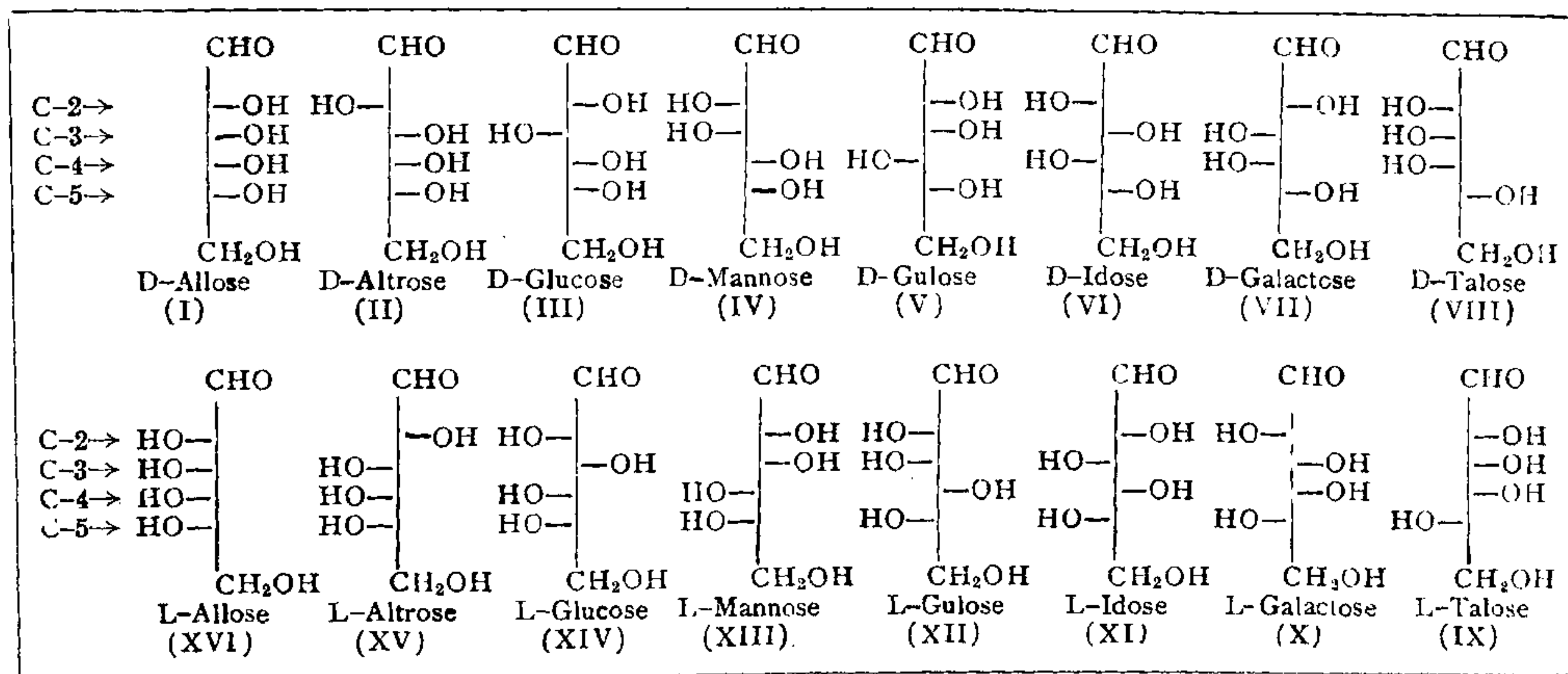


CHART I

mannose, gulose, idose, galactose and talose. For constructing the outline projection formulæ of the eight D-aldohexoses, one has to perform the following operation: The names of the eight sugars in the order in which they come according to the mnemonic are written one after the other in a line and above each

While the above method of representation is convenient when the projection formulæ of all the eight possibilities of D-aldohexoses are to be represented using the mnemonic, it is not easy if one has to quickly visualize the stereochemistry of a less familiar sugar like L-idose or D-talose. It will usually be necessary to write the projection formulæ of all the eight D-sugars and then pick up the appropriate ones.

\* Presented at the Summer Institute in Chemistry held at Madurai during May-June 1969.

In the present paper, a convenient method for quickly representing the stereochemistry of not only the eight D-aldohexoses but of the enantiomeric L-sugars also is discussed. For this purpose, the method of *stereo numbers* forms the basis. Feldman<sup>3</sup> has introduced the idea of stereo numbers for designating the stereoisomers in the fields of steroids, higher sugars, etc. The main basis in this notation is the binary system of arithmetic which uses only two symbols in the code. The binary system has been used by Rosenblatt<sup>4</sup> as a basis for the panoramic approach to the proof of the configurations of aldohexoses. In Rosenblatt's paper, four criteria have been chosen as questions and the answers to these questions are allotted either number 1 or number 0 depending on whether the answer is 'yes' or 'no'. It may be noted from Table I (*vide infra*) that the four criteria used by Rosenblatt<sup>4</sup> do not lead to any systematic representation.

For the present discussion, the direction in which the OH group, attached to the asymmetric carbon atom, is oriented in the projection formula decides the number. Thus if the OH group is projected to the right, it is allotted number 1 and if to the left, it has the number 0. In the final binary code number, the first number from the left-hand side corresponds to the orientation of the fifth carbon atom (last of the asymmetric carbon atoms), the next number which follows the first number corresponds to the orientation of the OH group of C-4 atom and so on. On this basis, the binary code number of D-allose (I) is 1111 and for D-altrose (II) it is 1110. In this way we arrive at the binary numbers for all the sixteen aldohexoses which are given in Table I. Each of the binary code numbers can be transformed into its respective decimal equivalent which is given in column 3 of Table I. The decimal equivalent number of an aldohexose is known as its *stereo number*.

As already mentioned, Rosenblatt<sup>4</sup> made use of the binary system as a basis for the panoramic approach to the proof of configuration of aldohexoses. But the decimal equivalent of the binary code number derived by Rosenblatt based on four other criteria for each of the aldohexoses does not follow any order (see column 5 of Table I) unlike the present approach (see column 3 of Table I).

Another method<sup>3</sup> of expressing binary numbers in a shorter form is the use of the

equivalent octal numbers.† If the octal system is used in the present case, the binary numbers of the sixteen aldohexoses turn out to be as indicated in column 4 of Table I. Though there is a certain degree of order in the octal system also when we go from D-allose to D-talose and then from L-talose to L-allose, the decimal system is better since on going from D-allose through D-talose and then through L-talose to L-allose, the decimal equivalent number (stereo number) goes on decreasing from 15 to 0.

TABLE I

Name of sugar	Binary code number	Decimal equivalent of binary code number (Stereo number)	Octal equivalent of binary code number	Decimal equivalent of binary code number based on Rosenblatt's procedure <sup>4</sup>
(1)	(2)	(3)	(4)	(5)
D-Allose (I)	.. 1111	15	17	2
D-Altrose (II)	.. 1110	14	16	8
D-Glucose (III)	.. 1101	13	15	11
D-Mannose (IV)	.. 1100	12	14	15
D-Gulose (V)	.. 1011	11	13	10
D-Idose (VI)	.. 1010	10	12	14
D-Galactose (VII)	.. 1001	9	11	3
D-Talose (VIII)	.. 1000	8	10	9
L-Talose (IX)	.. 0111	7	7	9
L-Galactose (X)	.. 0110	6	6	3
L-Idose (XI)	.. 0101	5	5	14
L-Gulose (XII)	.. 0100	4	4	10
L-Mannose (XIII)	.. 0011	3	3	15
L-Glucose (XIV)	.. 0010	2	2	11
L-Altrose (XV)	.. 0001	1	1	8
L-Allose (XVI)	.. 0000	0	0	2

The sum of the stereo numbers of two enantiomeric compounds is equal to  $2^n - 1$  where  $n$  is the number of asymmetric carbon atoms in the molecule. Thus the sum of stereo numbers of members of a pair of enantiomeric aldohexoses is  $2^4 - 1 = 15$ , based on the decimal equivalent representation of the binary system of arithmetic.

† In the octal system, the numbers run from 0 to 7 as shown below :

Binary number	..	000	001	010	011	100	101	110	111
Octal number	..	0	1	2	3	4	5	6	7

To get the octal number of a binary number like 101001, the binary number is broken into groups of three from the right. Thus the equivalent octal number of the above binary number is 51 (*i.e.*, 101/5, 001/1). Similarly, the octal number of 01011 is 13.

The main advantage of the present approach is the ease with which one can write the Fischer projection formula of any aldohexose if the mnemonic suggested by Fieser and Fieser<sup>1</sup> is kept in mind. As an illustration, the stereochemistry of L-gulose can easily be represented as (XII) by the following steps. The stereo number of D-gulose is 11 since D-allose has this number as 15 and D-gulose is fifth in the order starting from D-allose as the first according to the mnemonic. Hence, the stereo number of L-gulose is  $15 - 11 = 4$ . On converting the decimal equivalent 4 into the binary number, it will be 0100 which means that the hydroxyl groups of the C-5, C-3 and C-2 are projected to the left and that of C-4 to the right. Similarly, one can work

out the stereochemical representation of L-glucose which corresponds to (XIV) since the binary code number of L-glucose is 0010, its stereo number being 2.

#### ACKNOWLEDGEMENT

The author's thanks are due to Professor M. Venkataraman, Head of the Department of Mathematics, Madurai University, for the useful discussions on this paper.

1. Fieser, L. F. and Fieser, M., *Organic Chemistry*, Reinhold, N.Y., 3rd Edn., 1959, p. 359; *Advanced Organic Chemistry*, Asia Publishing House, Bombay, 1961, p. 947.
2. Dyke, S. F., *The Carbohydrates*, Interscience Publishers, N.Y., 1960, p. 24.
3. Feldman, A., *J. Org. Chem.*, 1959, **24**, 1556.
4. Rosenblatt, D. H., *J. Chem. Edn.*, 1965, **42**, 271.

### COSMIC RAY STUDIES\*

THERE have been, over the recent past, spectacular developments in various areas of astronomy, astrophysics and cosmology such as the discovery of quasars, of pulsars, of the apparently universal radiation in the microwave and infrared regions, of the existence of violent explosive phenomena in the universe, problems of nucleosynthesis, and a great deal else that cannot be compressed into a few words here. It has become increasingly clear that the detailed features of cosmic ray phenomena are closely tied up with the various astrophysical parameters and processes, particularly those concerning these new discoveries.

This book reproduces the proceedings of a Colloquium which was organised and held in Bombay from November 11 to 16, 1968, by the Tata Institute of Fundamental Research, Bombay, primarily to identify, and to focus attention on, the important connections and overlapping areas of interest created as a result of recent advances in cosmic ray research on the one hand, and spectacular developments in astronomy, astrophysics and cosmology on the other. In the Colloquium, about equal working time was devoted to invited talks and panel discussions.

This book includes all the invited talks and reports of the panel discussions.

The titles of the invited talks and their respective speakers are: 1. Abundances of the Elements, by A. G. W. Cameron; 2. Nucleosynthesis, by W. A. Fowler; 3. Composition of Cosmic Rays, by S. Biswas; 4. Cosmic Ray Nuclei of Charge Greater than 20, by D. Lal; 5. On the Propagation of Cosmic Rays, by Yash Pal; 6. X-Ray and Gamma-Ray Astronomy, by B. Rossi; 7. Background X-rays and Gamma-Rays—Interpretations, by S. Hayakawa; 8. Interstellar Matter, by H. C. van de Hulst; 9. Radio Continuum, by J. R. Shakeshaft; 10. The Microwave Background Radiation, by W. H. McCrea; 11. Cosmic Rays at Energies beyond  $10^{12}$  eV, by B. V. Sreekantan; 12. Cosmic Ray Electrons, by R. R. Daniel; 13. Dynamics of the Galactic Disc, by E. N. Parker; 14. Quasars—Observational, by M. K. V. Bappu; 15. Quasars—Interpretative, by W. H. McCrea; 16. Observations of Pulsars, by J. R. Shakeshaft; 17. Solar Neutrinos, by W. A. Fowler; and 18. Radio Source Counts, by J. R. Shakeshaft.

The subjects dealt with under panel discussions are: 1. Nuclear Abundances; 2. Spectrum and Composition; 3. X-rays, Gamma-Rays and Electrons; 4. Cosmic Ray Origin; 5. Problem of Helium Abundance; 6. Pulsars; 7. Neutrinos in Astrophysics; and 8. Cosmology.

This volume will be of great interest and value to all those working in this field.

C. V. R.

\* *Cosmic Ray Studies* in relation to recent developments in Astronomy and Astrophysics, Edited by R. R. Daniel, P. J. Lavakare and S. Ramadurai. (Published by the Tata Institute of Fundamental Research, Bombay, India), 1969. Pp. 874. Price: to Colloquium Participants: Rs. 10 and to all others: Rs. 50 or \$ 7.00 or £ 3-0 sh.-0 d.