DIRECT AND SIMPLE APPROACH FOR ASSIGNING ABSOLUTE CONFIGURATION IN WEDGE DASH PROJECTION

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ABSTRACT

The procedure of assignment of absolute configuration to optical stereoisomers in various projections has been already described in literature. Most common methods utilize the Fischer Projection as the standard and hence demands a three dimensional structure (wedge dash projection, newmann projection, sawhorse projection) to be inter converted to two dimensional planar Fischer Projection. This adds on an extra exercise which may sometimes cause error while specifying Absolute Configuration to a molecule originally represented in three dimensional projections. Hence this assignment of configuration to optical isomers should be directly taught to undergraduates through three dimensional representation of the molecule as stereochemistry deals with three dimensional aspects of an organic compound. This method assigns absolute configuration to the chiral molecules directly in wedge dash projection without interconverting to Fischer Projection. *[African Journal of Chemical Education—AJCE 11(2), July 2021]*

INTRODUCTION

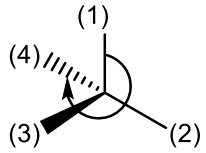
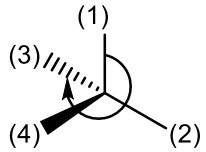
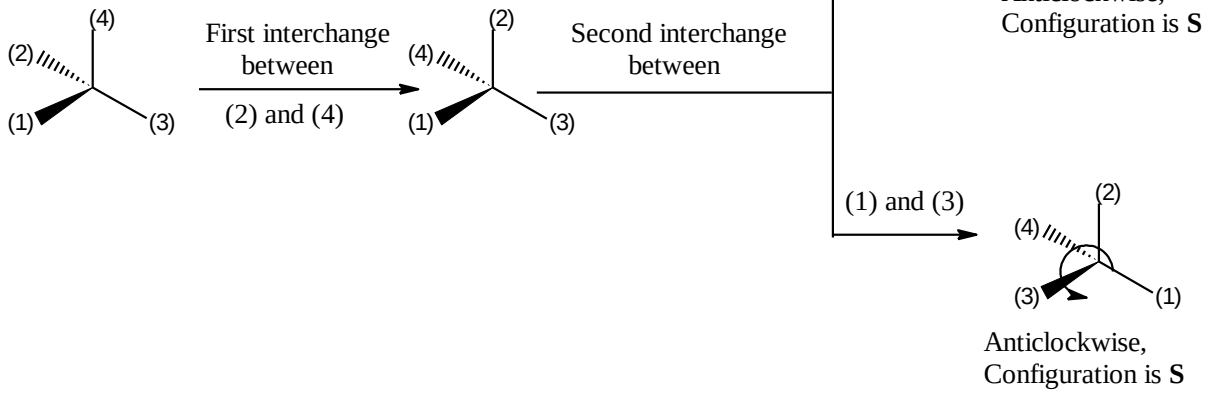
Absolute configuration is defined as stereochemical description of a chiral molecule with reference to the atoms and groups attached to the chiral center. The determination of absolute configuration to optical isomers is necessary as they differ in configuration. Though optical isomers differ in sign of rotation yet the arrangement of atoms or groups around a chiral center cannot be known. This is important as two stereoisomers may have same sign of optical rotation but may differ in their relative spatial arrangements of atoms or groups around a stereogenic center. Before 1951, chemists used to determine the configuration of compounds through chemical interconversions by the Method of Relative Configuration. [1-2].

The method suffered from serious drawbacks until the method of absolute configuration was introduced. This requires the application of sequence rules as devised by Cahn Ingold and Prelog [3-4]. The molecule is originally represented in wedge dash projection is converted to Fischer projection and then is subjected to assignment of absolute configuration. Though the method is successful yet it involves laborious steps of rotation and interconversion which makes it time consuming. When it comes to solve problems, the undergraduate students face difficulty in visualization during interconversion and waste their precious time. Till date, many modifications in the procedure of assigning absolute configuration have been reported [5-10] but either they involve visualization, interconversion to two dimensional projection or computational/mathematical calculations. From students' point of view these methods are not simple, time consuming and thus require extra efforts for results.

This manuscript describes a student friendly direct and simple method of assigning absolute configuration to a chiral molecule in three dimensional wedge representation via application of sequence rules. The modified general procedure for assigning absolute configuration

(R/S) to a chiral center in wedge-dash projection is given in Table-1 with illustrations (Scheme-1 and Scheme 2). Four groups or atoms directly attached to the chiral center are assigned priorities according to Cahn Ingold, Prelog (Sequence rule) from highest (1) to lowest (4).

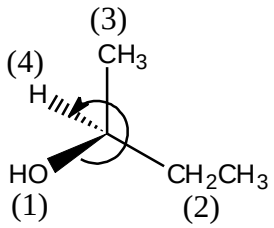
Table-1 Simple and Direct Procedure for assigning absolute configuration

S. No.	Position of the lowest priority group or atom	Position of atoms in a molecule in 3D or space	Direction of path	Configuration
1.	Away from the viewer (on dotted /dash line) Out of plane		Clockwise	**R**
2.	Towards the viewer (wedge/ solid wedge) Out of plane		Clockwise	Fictious- ~~R~~ Actual- **S**
3.	Plane of the paper (on the straight line)  Change the position of lowest priority group from plane of paper (straight line) to away from the viewer (dash) by making even number of interchange.			

ILLUSTRATION

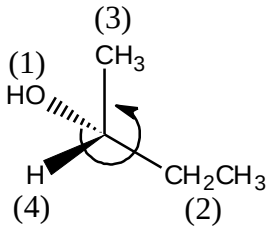
Absolute configuration (R/S) in different wedge dash projection of butane-2-ol is as follows.

(a)



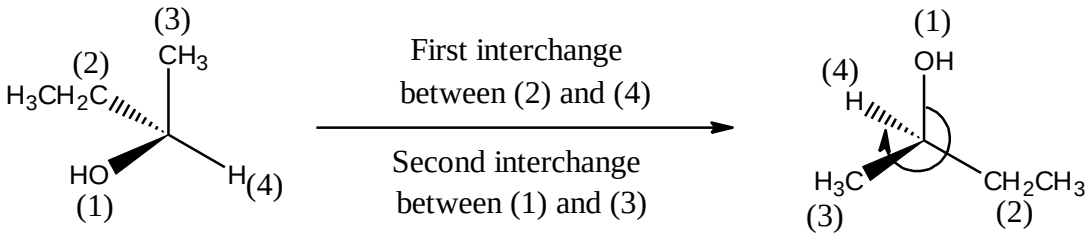
Direction of path
is anticlockwise,
Configuration-**S**

(b)



Direction of path
is anticlockwise,
Fictious Configuration-~~S~~
Actual Configuration-**R**

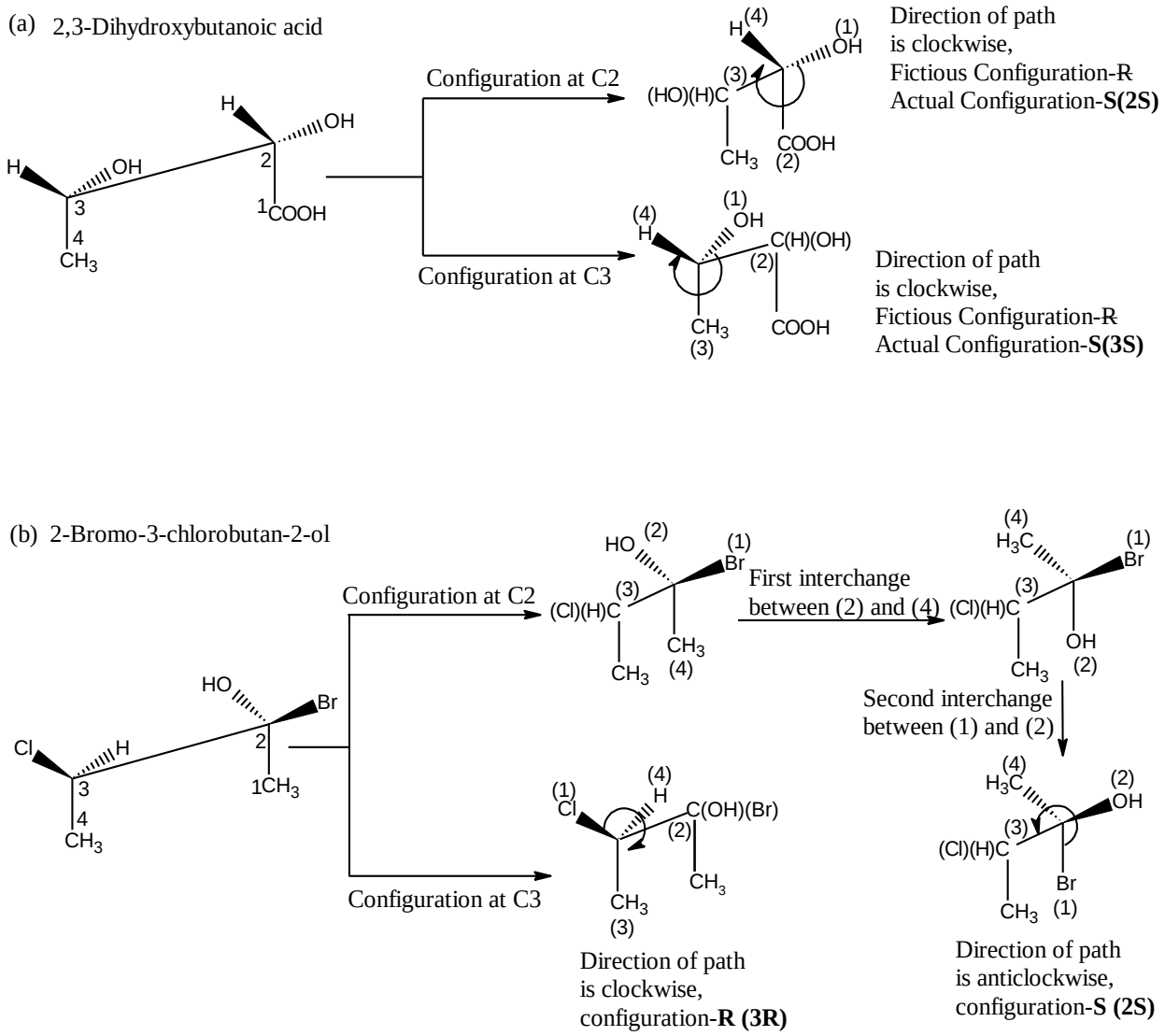
(c)



Direction of path
is clockwise,
Actual Configuration-**R**

Scheme-1

Similarly, absolute configuration (R/S) in wedge-dash projection for two chiral centers can also be assigned (Scheme-2).



Scheme-2

CONCLUSION

A direct method of assigning absolute configuration to a chiral center in wedge dash projection only utilizes the Cahn Ingold rule of assigning priority and then tracing the path irrespective of the position of lowest priority group. This method works well in wedge dash Projection of chiral molecules with one or more chiral centers. It avoids the use of three dimensional models and extra steps of interconversion and rotation of the molecule followed by

exchange of groups or atoms as required in conventional procedure. Students at times spend time in visualization and interconversion. This procedure is fast, reliable and provides a learning tool for assigning absolute configuration to three dimensional chiral molecules in a two dimensional perspective.

DECLARATIONS

Funding

No funding was received to assist with the preparation of this manuscript.

Conflict of Interest/Competing Interests

The authors have no conflict of interests.

Authors Contributions

All authors contributed to the study conception and design. Conceptualization Idea and manuscript preparation was by Sonia Ratnani. Figure preparation and formatting by Sarika Malik. Proof Reading and literature findings by Shriniwas Gurjar. All authors read and approved the final manuscript.

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