Determining R/S configurations of a chiral molecule with the Newman projection formula

Determinación de R/S configuraciones de una molécula quiral con la fórmula de proyección de Newman

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Abstract:

The R/S configuration of a chiral molecule with the Newman projection formula can be determined by a new method. The method includes different steps, and configurations of stereogenic centers are determined on one model. However, there is neither mental orientation of the molecule nor transformation of the molecule with 3D structure into Fischer projection formulas needed using this method.

Key words: *chirality, Newman projection formula, organic chemistry, stereochemistry.*

Resumen

La configuración de R/S de una molécula quiral con la fórmula de proyecciones de Newman puede determinarse por un nuevo método. El método incluye los pasos diferentes, y las configuraciones de centros quirales determinadas en un modelo. Sin embargo, no es necesaria la utilización ni orientación mental de la molécula, ni transformación de la molécula con 3D estructura en las fórmulas de proyecciones de Newman.

Palabras clave: *quiralidad, fórmula de proyecciones de Newman, química orgánica, esterioquímica.*

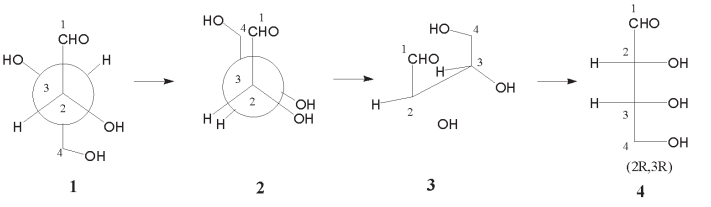
INTRODUCTION

The most widely accepted method for specifying the configuration about a stereogenic center is the R/S system. The stereogenic center is used as a chiral center (Mislow, et al., 1984; Wang, et al., 1992). This determination involves a two-step process. The first step requires an assignment of priority to each group about the stereogenic center. The second step involves a mental transfer of the two-dimensional figure into a three-dimensional model, followed by the determination of R or S.

Some investigations have been published about specifying the R/S configuration of a stereogenic center (Mislow, et al., 1984; Wang, et al., 1992; Dietzel, 1979; Idoux, 1982; Epling, 1982; Ayorinde, 1983; Mattern, 1985; Eliel, 1985; Ruekberg, 1987; Yongsheng, et al., 1992). However, not only many students but also some experienced chemists still find it difficult to assign R or S descriptions to stereogenic centers by inspection of a stereoformula such as Newman projection formulas. The illustration of molecules was studied as a the Newman projection formula (Silverman, et al., 1999; Tavernier, 1986). Wang and Yang used the rule of multiplication for determining the R/S configuration of a chiral molecule with the Newman formula (Wang, et al., 1992). In a molecule, the configuration of the molecule with two vicinal stereogenic centers, which is similar to the Newman projection formula, is assigned by Mandal, who proposed that after the priority order of ligands is determined for each stereogenic center, these centers be separately converted into two Fischer projection formulas, and then their configurations be assigned (Mandal, 2000).

As shown in scheme 1, determination of the R/S configurations of the Newman projection formulas may be determined by transformations of them into Fischer projection formulas (Morris, 2001). They can be figured out through the following steps: 1) After the Newman projection formula is rotated to an eclipsed conformation, a Fischer projection formula is made. 2) Priority order of all substituents is determined for each stereogenic center (C-2 and C-4) and then the R- and S- configurations of them are assigned.

Many students fall into error through "mental orientation of the molecule so that the group of lowest priority (fourth) is pointing directly back, away from us" or "transformations of the molecule with 3D structure into Fischer projection formulas". Determination of the R/S configuration of a chiral molecule with the Newman projection formula was studied without using mental orientation of the molecule.

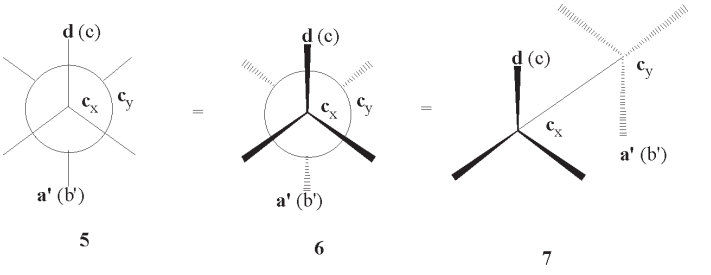


Scheme 1

RESULTS AND DISCUSSION

It is important that any phenomenon such as aromaticity, oxidation-reduction or order of atomic orbitals may be easily written, learned, and remembered (Quigley, 1992; Menzek, 1999; Menzek, 2002; Halkides, 2000). We have developed a method for determining the R/S configurations of stereogenic centers of the chiral molecule with the Newman formula.

We can consider the Newman projection formula 5 of a molecule. It has a gauche conformation, and its Cx and Cy are stereogenic centers. Therefore, a, b, c and d are groups attached to the stereogenic center Cx. At the same time, a', b', c' and d' are groups attached to the stereogenic center Cy. d represents the lowest priority group, excluding Cy, and a' represents the highest priority group, excluding Cx. Cy and Cx may be d and a', respectively, in one possible structure. Therefore, c and b' may be found in the case of d and a', respectively, in these formulas.



Scheme 2

As shown in 6 and 7, the groups attached to Cx, excluding Cy, are the groups coming toward us out of the paper, whereas Cy attached to Cx is a group going away from us behind the paper. The groups attached to Cy, excluding Cx, are the groups going away from us behind the paper, whereas Cx attached to Cy is a group coming toward us out of the paper.

The configurations of Cx and Cy of the Newman formula are determined easily and rapidly via structure 8 (Figure 1) of the Newman projection formula. c_x, d (c), Cx, Cy and a' (b') are shown on the same line in structure 8. In this structure, Cx-Cy and d (c)-c_x show Cx-Cy and Cy-Cx bonds, respectively.

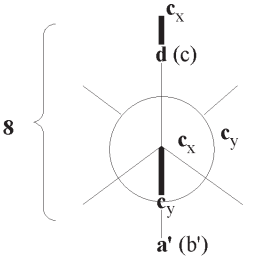


Figure 1

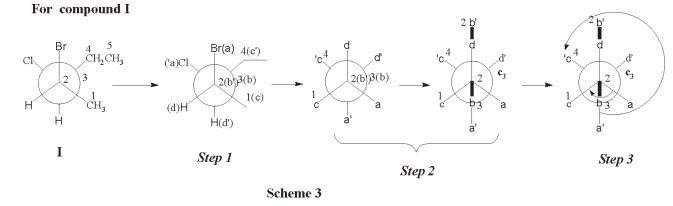
Determination of the R/S configurations of the Newman projection formulas:

Step 1. Draw the Newman projection formula of a molecule in gauche conformation. Assign the priority sequence for the groups attached to stereogenic centers based on Cahn-Ingold-Prelog sequence rules, and express the sequence by a, b, c and d (where a represents the highest priority group). Represent a, b, c and d as groups attached to a stereogenic center, such as C_x that is nearer to you, and a', b', c' and d' as groups attached to stereogenic center that is more distant from you, such as C_y

Step 2. Represent d and a' as vertical lines (in the same direction). If d and a' are the stereogenic center and the highest priority group, respectively, c and b' are represented in the case of d and a', respectively. Place the stereogenic center Cx that is nearer to you and the stereogenic center Cy that is more distant from you between Cx-d (c) and Cy-a'(b') and the end of d (c) as a bold line in the structure 8.

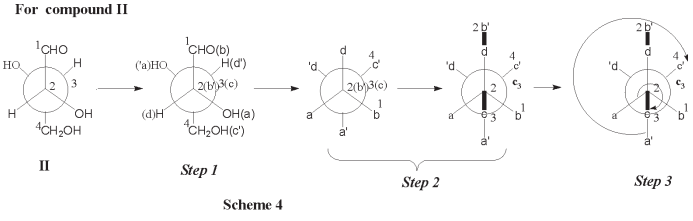
Step 3. Now mentally move from (a) to (b) to (c) and (a') to (b') to (c'). Ignore groups (d) and (d'). If the direction of your motion is clockwise, the configuration is R. If the direction of your motion is counterclockwise, the configuration is S. If Cx attached to Cy is d', the configuration of Cy is opposite (such as R in case S) of that found from 8. Name the original molecule.

Examples, for determination of the R/S configurations of a molecule with Newman projection formula:



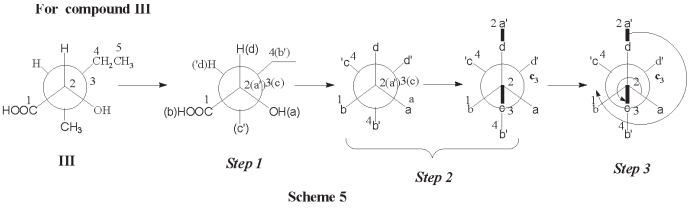
Scheme 3

The name of compound I is (2R,3S)-2-bromo-3-choloropentane.



Scheme 4

The name of compound II is (2R,3R)-2,3,4-trihydroxybutanal.



Scheme 5

The name of compound III is (2S,3R)-2-hydroxy-3-methylpentanoic acid.

The above steps may be shortened and the configurations of Newman projection formulas may be more rapidly determined.

CONCLUSIONS

The R/S configurations of Newman projection formulas may be determined by this method. This method is new and includes different steps. The R/S configurations of stereogenic centers are determined on one model. There is no mental orientation of the molecule and transformation of the molecule with 3D structure into Fischer projection formulas, using this method. Therefore, students may fall into less error in the determination of the R/S configuration of a chiral molecule with the Newman projection formula.

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What content for biological education is in Sub-saharan Africa today?
¿Cuál es el contenido moderno de la educación biológica en África Subsahariana?

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Abstract

Nowadays Sub-saharan Africa is characterized by a lot of problems linked to underdevelopment:

-Every year the size of the population grows significantly while food resources are not adequate; there is a large food deficit (malnutrition, famine, etc.).

-A major environmental deterioration, which is due to deforestation, resulting in a reduction of the biodiversity, desertification, and uncontrolled urbanization.

-Several endemic diseases like AIDS and malaria are causes of death in most of the countries. There is a low life expectancy (45-50 years) and a high maternal and infant mortality. To face this situation and set a sustainable rate of development, Subsaharan Africa has to struggle first, against the high illiteracy of most of the population by defining new educational curricula in schools in areas related to knowledge, skills for the resolution of practical problems, and positive attitudes. In facing such a challenge, biological education has a large part to play in order to give to every citizen the minimum of scientific knowledge which is necessary to live in harmony with