The Keval’s Method – Determination of Absolute Configuration Using Calculations

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Abstract
“The Keval’s Method” is developed for the determination of absolute configuration of a chiral carbon in a Fisher Projection and Wedge-Dash Projection just by simple calculations. This method is easily applicable over both Fisher as well as Wedge-Dash Projection.

INTRODUCTION
5.1. Number all 4 elements using CIP(CAHN-INGOLD-PREGOLD) Convention

5.2. The Coordinate system postulates of Keval’s Method
5.2.1. Fisher
• Take the vertical line of Fisher Projection as Y-axis (a-c), so, Take ‘a’ Positive and ‘c’ Negative.
• Take the horizontal line of Fisher Projection as X-axis (d-b), so, Take ‘b’ Positive and ‘d’ Negative.

5.2.2. Wedge-Dash
• Take ‘Dash’ as Negative Y-axis
• Take opposite ‘Line’ or opposite ‘Dash’ as Positive Y-axis.
5.3. Calculations

K = (Y1)*(X1) + (X1)(-Y2) + (-Y2)(-X2) + (-X2)(Y1)
Check if K is Positive or Negative.

M = |(Y1)-(Y2)|
Check if M is Odd or Even.

Then,
M->Odd => T=(-K)
M->Even => T=(K)

5.3.1. (Table-1) Absolute Configuration will be according to the table

<table>
<thead>
<tr>
<th>K</th>
<th>M</th>
<th>T</th>
<th>Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Positive</td>
<td>Odd</td>
<td>Negative</td>
<td>R</td>
</tr>
<tr>
<td>Positive</td>
<td>Even</td>
<td>Positive</td>
<td>S</td>
</tr>
<tr>
<td>Negative</td>
<td>Odd</td>
<td>Positive</td>
<td>S</td>
</tr>
<tr>
<td>Negative</td>
<td>Even</td>
<td>Negative</td>
<td>R</td>
</tr>
</tbody>
</table>

(Table showing mathematical conditions according to Keval’s Method and respective configurations.)
6. Examples

6.1. Fisher

6.1.1. S-1-Bromo-1-Chloroethane

\[ K = (2)(3) + (3)(-1) + (-1)(-4) + (-4)(2) \]
\[ = 6 - 3 + 4 - 8 \]
\[ = -1, \text{ So, } K \text{ is Negative} \]

\[ M = |(2) + (-1)| \]
\[ = 1, \text{ So, } M \text{ is Odd} \]

\[ T = (-K) = (-(-1)) \]
\[ = 1, \text{ So, } T \text{ is Positive.} \]

According to the table, Configuration is ‘S’.

6.1.2. R-1-Bromo-1-Chloroethane

\[ K = (1)(3) + (3)(-2) + (-2)(-4) + (-4)(1) \]
\[ = 3 - 6 + 8 - 4 \]
\[ = +1, \text{ So, } K \text{ is Positive.} \]

\[ M = |(1) + (-2)| \]
\[ = 1 \]

\[ So, M \text{ is Odd.} \]

\[ T = (-K) = -1 \]
\[ = (-1), \text{ So, } T \text{ is Negative.} \]

According to the table, Configuration is ‘R’.

6.1.3. R-1-Bromo-1-Chloroethane
K = (4)(1) + (1)(-2) + (-2)(-3) + (-3)(4) 
= 4 - 2 + 6 - 12 
= (-4), So, K is Negative.
M = |(4) + (-2)| 
= 2, So, M IS Even.
T = (-K) = (+(-4)) = (-4) 
= (-4), So, T is Negative. 
According to the table, 
Configuration is ‘R’.
6.2. Wedge-Dash
6.2.1. R-1-Bromo-1-Chloro-1-Floromethane

K = (1)(3) + (3)(-2) + (-2)(-4) + (-4)(1) 
= 3 - 6 + 8 - 4 
= (+1), So, K is Positive.
M = |(-2) + (1)| 
= 1, So, M is Odd.
T = (-K) = (+(-1)) = (-1) 
= (-1), So, T is Negative. 
According to the table, 
Configuration is ‘R’.
6.2.2. R-1-Bromo-1-Chloroethane
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6.2.3.5-1-Bromo-1-Chloroethane

K=(3)(4)+(4)(-1)+(-1)(-2))+(-2)(3)
=12-4+2-6
=(4), So, K is Positive.
M=|(3)+(-1)|
=2, So, M IS Even.
T=(K)=(+(4))=+(4)
=(+4), So, T IS Positive.
According to the table,
Configuration is ‘S’.

7. Conclusion
The Keval’s Method described in this manuscript for assigning R,S-configuration, is the first method which assumes chiral carbon molecule as co-ordinate system with carbon as origin And it’s the method which uses
Mathematical Calculations to determine absolute configuration of a chiral molecule. As demonstrated above, the method works equally well for either of the commonly used representations of the three-dimensional geometry: Fisher Projection as well as Natta (wedge-dash) Projections. Absolute configuration from the Fischer Projections & Wedge-Dash is easily determined by the method without exchanging groups as required by the exchange rules. Students will always find conceptualizing spatial arrangement in three dimensions to be challenging. The method described in this manuscript is a fast, comprehensive, reliable and a rapidly learnable method for students to use as this method does not require any knowledge of spatial arrangement in three dimensions. Students should find it very easy to use a method, which just uses simple calculations versus traditional one hand or two hand methods, when taking exams and studying.

Also, this method is very useful because it can also be used to make “computer software” to find absolute configuration of a chiral molecule as the method just uses simple calculations.

References