Folding Techniques in Alcohol Chemical Structures

K. Thiagarajan, N. Subashini, S.K. Chithralekha Devi

Abstract: ***In this paper, we have observed the definitions of point folding and edge folding from the graph theory in mathematics. Also we have derived newly semi- edge folding techniques to get new applications in Alcohol chemical world. The proposed methodology is very useful for Alcohol chemical compounds like methanol, ethanol etc after applying appropriate procedure to get decided meaningful concept in Chemistry through folding technique.***

Keywords: Alcohol Chemical Structures, Edge Folding, Folding, Point Folding, Semi Edge Folding.

I. INTRODUCTION

Theories of chemical structure were first developed by August Kekule, Archibald Scott Couper, and Aleksandr Butlerov, among others, from about 1858.

These theories were first to state that chemical compounds are not a random cluster of atoms and functional groups, but rather had a definite order defined by the valency of the atoms composing the molecule, giving the molecules a three dimensional structure that could be determined or solved.

In this paper, we correlate alcohol chemical structure and folding techniques [8] for some special alcohol chemical structures in algorithmic way.

The folding Technique is applicable for some special type of alcohol chemical structure in the field of chemistry. Complete electronic structure descriptions include specifying the occupation of a molecule's molecular orbitals.

Structure determination can be applied to a range of targets from very simple molecules (e.g., diatomic oxygen or nitrogen), to very complex ones (e.g., such as of protein or DNA).

II. PRELIMINARIES : [1],[2]& [3]

Definition 1:

Chemical Structures

Molecular geometry refers to the spatial arrangement of atoms in a molecule and the chemical bonds that hold the atoms together and can be represented using structural formulae and by molecular models;

Definition 2: [8]

Semi graph Folding

A Semi graph map F: $SG_1 \rightarrow SG_2$ a semi graph folding, if and only if F maps vertices to vertices, semi vertices to semi vertices, edges to edges and semi edges to semi edges.

Definition 3: [8]

Point Folding

A graph map F: $G_1 \rightarrow G_2$ a point folding, if and only if F maps vertices to vertices and edges to edges when numbers of vertices are odd.

Definition 4: [8]

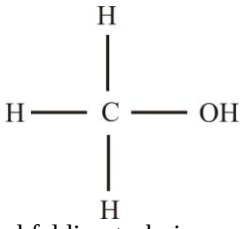
Edge Folding

A graph map F: $G_1 \rightarrow G_2$ a edge folding, if and only if F maps vertices to vertices and edges to edges when number of vertices are even.

III. FOLDING TECHNIQUES IN ALCOHOL CHEMICAL STRUCTURES HAVING ODD NUMBER OF CARBONS

Example 1:

Consider Methanol Alcohol, the following chemistry structure is followed

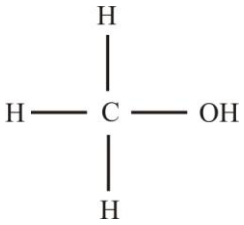


This can be derived folding technique namely point folding, edge folding and semi edge folding in the following algorithm I.

Algorithm I:

Step I:

Given $CH_3 - OH$ can be referred as



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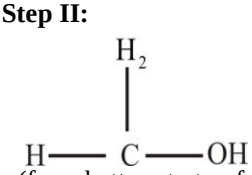
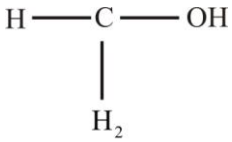
Step II:



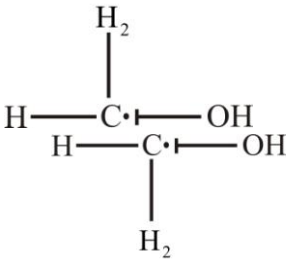
(from bottom to top folding)



(from top to bottom folding)

Here point folding is applied from bottom to top folding (or) top to bottom folding justification. This shown in the above structure.

Step III:



(or)

Here semi folding is introduced at which [number of carbons+1]/2th place proceeding (or) succeeding by carbon.

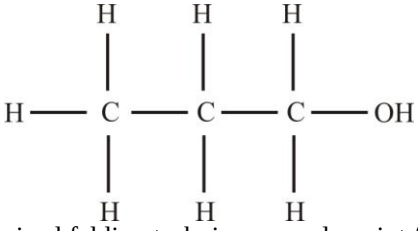
Step IV:

Here point folding is applied at which [number of carbons+1]/2th place proceeding (or) succeeding by carbon.

Step V:

Step IV can be written as $CH_3 - OH$ and hence aims completes to get CH_3OH .

Example 2: Consider proponal, the following chemical structure is followed.

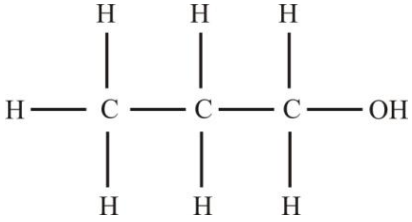


This can be derived folding technique namely point folding, edge folding and semi edge folding in the following algorithm II.

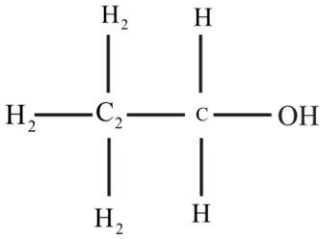
Algorithm II:

Step I:

Given $C_3H_7 - OH$ can be referred as

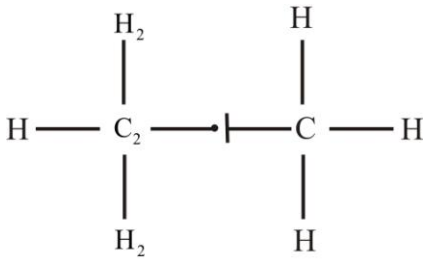


Step II:



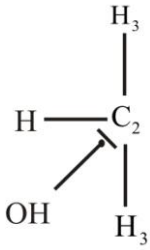
Here point folding is applied at which [number of carbons+1]/2th place proceeding (or) succeeding by carbon.

Step III:



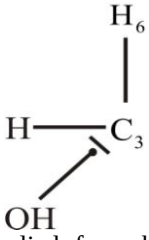
Here, semi edge folding is introduced at which [number of carbons]/2th place proceeding (or) succeeding by carbon. Since the numbers of carbons are even. Hence, edge folding is not possible.

Step IV:



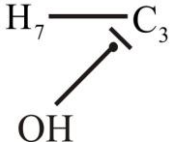
Here, semi edge folding is applied from right to left folding.

Step V:



Here point folding is applied from bottom to top with respect to C_3 which is available at the [number of carbons+1]/2th place.

Step VI:



Here point folding is applied with respect to C_3 which is available at the [number of carbons+1]/2th place.

Step VII:

Step VI can be written as

Hence, aim completes to get $C_3H_7 - OH$.

Theorem 1:

In any simple discussed alcohol chemical structure if the number of carbons are odd then, [(number of carbons+1)/2]th carbon will be acting as the domination carbon to apply point folding and also semi edge folding technique.

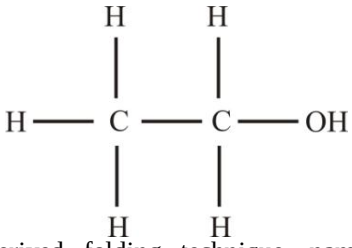
Proof:

From Examples 1 & 2.

IV. FOLDING TECHNIQUES IN ALCOHOL CHEMICAL STRUCTURES HAVING EVEN NUMBER OF CARBONS

Example 3:

Consider Ethanol, the following chemical structure is followed:

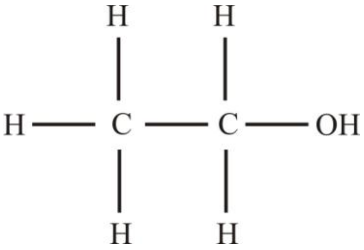


This can be derived folding technique, namely, edge folding, semi edge folding in the following algorithm III.

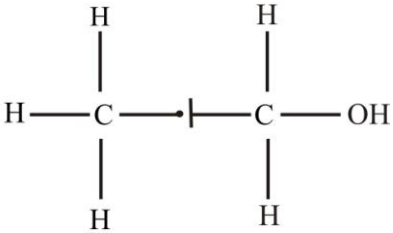
Algorithm III:

Step I:

Given $C_2H_5 - OH$ can be referred as

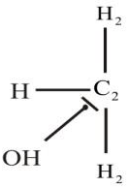


Step II:



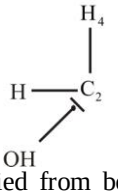
Here, semi-edge folding is introduced at which [number of carbons]/2th place proceeding (or) succeeding by carbon. Since the numbers of carbons are even. Hence, edge folding is not possible.

Step III:



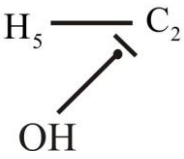
Here edge folding is applied from right to left folding.

Step IV:



Here, point folding is applied from bottom to top folding with respect to C_2 which is available at [number of carbons+1]/2th place.

Step V:

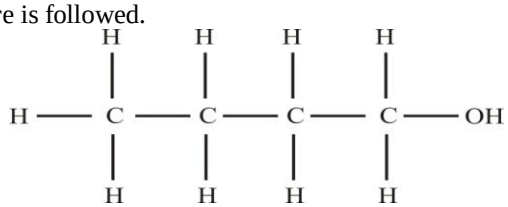


Here, point folding is applied with respect to C_2 which is available at [number of carbons+1]/2th place.

Step VI: Step V can be written as

Hence the aim completes to get $C_2H_5 - OH$.

Example 4: Consider the Butanol the following chemical structure is followed.

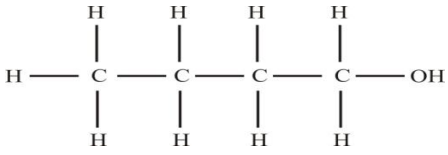


This can be derived folding technique namely, point folding, edge folding, semi edge folding in the following algorithm IV.

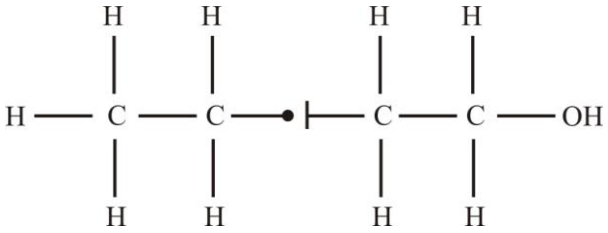
Algorithm IV:

Step I:

Given $C_4H_9 - OH$ can be referred as

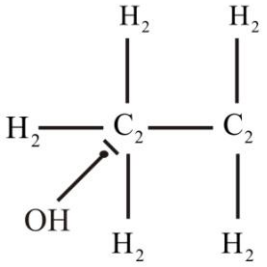


Step II:



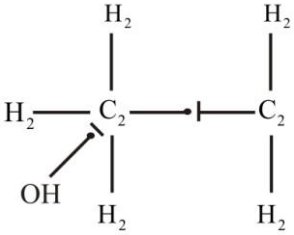
Here, semi-edge folding is introduced at which [number of carbons]/2[th] place proceeding (or) succeeding by carbon. Since the numbers of carbons are even. Hence, edge folding is not possible.

Step III:



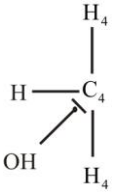
Here semi edge folding is applied from right to left folding.

Step IV:



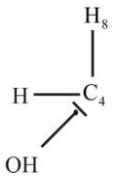
Here, semi-edge folding is applied at which [number of carbons]/2[th] place proceeding (or) succeeding by carbon. Since the number of carbons are even and edge folding is not possible.

Step V:



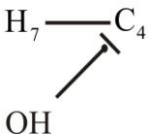
Here, semi-edge folding is applied at which [number of carbons]/2[th] place proceeding (or) succeeding by carbon. Since the number of carbons are even and edge folding is not possible.

Step VI:



Here, point folding is applied from bottom to top folding with respect to C_4 which is available at [(number of carbons + 1)/2][th] place.

Step VII:



Here, point folding is applied with respect to C_4 which is available at [(number of carbons + 1)/2][th] place.

Step VIII:

Step VII can be written as

Hence, the aim completes to get $C_4 H_7 - OH$.

Theorem 2:

In any simple discussed alcohol chemical structure if the number of carbons are even then, [number of carbons / 2][th] will be acting as the domination carbon. We can apply semi edge folding technique and also point folding technique.

Proof:

From examples 3 & 4.

V. CONCLUSION

In this paper, we have derived point folding techniques, edge folding techniques and semi edge folding techniques in some special alcohol chemical structures. Also, we have derived some theorems based on folding techniques in some special alcohol chemical structures and this proposed methodology will be very useful in alcohol chemical compounds in the field of chemistry.

VI. FUTURE WORK

In future, this folding approach may be extended for some other special alcohol chemical structures.

VII. ACKNOWLEDGEMENT

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