Folding Techniques in 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 chemical world. The proposed methodology is very useful for chemical compounds like methane, ethane etc after applying appropriate procedure to get decided meaningful concept in Chemistry through folding technique.***

Keywords: 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 chemical structure and folding techniques [8] for some special chemical structures in algorithmic way.

The folding Technique is applicable for some special type of 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]

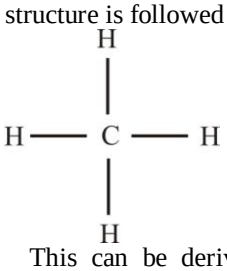
Edge Folding

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 CHEMICAL STRUCTURES HAVING ODD NUMBER OF CARBONS

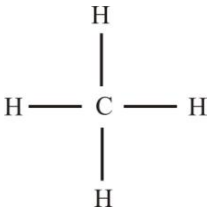
Example 1:

Consider Methane CH_4 in chemistry, the following structure is followed by

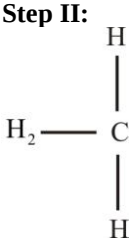


This can be derived in folding techniques using point folding [4], edge folding ([5], [6], [7])and semi edge folding [8] explained in algorithm I.

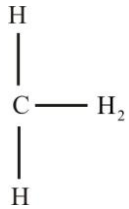
Algorithm I: Step I: Given CH_4 can be referred as



Step II:



(from right side to left side folding) (or)



(from left side to right side folding)

Revised Manuscript Received on May 07, 2019.

K. Thiagarajan, Professor-Academic Research, Jeppiaar Engineering College, Chennai-119, Tamilnadu, India.

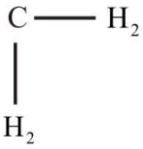
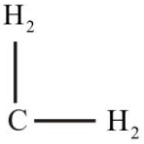
N. Subashini , Research Scholar, Mother Teresa Women's University, Kodaikanal, Tamilnadu, India. Dept. of Mathematics, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India.

S.K. Chithralekha Devi Professor, Department of Chemistry, Jeppiaar Engineering College, Chennai-119, Tamilnadu, India.

Here point folding is applied from right to left justification. It may be applied from left to right also. This shown in the folding structure.

Step III: Similarly, the above folding technique is applied from top to bottom folding (or) bottom to top folding.

Top to Bottom folding (or) Bottom to top folding

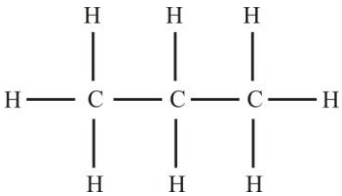
Step IV: The step III can be written as $H_2 - C - H_2$ .Then point folding technique is applied with respect to C from right to left folding(or) from left to right folding, we get $C - H_4$ (or) H_4-C

Step V:

Hence, the aim completes to get CH_4 .

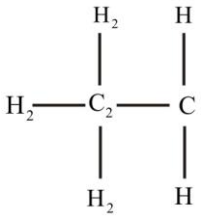
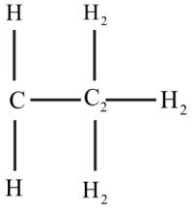
Example 2: Consider C_3H_8 in chemistry [3], the following structure is followed algorithm II.

Algorithm II: Step I: Given C_3H_8



Step II:

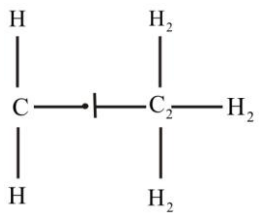
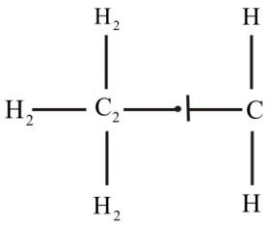
To apply point folding with respect to C which is available at centre of the structure calculated through [(Number of carbons + 1)/2, here Number of carbons=3(odd)]

(from right to left folding) (or) (from left to right folding)

Step III:

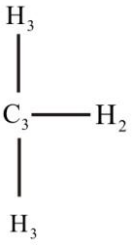
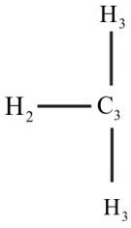
In this introduce semi edge folding between two carbons (since,the number of carbons are even and edge folding is not possible).

(or)

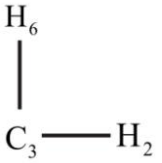
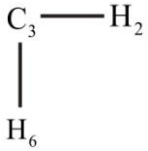
Step IV:

To apply semi edge folding then, we shall have '2' ways

(or)

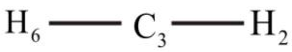
Step V: In this, to apply point folding with respect to C_3 from top to bottom (or) from bottom to top, we get

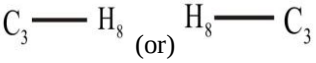
(or)

(from bottom to top folding) (from top to bottom folding)

The above structure can be written as



Step VI: Now, in this, we apply point folding from right to left folding (or) from left to right folding with respect to C_3 , we get



(or)

Step VII: Hence, the aim completes to get $C_3 - H_8$.

Theorem 1: In any simple discussed 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 technique and also, in this case, point symmetry only is possible for folding.

Proof: From Examples 1 & 2.

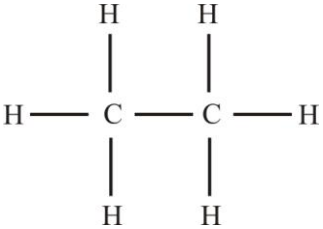
IV. FOLDING TECHNIQUES IN CHEMICAL STRUCTURES HAVING EVEN NUMBER OF CARBONS

Example 3:

Consider C_2H_6 - Ethane in Chemistry

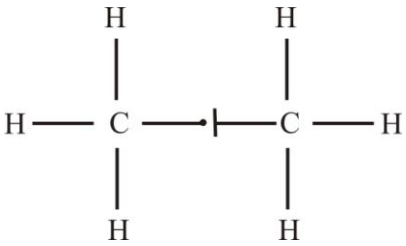
Step I:

Given C_2H_6



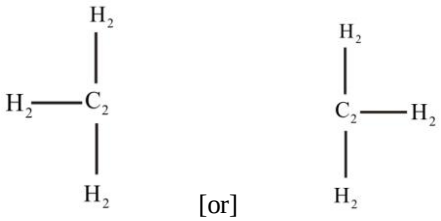
Step II:

Introduce semi-edge folding between two carbons (Q Here, edge folding is not possible). Then, the above structure can be reformed as



Step III:

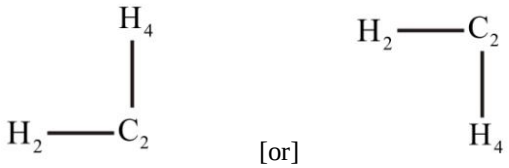
Folding technique is applied with respect to semi edge on the above reformed structure.



(from right to left folding) [or] (from left to right folding)

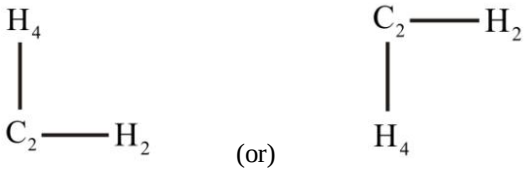
Step IV:

In the above structure, point folding is applied from top to bottom folding (or) bottom to top folding with respect to C_2 .This shown in the following structure



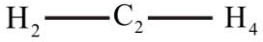
(from bottom to top folding) [or] (from top to bottom folding)

On the other way, we shall have

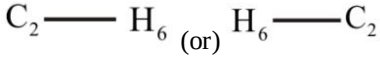


(from bottom to top folding) (or) (from top to bottom folding)

This can be written as



Step V: To apply point folding technique from right to left folding (or) from left to right folding with respect to C_2, we get



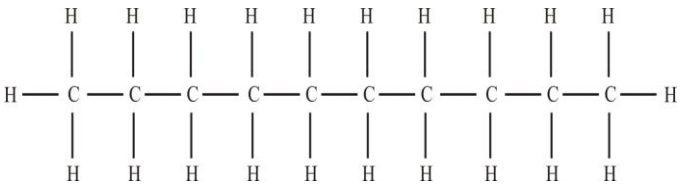
Step VI: Hence, the aim completes to get C_2H_6 .

Example 4:

Consider $C_{10}H_{22}$ - Decane in Chemistry

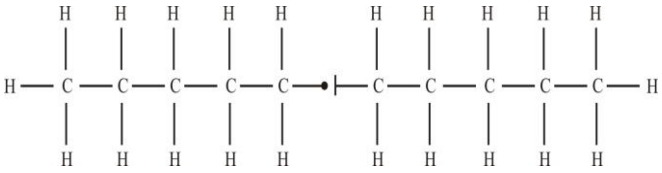
Step I:

Given $C_{10}H_{22}$



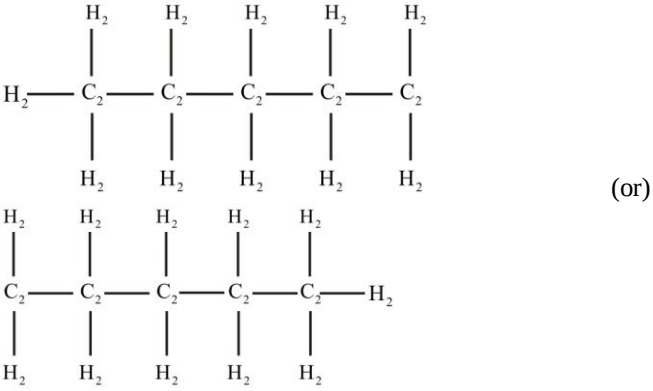
Step II:

Introduce semi edge at (Number of Carbons/2)th place and apply folding between two carbons [Q Here edge folding is not possible] .Here number of carbons are 10 , therefore semi edge will be possible to introduce carbons between 5th & 6 th then the above structure can be reformed as



Step III:

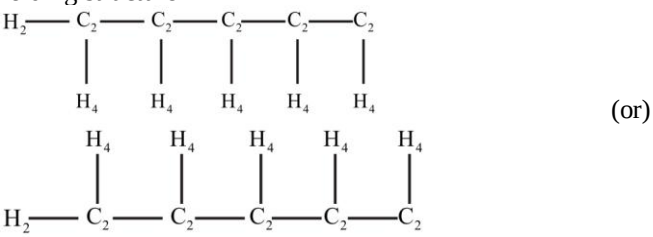
Folding technique is applied with respect to semi edge on the above reformed structure



(from right to left folding) (from left to right folding)

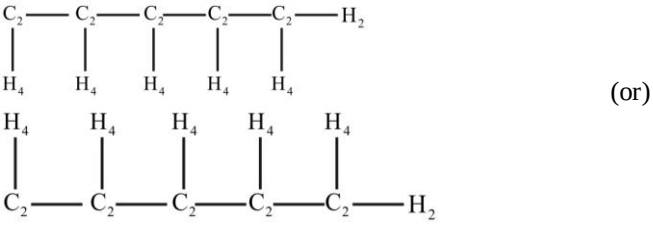
Step IV:

In the above structure, point folding is applied from top to bottom folding (or) bottom to top folding with respect to C_2 which is available at the [(number of carbons + 1)/2]th place of the above structure. This shown in the following folding structure



(from top to bottom folding) (from top to bottom folding)

On the other way, we will have

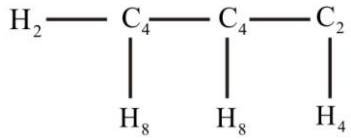


(from top to bottom folding) (from top to bottom folding)

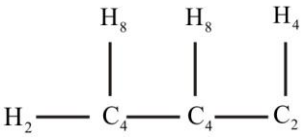
Step V:

In the above structure, point folding is applied from right

to left folding (or) left to right folding with respect to C_2 which is available at the [(number of carbons + 1)/2]th place of the above structure. This shown in the following structure

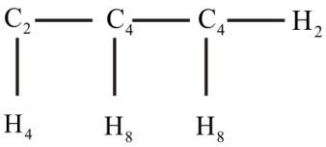


(or)

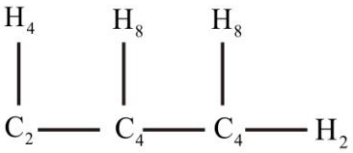


(from right to left folding) (from left to right folding)

On the other way, we will have

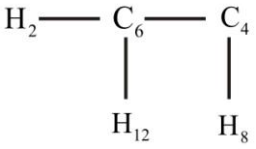


(or)

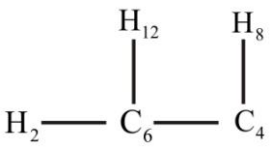


(from right to left folding) (from left to right folding)

Step VI: In the above structure, point folding is applied from right to left folding (or) left to right folding with respect to C_4 which is available at the [(number of carbons + 1)/2]th place of the above structure. This shown in the following structure:

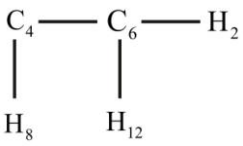


(or)

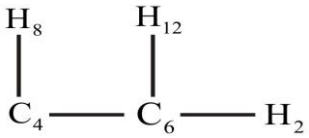


(from right to left folding) (from left to right folding)

On the other way, we shall have,



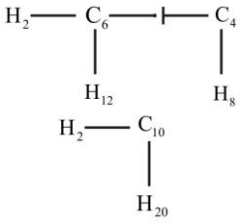
(or)



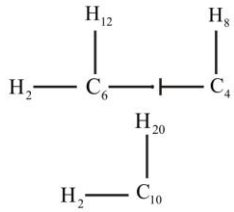
(from right to left folding) (from left to right folding)

Step VII:

In the above structure, we introduce semi edge folding between '2' carbons at the [(number of carbons / 2]th place of the above structure. (Since edge folding is not possible) from right to left folding (or) left to right folding. This shown in the following structure:

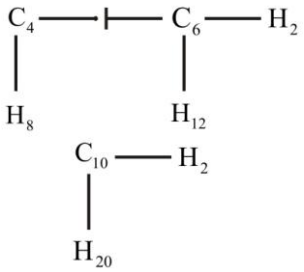


(or)

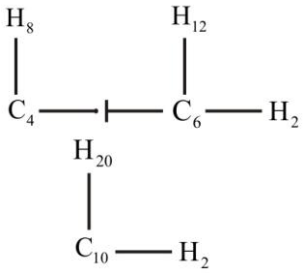


(from right to left folding) (from left to right folding)

On the other way, we will have,



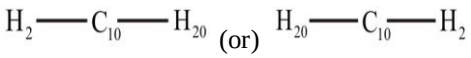
(or)



(from right to left folding) (from left to right folding)

Step VIII:

The above structure can be written in two ways. This shown in the following structure



Step IX:

In the above structure, point folding is applied with respect to C_{10} at the [(number of carbons + 1)/ 2]th place from right to left folding (or) left to right folding. This shown in the following structure

$C_{10} - H_{22}$ (or) $H_{22} - C_{10}$

Step X: Hence, the aim completes to get $C_{10}H_{22}$.

Theorem 2: In any simple discussed 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 after 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 chemical structures. Also, we have derived some theorems based on folding techniques in some special chemical structures and this proposed methodology will be very useful in chemical compounds in the field of chemistry.

Retrieval Number G6353058719/19©BEIESP

Published By:
Blue Eyes Intelligence Engineering
& Sciences Publication

VI. FUTURE WORK

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

VII. ACKNOWLEDGEMENT

The authors would like to thank **Dr. Ponnammal Natarajan,** Former Director – Research & Development, Anna University- Chennai, Tamilnadu, India, for her initiative ideas and fruitful discussions with respect to the paper's contribution.

REFERENCES

1. Frank Harary, Graph Theory, Addison Wesley Publishing Company, Third Printing (1972).
2. Narsingh Deo, Graph Theory With Applications To Engineering And Computer Science, PHI Publications, New Delhi (1995).
3. Gallian J.A., A Dynamic survey of graph labeling, Electronic Journal of combinatorics (2010)
4. Proceedings of sixth international conference on "Frontiers In Intelligent Computing Theory And Applications"(FICTA 17), KIIT University, Bhubaneswar.
5. Proceedings of Sixth International Conference on "Contemporary Engineering and Technology-2018"(ICCET18), Prince Shri Venkateswara Padmavathy Engineering College, Ponmar, Chennai, Tamilnadu.
6. Proceedings Of Thirteenth International Conference On Science, Management And Engineering (ICSME 17), Kerala, India.
7. Bondy J.A., Murthy U.S.R., Graph theory with Applications, American Elsevier Publishing Company, Inc., New York, New York (2015).
8. Thiagarajan K and Padmashree J, "Study on Finite Words in Semi graph Folding", Journal of Applied Sciences Research, 2015, Volume 11, Number 14, pp.30-35.