Folding Automaton Techniques in Chemical Structures

K. Thiagarajan, N. Subashini

Abstract**:** ***In this paper, we have observed the definitions of point folding technique and edge folding technique and semi-edge folding techniques from the graph theory in mathematics to get new applications for chemical world. Folding automaton derived for chemical structure. Some theorems are derived based on the folding techniques for chemical structures. The proposed methodology is very useful for chemical compounds.***

Index Terms: Automaton, Chemical Structures, Edge Folding, Folding, Folding automaton, Point Folding, Semi Edge Folding**.**

I. INTRODUCTION

Speculations of concoction structure were first created by August Kekule, Archibald Scott Couper, and Aleksandr Butlerov, among others, from around 1858.These speculations were first to express that concoction mixes are not an arbitrary bunch of iotas and utilitarian gatherings, yet rather had a distinct request characterized by the valency of the particles forming the atom, giving the particles a three dimensional structure that could be resolved or illuminated.
In this paper, we correspond substance structure and collapsing machine methods [8] for some extraordinary compound structures in algorithmic way.The collapsing Technique is material for some exceptional kind of concoction structure in the field of science. Complete electronic structure depictions incorporate indicating the control of a particle's sub-atomic orbitals. Structure assurance can be connected to a scope of focuses from basic atoms (e.g., diatomic oxygen or nitrogen), to extremely complex ones (e.g, for example, of protein or DNA). The investigation of limited automata (FA) respectable, or programmed, structures started underway by Hodgson (Th'eories d'ecidables standard computerize fini, Annales de Sciences Math'ematiques, 1983), and afterward carried on in Khoussainov and Nerode[10].Automata assumes a fundamental job in principle of calculation, compiler development, man-made consciousness, voyaging and formal confirmation. Likewise limited automata are utilized in content handling, compilers, and equipment.

II. PRELIMINARIES

Definition 1: [1],[2]& [3]

Chemical Structures

Sub-atomic geometry alludes to the spatial course of action of particles in an atom and the compound bonds that hold the iotas together and can be spoken to utilizing auxiliary formulae basic formulae and by sub-atomic models.

Definition 2: [8]

Semi graph Folding

A Semi chart map F: $SG_1 \rightarrow SG_2$ a semi diagram collapsing, if and just if F maps points to points, semi points to semi points, lines to lines and semi lines to semi lines.

Definition 3: [8]

Point Folding

A chart map F: $G_1 \rightarrow G_2$ a point collapsing, if and just if F maps points to points and lines to lines when quantities of points are odd.

Definition 4: [8]

Edge Folding

A chart map F: $G_1 \rightarrow G_2$ an edge collapsing, if and just if F maps points to points and lines to lines when quantities of points are even.

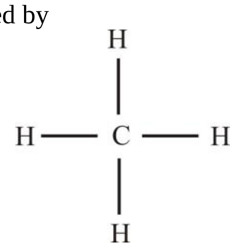
Definition 5: Finite Automaton [9]

A limited robot is spoken to formally by the 5-tuple (Q, Σ, δ, q0, F),Where Q is a limited arrangement of states, Σ is a limited arrangement of Input images, δ is the change work, that is, $\delta : Q \times \Sigma \rightarrow$ Q,q0 is the begin state, F is a lot of definite conditions of Q.

Folding Techniques in Chemical Structures having Odd Number of Carbons

Example 1:

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

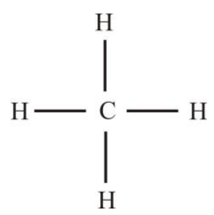


This can be derived in folding techniques using point folding technique [4], edge folding technique ([5], [6], [7]) and semi edge folding technique [8] explained in algorithm I.

Algorithm I for Example 1:

Step I:

Given CH_4 can be referred as follows,

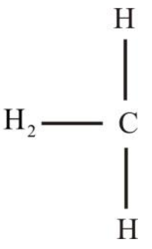


Revised Manuscript Received on December 22, 2018.

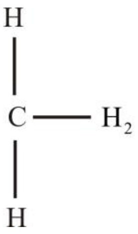
K. Thiagarajan, *Academic Research, Jeppiaar Engineering College, Chennai-119, Tamilnadu, Indi, vidhyamannnan@yahoo.com.*

N. Subashini, research scholar, *Mother Teresa Women's University, Kodaikanal, Tamilnadu, India and Dept. of Mathematics, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, subashini.sams@gmail.com.*

Step II:
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.

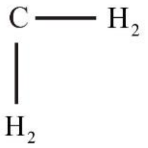


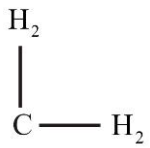
(from right side to left side folding)

(or) 

(from left side to right side folding)

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

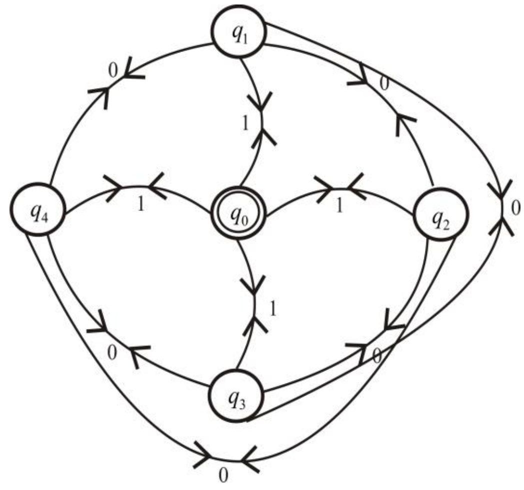




Step IV:
The step III can be written as H_2-C-H_2 .Then point folding technique is applied with respect to C from right to left folding technique (or) from left to right folding technique, we get $C-H_4$ (or) H4-C.

Step V:
Hence, the aim completes to get CH_4 .

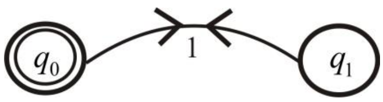
Automaton for Example 1:



Transition Table for Example 1:

	q_0	q_1	q_2	q_3	q_4
q_0	-	1	1	1	1
q_1	1	-	0	0	0
q_2	1	0	-	0	0
q_3	1	0	0	-	0
q_4	1	0	0	0	-

Folding Automaton for Example 1:

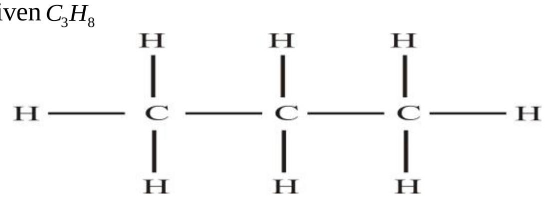


Transition Table for Example 1:

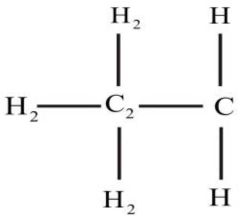
	q_0	q_1
q_0	-	1
q_1	1	-

Example 2:
Consider C_3H_8 in chemistry [3], This can be derived in folding techniques using point folding technique [4], edge folding technique ([5], [6], [7])and semi edge folding technique [8] explained in algorithm II.

Algorithm II for Example 2:
Step I:
Given C_3H_8

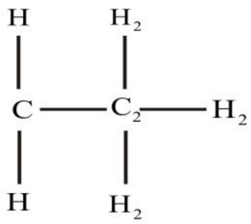


Step II:
To apply point folding technique with respect to C which is available at centre of the structure calculated through [(Number of carbons + 1)/2, here Number of carbons=3 (odd)]



(from right to left folding)

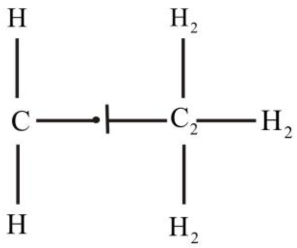
(or)



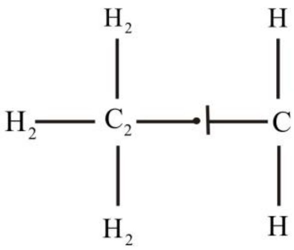
(from left to right folding)

Step III:

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

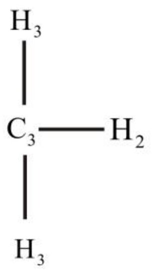


(or)

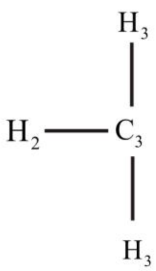


Step IV:

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

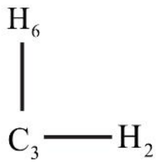


(or)

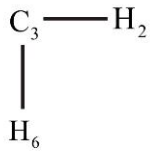


Step V:

In this, to apply point folding technique 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

$$H_6 — C_3 — H_2$$

Step VI:

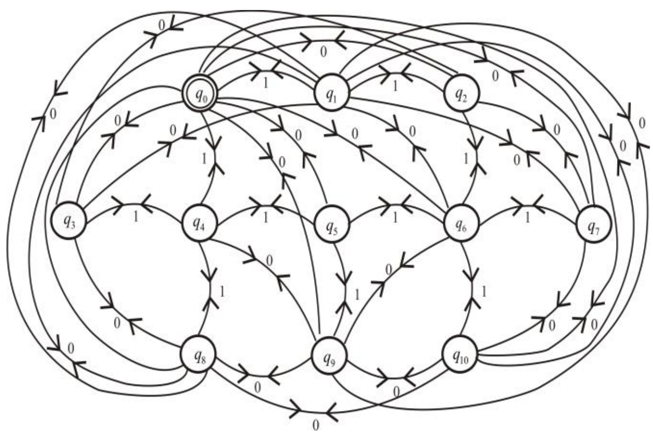
Now, in this, we apply point folding technique from right to left folding (or) from left to right folding with respect to C_3, we get

$$C_3 — H_8 \quad \text{(or)} \quad H_8 — C_3$$

Step VII:

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

Automaton for Example 2:



Top to Bottom folding technique (or) Bottom to top folding technique

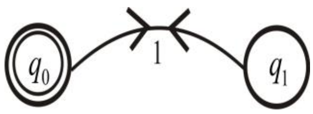
Transition Table for Example 2:

	q_0	q_1	q_2	q_3	q_4	q_5	q_6	q_7	q_8	q_9	q_{10}
q_0	-	0	0	0	1	0	0	0	0	0	0
q_1	0	-	0	0	0	1	0	0	0	0	0
q_2	0	0	-	0	0	0	1	0	0	0	0
q_3	0	0	0	-	1	0	0	0	0	0	0
q_4	1	0	0	1	-	0	0	0	0	0	0
q_5	0	1	0	0	1	-	1	0	0	1	0
q_6	0	0	1	0	0	1	-	1	0	0	1

Published By:
Blue Eyes Intelligence Engineering
& Sciences Publication

q_7	0	0	0	0	0	0	1	-	0	0	0
q_8	0	0	0	0	1	0	0	0	-	0	0
q_9	0	0	0	0	0	1	0		0	-	0
q_{10}	0	0	0	0	0	0	1	0	0	0	-

Folding Automaton for Example 2:



Transition Table for Example 2:

	q_0	q_1
q_0	-	1
q_1	1	-

Theorem 1:

In any simple chemical structure if the number of carbons are odd then, [(number of carbons+1)/2]th carbon will be acting as the domination carbon. Then point folding technique and point symmetry folding is possible only at this domination carbon.

Proof:

From Examples 1 & 2.

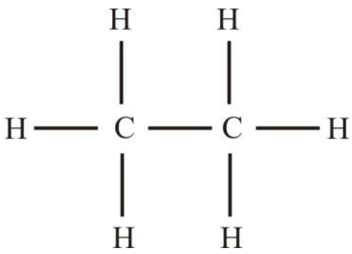
III. FOLDING TECHNIQUES IN CHEMICAL STRUCTURES HAVING EVEN NUMBER OF CARBONS

Example 3:

Consider C_2H_6 - Ethane in Chemistry. This can be derived in folding techniques using point folding technique [4], edge folding technique ([5], [6], [7]) and semi edge folding technique [8] explained in algorithm III.

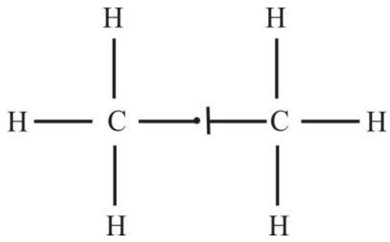
Algorithm III for Example 3:

Step I: Given C_2H_6



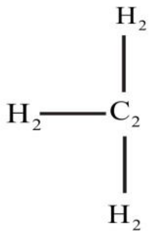
Step II:

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

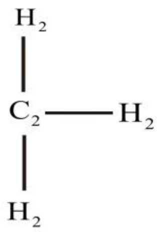


Step III:

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)

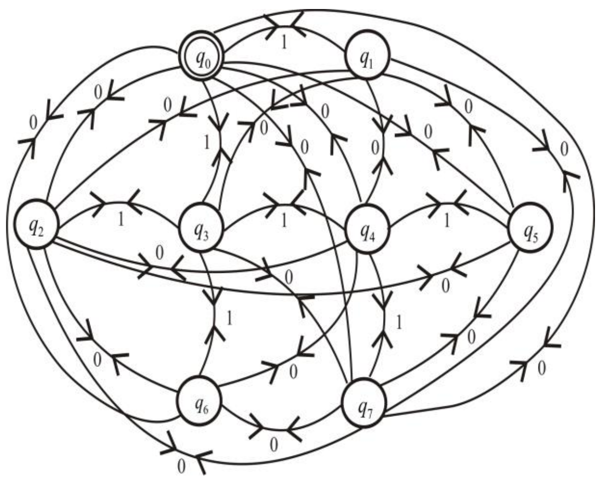
Step IV:

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.

Step VI:

Hence, the aim completes to get C_2H_6 .

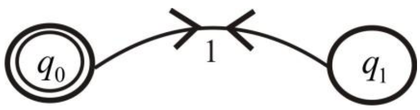
Automaton for Example 3:



Transition Table for Example 3:

	q_0	q_1	q_2	q_3	q_4	q_5	q_6	q_7
q_0	-	0	0	1	0	0	0	0
q_1	0	-	0	0	1	0	0	0
q_2	0	0	-	1	0	0	0	0
q_3	1	0	1	-	1	0	1	0
q_4	0	1	0	1	-	1	0	0
q_5	0	0	0	0	1	-	0	0
q_6	0	0	0	1	0	0	-	0
q_7	0	0	0	0	1	0	0	-

Folding Automata for Example 3:



Transition Table for Example 3:

	q_0	q_1
q_0	-	1
q_1	1	-

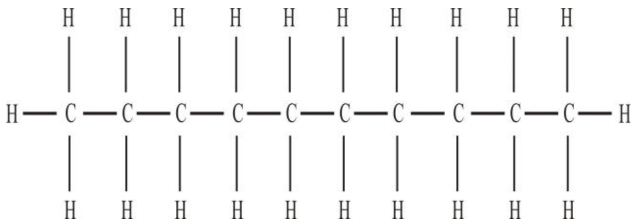
Example 4:

Consider $C_{10}H_{22}$ - Decane in Chemistry. This can be derived in folding techniques using point folding technique [4], edge folding technique ([5], [6], [7]) and semi edge folding technique [8] explained in algorithm IV.

Algorithm IV for Example 4:

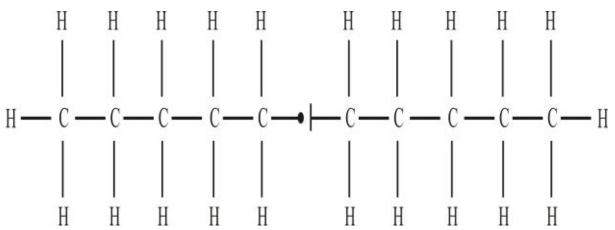
Step I:

Given $C_{10}H_{22}$



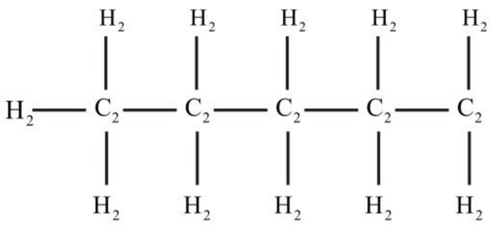
Step II:

Introduce semi edge at (Number of Carbons/2)th place and apply folding between two carbons [∵ 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

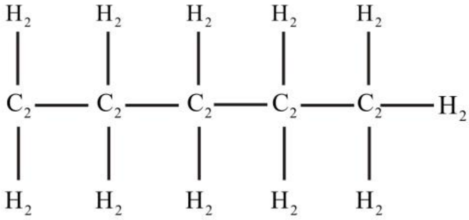


Step III:

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



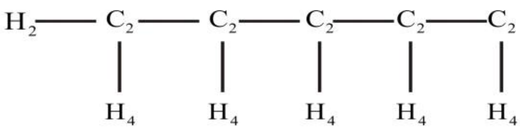
(or)



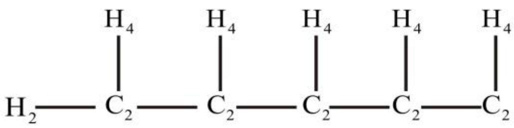
(from right to left folding) (from left to right folding)

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.

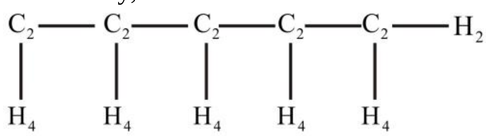


(or)

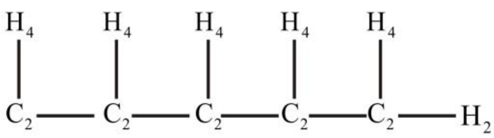


(from top to bottom folding) (from top to bottom folding)

On the other way, we will have



(or)

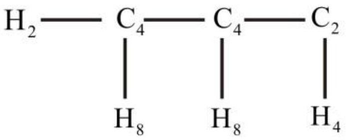


(from top to bottom folding) (from top to bottom folding)

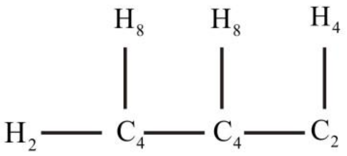
Step V:

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

Published By:
Blue Eyes Intelligence Engineering
& Sciences Publication

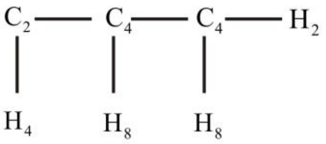


(or)

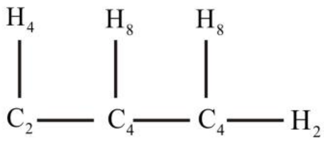


(from right to left folding) (from left to right folding)

On the other way, we will have



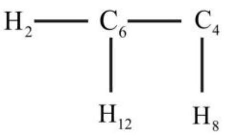
(or)



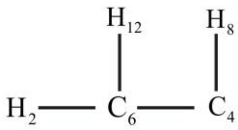
(from right to left folding) (from left to right folding)

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:

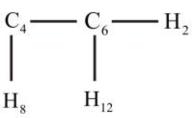


(or)

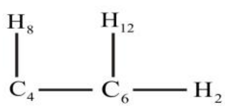


(from right to left folding) (from left to right folding)

On the other way, we shall have,



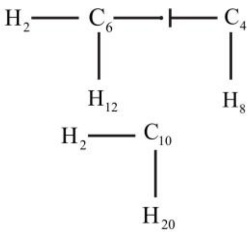
(or)



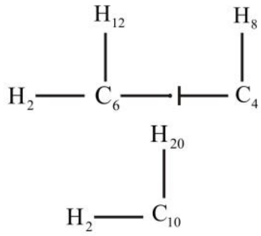
(from right to left folding) (from left to right folding)

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:

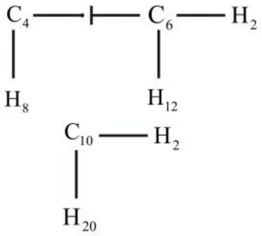


(or)



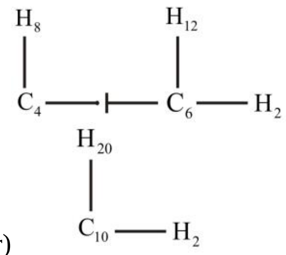
(from right to left folding) (from left to right folding)

On the other way, we will have,



(from right to left folding)

(or)



(from left to right folding)

Step VIII:

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

$$H_2 - C_{10} - H_{20} \text{ (or) } H_{20} - C_{10} - H_2$$

Step IX:

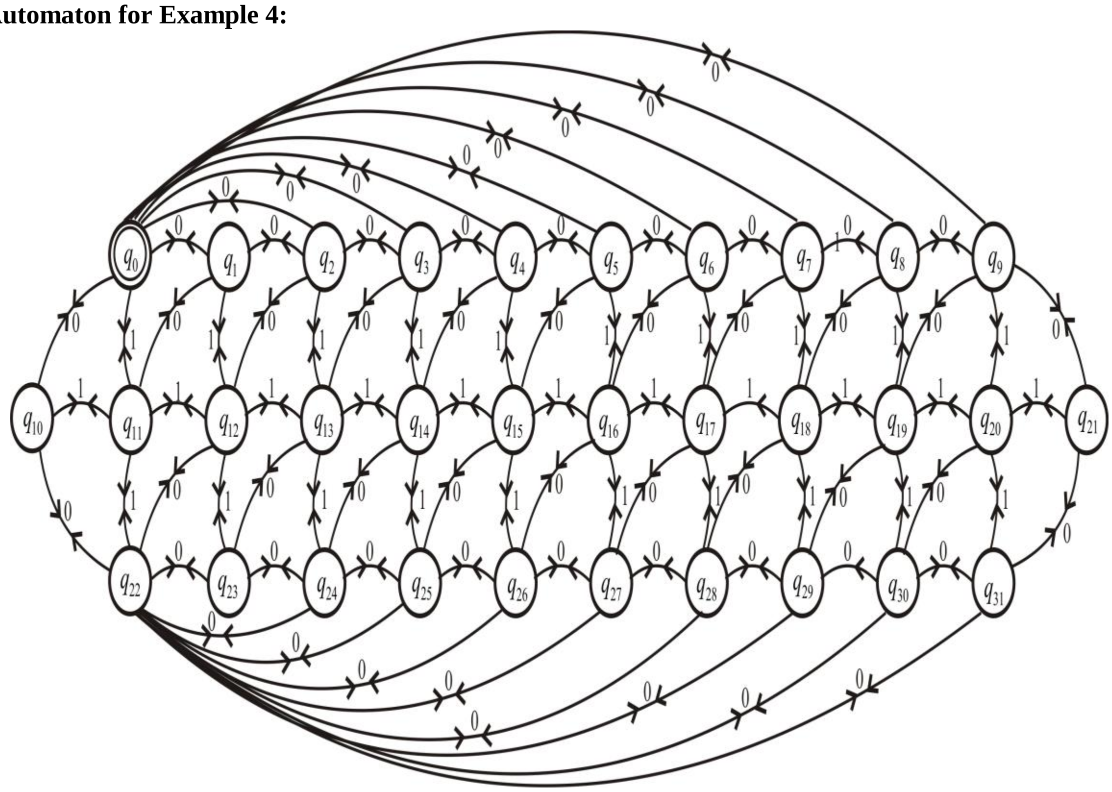
In the above structure, point folding is applied with respect to C_{10} at the [(number of carbons + 1)/ 2]th place from right to left folding (or) left to right folding. This shown in the following structure

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

Step X:

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

Automaton for Example 4:



Transition Table for Example 4 :

	q_0	q_1	q_2	q_3	q_4	q_5	q_6	q_7	q_8	q_9	q_{10}	q_{11}	q_{12}	q_{13}	q_{14}	q_{15}	q_{16}	q_{17}	q_{18}	q_{19}	q_{20}	q_{21}	q_{22}	q_{23}	q_{24}	q_{25}	q_{26}	q_{27}	q_{28}	q_{29}	q_{30}	q_{31}
q_0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
q_8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
q_9	0	0	0	0	0	0	0	0	0	0	0	00	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
q_{10}	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_{11}	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
q_{12}	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
q_{13}	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
q_{14}	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
q_{15}	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
q_{16}	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
q_{17}	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
q_{18}	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
q_{19}	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
q_{20}	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
q_{21}	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_{22}	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_{23}	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_{24}	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_{25}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_{26}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_{27}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_{28}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
q_{29}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
q_{30}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
q_{31}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0

Published By:
Blue Eyes Intelligence Engineering
& Sciences Publication

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. Then semi edge folding technique after point folding technique is possible at domination carbon.

Proof:

From examples 3 & 4.

IV. CONCLUSION

In this methodology, we have connected point collapsing systems, edge collapsing strategies and semi edge collapsing procedures for some concoction structures. likewise, we have determined a few hypotheses dependent on collapsing procedures for compound structures. the proposed approach will be valuable to get want structure for substance mixes in the field of science. we plan distinctive applications which are accessible in automata hypothesis to produce robot for concoction structures. the connection of concoction structure and its relating robot is determined for some compound structure and the distinctive kinds collapsing method is talked about to acquire chose substance structures.

FUTURE WORK

In future, this collapsing robot approach might be stretched out for some other extraordinary substance structures.

ACKNOWLEDGMENT

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.
9. Introduction to Automata Theory, Languages, and Computation(3rd Edition Pearson Publication) -John E. Hopcroft, Rajeevmotwani, Jeffrey D. Ullman.
10. B. R. Hodgson, Th´eories d´ecidables par automate fini, Annales de Sciences Math´ematiques, 7:39–57, 1983. 14.