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Chemical Formula Encryption - using Hamiltonian Circuits and Graph Valued Functions

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***Abstract*: The ever expanding nature of graph theory has made it a convenient tool for a wide range of practical applications. This study prescribes an algorithmic approach of cryptographic decoding of chemical formula using Jump graphs and Line graphs. Hamiltonian graphs are used as the key for encryption and decryption.**

***Keywords* : Chemical Formula, Hamiltonian circuit, Line graph, Jump graph, Encryption, Decryption.**

I. INTRODUCTION

The development of science and technology has paved way for new inventions very often. At the same time technology provides a huge threat due to rivalry in every field. The invention of any new product which is intended to make human life simpler is mostly structured on chemical formulas. Most commonly these chemical formulas play a vital role in the field of medical science to develop new drugs (medicines) and to modify the existing drugs. Since, health and well-being tops the wish list of man-kind among all his priorities, the development and maintaining the secrecy of the chemical formulae of the drugs has become more important in order to avoid piracy.

Cryptography is the science of using mathematics to encrypt and decrypt. Encryption is a method of transmitting massages or information's in such a way that only the personals or parties concerned in the process can read by decoding[7]. Thus it is a simple technique of hiding the true meaning of information's from any intruders. The origin of cryptography may be traced back to the stone-age era, which makes this part of science as the one of the very old branch of sciences. The modern cryptographic techniques uses advanced mathematical and computer technologies to provide a challenge to any hackers on its way.

A collection of chemical symbols that represent the type and number of atoms present in a molecule of a substance is termed as chemical formula.

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Thus, every chemical formula consists of two main components, the alphabetic terms and the numerical terms [6]. Graph Theory is one among the many branches of Discrete Mathematics that has attracted the interest of researchers in the recent years due to its many useful applications. The interesting operations on a graph that yields a new graph is termed as graph valued functions[1].M.Yamuna at el.[2,3] has developed a method for encrypting the molecular formula of a drug using the graph domination number and molecular biology. Another approach of chemical formula encryption using binary periodic table has been prescribed in [4]. In 2013, M.Yamuna et al.[5] formulated an algorithm using Hamiltonian circuits for encrypting multiple massages. This paper suggests another method of encrypting the chemical components of a drug using the Hamiltonian circuits of a complete graph and its graph valued functions.

II. PRELIMINARY NOTE

2. Preliminary Note:

In this section we give the basics required for easy understanding of the paper.

2.1 Graph.

A graph G is a non-empty set of points or vertices denoted by V(G) connected by a set of lines or edges denoted by E(G).

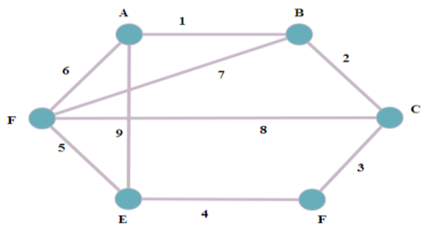


Fig:1. A graph G.

2.2 Line graph of a graph.

Let G(V,E) be simple connected graph with order p and size q. A Line graph L(G) of G is drawn by taking E(G)as V(L(G)).In L(G) two vertices are adjacent if and only if their corresponding edges are adjacent in G.

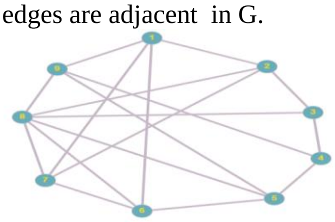


Fig:2. Line graph L(G).

2.3 Jump graph of a graph.

A graph whose order is the size of a graph G where two vertices are adjacent if and only if the corresponding edges are non-adjacent in G is called the jump graph J(G) of the graph G. Thus, the complement graph of a line graph L(G) isthe jump graph J(G) of G.

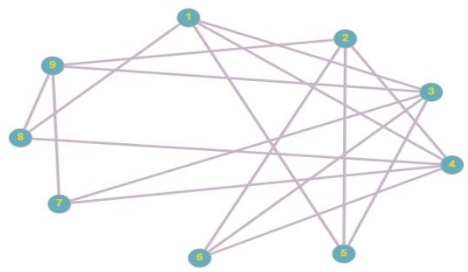


Fig:3. Jump graph J(G).

2.4 Hamiltonian graph.

A circuit comprising of all the vertices of a graph is the Hamiltonian circuit of the graph. A graph containing a Hamiltonian circuit is called as Hamiltonian graph. In any graph with order p(p, an odd number) will have$\left(\frac{p-1}{2}\right)$edge disjoint circuits[8].

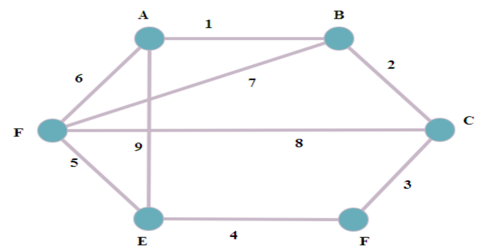


Fig:4. A Hamiltonian graph.

2.5 Chemical Formula.

A collection of chemical symbols that represent the type and number of atoms present in a molecule of a substance is termed as chemical formula.

Example.

Cocaine :$C_{17}H_{12}\,NO_4$.

Paracetamol: $C_8H_9NO_2$.

III. PROPOSEDENCRYPTION SCHEME

Consider any molecular formula to be encrypted and a complete graph K_p,(p≥5). Then the line graph of the graph $K_p$has been used for chemical encryption and the jump graph of the complete graph is used for numerical encryption. "Every complete graph with p vertices there are $\left(\frac{p-1}{2}\right)$ edge disjoint Hamiltonian circuits if p is an odd number p≥3"[8]. Thusthe complete graphK_p (for p=odd and p≥ 3) has $\left(\frac{p-1}{2}\right)$ edge disjoint Hamiltonian circuits. These Hamiltonian circuits are used as key for encryption and decryption.Label these circuits as $H_1, H_2, \dots \dots . . H_n$, $n = \left(\frac{(p-1)}{2}\right)$. The line graph of K_p will have $\left(\frac{p(p-1)}{2}\right)$ vertices. Any circuit in K_p will be a circuit in the line graph $L(K_p)$. So,H_i(i = 1…n) will be circuits in $L(K_p)$. Label these circuits in $L(K_p)$ as,

$H_1: e_{11}, e_{12}, \dots \dots \dots \dots . e_{1p}$,
$H_2: e_{21}, e_{22}, \dots \dots \dots \dots . e_{2p}$, …, $H_n: e_{n1}, e_{n2}, \dots \dots \dots \dots . e_{np}$.

Throughout the remaining sections, whenever K_p is a complete graph, the line graph of K_p is denoted by G_1 and the jump graph of $K_p$by G_2.$H_1, H_2, \dots \dots . . H_n$will be circuits in K_p and G_1.

3.1 Encoding chart

Every chemical formula consists of alphabets and numbers. We shall convert alphabets to numbers. We can use any encoding chart. In this paper we shall use the following conversion

A B C D E … X Y Z
↕↕↕↕↕↕↕↕↕
1 2 3 4 5 …24 25 26.

3.2 . Encryption Algorithm

As an example, let us choose the drug, Methamphatamine for encryption.

Its molecular formula is $C_{10}H_{15}N$.

Step 1

Let S be the chemical formula to be encrypted.

For the example S is, $S = C_{10}H_{15}N$.

Step 2

Split S into two sequences S_1 and S_2 where, S_1 is a sequence of chemicals and S_2 is a sequence of numbers in S.

For the example

S_1: C H N and

S_2: 10 15

Step 3

Convert S_1 into a sequence of numbers using the encryption chart to generate a sequence S_3.

For the example

S_3: 3 8 14

Step 4

Let $|S_3| = k_1$and $|S_2| = k_2$. Let $S_3 = w_1, w_2, \dots \dots w_{k_1}$and $S_2 = t_1, t_2, \dots \dots t_{k_2}$.

For the example

S_3 : w_1 w_2 w_3
↓ ↓ ↓
3 8 4

S_2 : t_1 t_2
↓ ↓
10 15

Step 5

Choose a complete graph with p vertices, p≥5 where p ≥$|S_1|$ or p≥$|S_2|$(Choose the larger number)

For the example

$|S_1|$= 3 and $|S_2|$= 2

So, choose a Hamiltonian circuit with atleast 5 vertices. That is, the considered complete graph must contain a Hamiltonian circuit with atleast 5 vertices. Assume the graph,$G = K_5$.

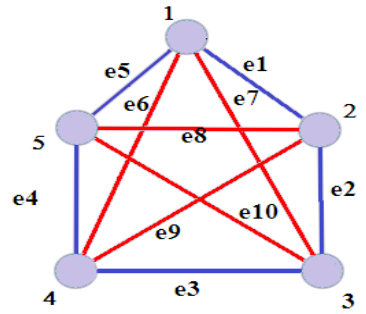


Fig.5:K_5

Then, the possible edge disjoint Hamiltonian circuits of$K_5$are (e_1-e_2-e_3-e_4-e_5) and (e_7-e_{10}-e_8-e_9-e_6)[They are high lightened by blue and red colour respectively].

Step 6

Consider the line graph G_1 and the jump graph G_2 for G= K_p.

For the example,G_1 and G_2 are as seen in Fig 6

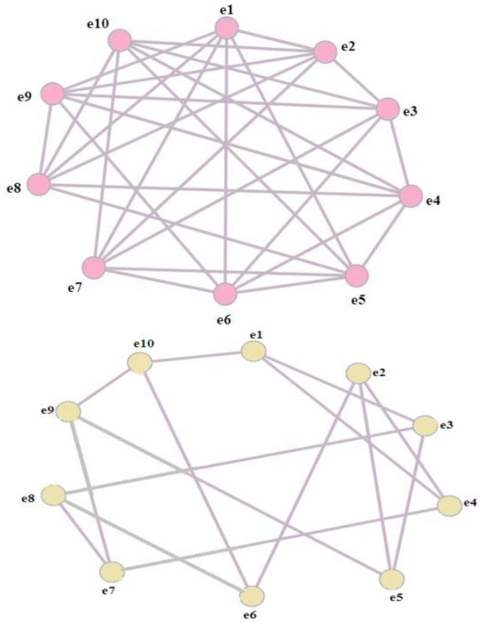


Fig.6:G_1 and G_2

Step 7

Choose any arbitrary Hamiltonian circuit H out of the $\binom{p-1}{2}$ Hamiltonian circuits of G.

For the example, choose the Hamiltonian circuit ($e_1 - e_2 - e3 - e4 - e5$ as H.

$$H = (e_1 - e_2 - e_3 - e_4 - e_5).$$

Step 8

The edges in H are adjacent in G. These edges will be vertices in G_1 and will form a circuit inG_1.Choose this circuit as H_i : $e_{i1}, e_{i2}, \ldots e_{ip}$ in G_1 (Length of H = Length of H_i).Note that here $e_{i1}, e_{i2}, \ldots e_{ip}$ represents vertices.

Encode S_3 along H_i (following the ordering of edges in H_i) i.e., edges $(e_{i1}, e_{i2}), (e_{i2}, e_{i3}) \ldots (e_{i(p-1)}, e_{ip})$ are assingned the weight $(w_1, w_2, \ldots w_{k_1})$, $k_1 \leq p$. The remaining edges if any (when$k_1 < p$), assign arbitrary weights (choose these weights as decimal numbers to differentiate the integer valuesin the molecular formula). Label the resulting graph as G_3.

For the example, H_1 is

$H_1 = e_1, e_2, e_3, e_4, e_5$

Edges are ordered as (e_1, e_2), (e_2, e_3),(e_3, e_4), (e_4, e_5). To these edges we assign weights 03, 08, 14, 0.1, 0.2. Note that $|H_1| = 5$but,$|S_3| = 3$. So, the last two edges receive decimal value. The resulting graph G_3 is as seen in Fig.7

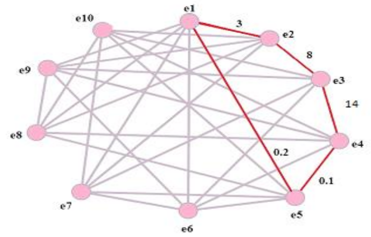


Fig.7:G_3

Step 9

Assign arbitrary weights to the remaining edges of G_3 to generate G_4.

For the example, the graphG_4 is as seen in Fig 8.

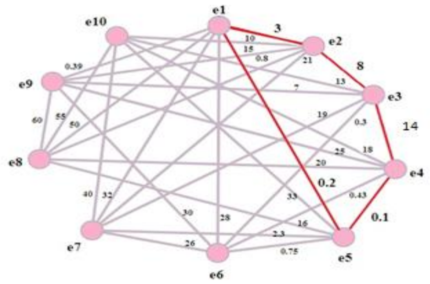


Fig.8:G_4

Step 10

Choose another arbitrary Hamiltonian circuit in G = K_p say $H_j \neq H_i$(out of $\binom{p-3}{2}$)

Let H_j: $e_{j1}, e_{j2}, \ldots \ldots e_{jn}$.

For the example considered here, the left overcircuit isH_2.

(i.e) $H_2 = e_7$,e_{10}, e_8,e_9,e_6.

Step 11

The edges in H_2 are adjacent in G. The vertices corresponding to these edges willform a circuit in G_1. Hence these vertices will be non-adjacent in G_2. Create a new graph G_5 by including edges (e_{j1}, e_{j2}) (e_{j2}, e_{j3}) ..... $(e_{j(p-1)}, e_{jp})$in G_2.

For the example, the resulting graph G_5 is as seen in Fig 9(The new edges are highlighted with red).

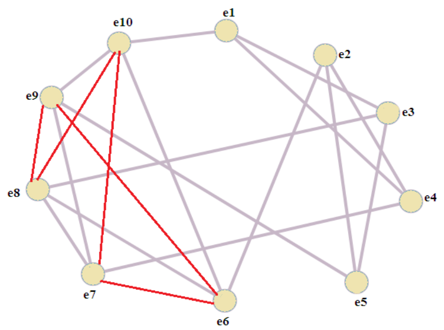


Fig.9:G_5

Step 12

Encode S_2along H_j(following the ordering of edges in H_j). i.e.,edges$(e_{j1}, e_{j2}), (e_{j2}, e_{j3}), \ldots (e_{j(p-1)}, e_{jp})$areassigned the weights $(t_1, t_2 \ldots t_{k_2}), K_2 \leq p$. The remaining edges if any (when $K_2 < p$) assign arbitrary weight (choose these weights as decimal numbers to differentiate the integer values in the molecular formula). Label the resulting graph as G_6.

For the example, H_2 is

$H_2 = e_7, e_{10}, e_8, e_9, e_6$

Edges are ordered as (e_7, e_{10}) $(e_{10}, e_8)(e_8, e_9)$ (e_9, e_6). To these edges assign weights 10, 15, 0.2, 0.3, 0.4. Note that $|H_2| = 5$ and $|S_2| = 2$, so the last three edges receives decimal values. The resulting graph G_6 is seen in Fig 10.

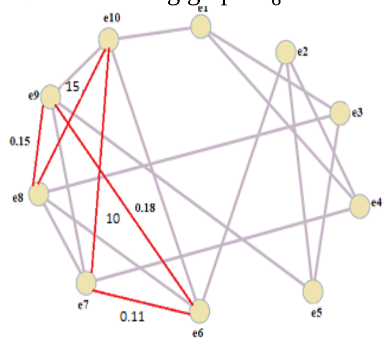


Fig.10:G_6

Step 13

Assign arbitrary weight to the remaining edges of $G_6$to generate G_7.

For the example,G_7 is as seen in Fig 11

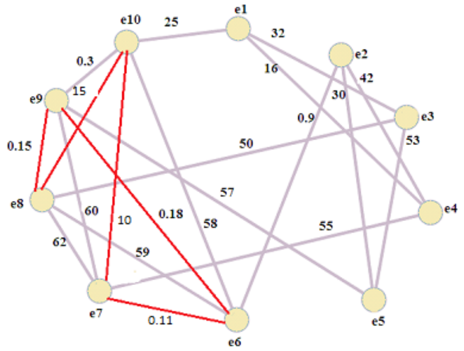


Fig.11:G_7

Step 14

Send G_4 *and* G_7 to the receiver.

Decoding is done by reversing the procedure. Suppose the received graphs are as seen in fig. 12((i.e) G_4 and G_7 is taken as Fig.12)

Since these graphs have 21 vertices, the graph used for encryption has to be the complete graph K_7 . AndK_7has three possible Hamiltonian circuits

H_1 =1-2-3-4-5-6-7-1.

H_2 = 1-4-2-6-3-7-5-1. H_3 =1-6-4-7-2-5-3-1.

Among these any two circuits would have been used for encryption. Assume that they are the circuits$H_2$and H_3. Their corresponding circuits in L(K_7) are

H_2 : e_8- e_3-e_2-e_6-e_5-e_{11}-e_{10}.

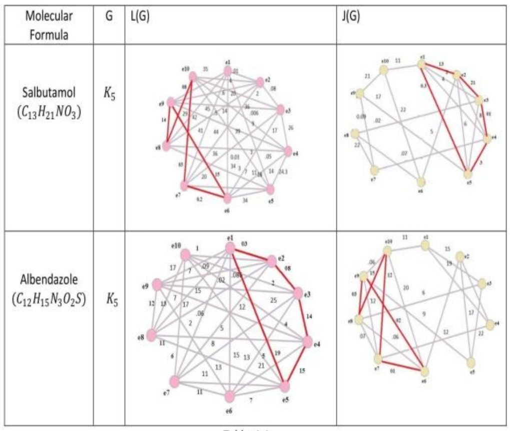
H_3 : e_{15}- e_{16}-e_{17}-e_{18}-e_{19}-e_{20}-e_{21}.

The edge weights corresponding to these circuits from fig 8 are 03, 08, 0312, 0.03, 0.02, 0.33, 0.34, 0.35 and 10, 06, 08, 0.16, 0.25, 0.26, 0.28, 0.55. Removing weights which are decimal values, the remaining strings are (03, 08, 03, 12) and (10, 06, 08). That is,S_3 = 03, 08, 03, 12 and S_2 = 10,06,08.

From the encoding chart, string S_3 represents C, H, Cl. Combining S_2 and S_3 the resulting molecular formula is $C_{10}H_6Cl_8$ which represents Chlorbane.

Example:1.1

Table 1.1 shows the encoded graphs for the drugs Salbutamol ($C_{13}H_{21}NO_3$) and Albendazole ($C_{12}H_{15}N_3O_2S$).



Molecular Formula	G	L(G)	J(G)
Salbutamol ($C_{13}H_{21}NO_3$)	K_5		
Albendazole ($C_{12}H_{15}N_3O_2S$)	K_5		

Table: 1.1

IV. CONCLUSION

This paper has proposed an algorithm to encode and decode the chemical formula of drug using the graph valued functions, line graph and jump graph of a graph by assuming the Hamiltonian circuits of a complete graph in them. Decoding of massages by any intruders is thus made secured by the combination of these graphs using the prescribed algorithm.

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