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Matrix Representation of Graph Theory in Hydrocarbons

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Abstract: Graph theory is one of the best-known research head subjects having many applications. Graph theory serves as a mathematical model to represent any system which has a binary relation. Chemical graph theory is branch of graph theory that is concerned with analysis of all consequences of connectivity in a chemical graph. An organic molecule can be represented by a graph, which can be converted to several matrices by using various graph characteristic, connecting of atoms through bonds lead to adjacency, incidence, cut-set, circuit and distance matrices. The object of this paper is to adopt graph theory matrix approach in hydrocarbons.
Key Word: Matrix (Adjacency, cycle, cut-set, edge, incidence and path) and Undirected graph.

1. Introduction

The graph theory is the study of graph, which is a collection of vertices or nodes and edges that connect pair of vertices and is a branch of graph theory that applies geometry to derive two-dimensional representation of graphs. Graph theory matrix approach is used in modeling and solving decision making problem with multiple and interrelated attributes.

1.1 Graph theoretical terms and chemical terms

Chemical system may be depicted by chemical graphs using a simple conversion rule,

Site ↔ Vertex
Connection ↔ Edge

1.2 Mapping of graph theoretical and chemical terms

	Graph theoretical terms		Chemical terms
•	Chemical/ Molecular graph	→	Structural formula
•	Vertex	→	Atom
•	Weighted vertex	→	Atoms of a specified element
•	Edge	→	Chemical bond
•	Weighted Edge	→	Chemical bond between specified element
•	Chain	→	Linear Alkanes/Alkenes/Alkynes
•	Cycle	→	Cycloalkanes

2. Matrix representation of structural graphs

The purpose of matrix representation of structural graph is the reflecting molecular topology and correlating structure. Graphs are converted into a mathematical expression which may be matrix and a polynomial. The first representation for characterizing graph and discussed below.

2.1 Adjacency Matrix

Adjacency matrix of a graph with n-vertices and no parallel edges, self-loops are allowed is an n×n order matrix $A=(a_{ij})$

Where,

$$a_{ij}=\begin{cases}1.\ if\ there\ is\ an\ edge\ between\ i^{th}\ and\ j^{th}\ vertices\\0,\ if\ there\ is\ no\ edge\ between\ i^{th}\ and\ j^{th}\ vertices\end{cases}$$

is weighted adjacency matrix of Aliphatic Hydrocarbons. The valency of carbon is 4 and valency of Hydrogen is 1.

2.2 Incidence Matrix

Let G=(V, E) be graph with n-vertices ($v_1,v_2,.....,v_n$) and m-edges ($e_1,e_2,.....,e_m$) and no Self-Loop. The matrix $A=(a_{ij})$ of order n×m, where,

$$a_{ij}=\begin{cases}1,\ if\ i^{th}\ edge\ e_j\ is\ incident\ nce\ on\ i^{th}\ vertex\ v_i\\0,\ otherwise\end{cases}$$

for a given graph G=(V,E), an incidence matrix depends on the ordering of the vertices of G and that edge of G. For different ordering of vertices and edges we get different incident matrix of the same graph G.

2.3 Path Matrix

A path matrix is defined for a specific pair of vertices in a graph say (u.v) and is denoted by P(u,v).
Let 'm' be the number of different paths between the vertices 'u' and 'v', 'n' be the number of edges path between the vertices (u,v).
Then path matrix will be,

$$P(u,v)=(P_{ij})=\begin{cases}1,\ if\ j^{th}\ edge\ lies\ in\ i^{th}\ vertex\\0,\ otherwise\end{cases}$$

The path matrix of any two vertices of alkenes is row matrix. At last, one of the path matrixes of any two carbons in alkenes is two rows. At last, one of the path matrixes of any two carbons alkynes are three rows.

2.4 Cycle Matrix

Let G be graph with 'm' edges and 'n' different circuits then a cycle matrix $C=(C_{ij})$ of order n×m is defined as

$$C_{ij}=\begin{cases}1,\ if\ i^{th}\ circuit\ includes\ j^{th}\ edge.\\0,\ otherwise\end{cases}$$

The cycle matrix is denoted by C(G). The cycle matrix of aliphatic hydrocarbons as

Cycle matrix of Alkanes does not exist.
Cycle matrix of Alkenes is 1.
Cycle matrix of Alkynes is 2.

2.5 Edge Cut-Set Matrix: -

Let the graph G have 'm' edge and 'n' be the number of different Cut-set in G. The Edge Cut-set matrix E(G) is given by

$$E(G)=(E_{ij})_{n\times m}\ \text{where}\ E_{ij}=\begin{cases}1,\ if\ i^{th}\ cutset\ includes\ j^{th}\ edge\\0,\ otherwise\end{cases}$$

The number of Edge cut-sets of alkanes are 4,7, 10,..,3n+1, alkenes are 5,8,11,.....,3n+2 and alkynes are 3,6,9,.....3n.

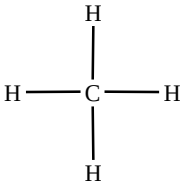
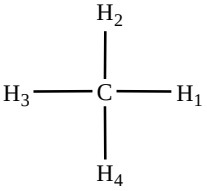
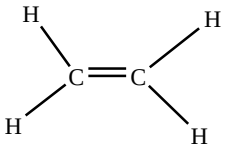
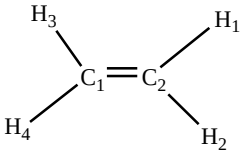
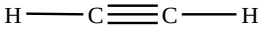
3. Hydrocarbons

Hydrocarbons in an organic compound made of carbons and hydrogens. It is possible for single (−), double (=) and triple (≡) bonds to form carbine atoms and hydrogen's. Aliphatic hydrocarbons are compound of hydrogen and carbon that do not contain benzene ring. There are three types alkanes, alkene and alkynes. The saturated hydrocarbons know as alkanes consist only carbon and hydrogen connected by single bond. The chemical formula is C_nH_{2n+2} where n represent the number of carbons and 2n+2 represents number of hydrogens.The unsaturated hydrocarbons are alkenes and alkynes. Alkenes are hydrocarbons that contain C=C, chemical formula for alkene is C_nH_{2n}.Alkynes are hydrocarbons that contains at least one triple bond between two carbon atoms, the number of hydrogen atoms is still less in alkynes as compared to alkanes or alkenes. The chemical formula of alkynes is C_nH_{2n-2}.

4. Different types of graphs matrix representation in aliphatic hydrocarbons

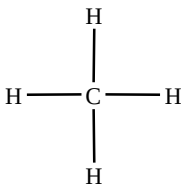
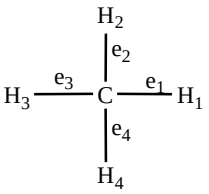
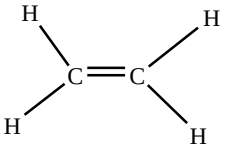
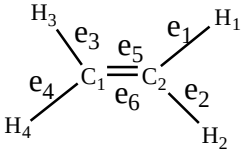
4.1. Adjacency Matrices

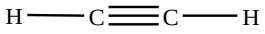
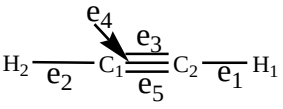
Table-4.1

Hydrocarbons	Structure	Structure into a graph	Adjacency Metrix
Methane(CH_4) (Alkane)			$W_1 = \begin{array}{c} \\ C \\ H_1 \\ H_2 \\ H_3 \\ H_4 \end{array} \begin{array}{c} \begin{array}{ccccc} C & H_1 & H_2 & H_3 & H_4 \end{array} \\ \begin{bmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$
Ethene (C_2H_4) (Alkene)			$W_2 = \begin{array}{c} \\ C_1 \\ C_2 \\ H_1 \\ H_2 \\ H_3 \\ H_4 \end{array} \begin{array}{c} \begin{array}{cccccc} C_1 & C_2 & H_1 & H_2 & H_3 & H_4 \end{array} \\ \begin{bmatrix} 0 & 2 & 1 & 1 & 0 & 0 \\ 2 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$
Ethyne (C_2H_2) (Alkyne)			$W_3 = \begin{array}{c} \\ C_1 \\ C_2 \\ H_1 \\ H_2 \end{array} \begin{array}{c} \begin{array}{cccc} C_1 & C_2 & H_1 & H_2 \end{array} \\ \begin{bmatrix} 0 & 3 & 0 & 1 \\ 3 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \end{array}$

4.2. Incidence Matrix

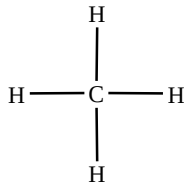
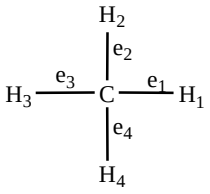
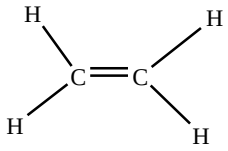
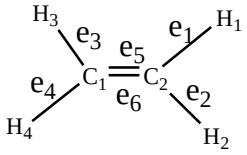
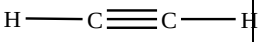
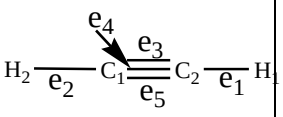
Table-4.2

Hydrocarbons	Structure	Structure into a graph	Adjacency Metrix
Methane (CH_4) (Alkane)			$W_1 = \begin{array}{c} \\ C \\ H_1 \\ H_2 \\ H_3 \\ H_4 \end{array} \begin{array}{c} \begin{array}{cccc} e_1 & e_2 & e_3 & e_4 \end{array} \\ \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \end{array}$
Ethene (C_2H_4) (Alkene)			$W_1 = \begin{array}{c} \\ C_1 \\ C_2 \\ H_1 \\ H_2 \\ H_3 \\ H_4 \end{array} \begin{array}{c} \begin{array}{cccccc} e_1 & e_2 & e_3 & e_4 & e_5 & e_6 \end{array} \\ \begin{bmatrix} 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix} \end{array}$

Ethyne (C_2H_2) (Alkyne)			$W_1 = \begin{array}{c} \\ C_1 \\ C_2 \\ H_1 \\ H_2 \end{array} \begin{array}{c} \begin{array}{ccccc} e_1 & e_2 & e_3 & e_4 & e_5 \end{array} \\ \begin{bmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix} \end{array}$

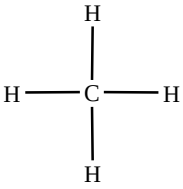
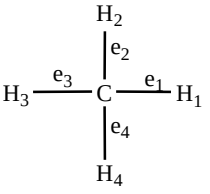
4.3. Path matrix

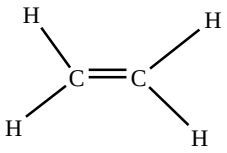
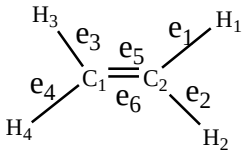
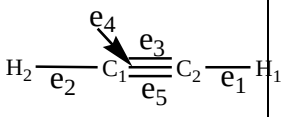
Table-4.3

Hydrocarbons	Structure	Structure into a graph	Adjacency Metrix
Methane (CH_4) (Alkane)			Path matrix of Methane with vertices C,H_1 whose order is 1×4 is denoted by $P(C, H_1) = P_1 \begin{array}{c} \begin{array}{cccc} e_1 & e_2 & e_3 & e_4 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix} \end{array}_{1\times4}$
Ethene (C_2H_4) (Alkene)			Path matrix of ethane with vertices C_1 and C_2 whose order is 2×6 is denoted by $P(C_1, H_1) = P_1 \begin{array}{c} \begin{array}{cccccc} e_1 & e_2 & e_3 & e_4 & e_5 & e_6 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array}_{2\times6}$
Ethyne (C_2H_2) (Alkyne)			Path matrix of ethane with vertices C_1 and C_2 whose order is 3×6 is denoted by $P(C_1, H_1) = P_1 \begin{array}{c} \begin{array}{ccccc} e_1 & e_2 & e_3 & e_4 & e_5 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array}_{3\times5}$

4.4. Edge Cut Set matrix

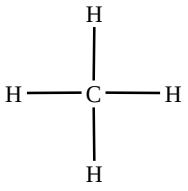
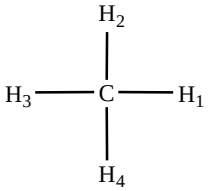
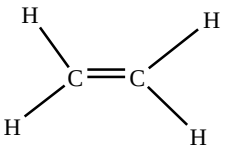
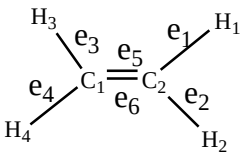
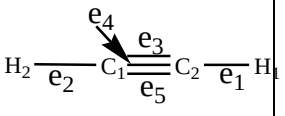
Table-4.4

Hydrocarbons	Structure	Structure into a graph	Adjacency Metrix
Methane (CH_4) (Alkane)			Edge Cut-sets of methane are $C_1=\{e_1\}$, $C_2=\{e_2\}$, $C_3=\{e_3\}$ and $C_4=\{e_4\}$ So, the Edge Cut Set matrix pf methane is of order 4×4 is $C(G) = \begin{array}{c} \\ C_1 \\ C_2 \\ C_3 \\ C_4 \end{array} \begin{array}{c} \begin{array}{cccc} e_1 & e_2 & e_3 & e_4 \end{array} \\ \begin{bmatrix} 0 & 3 & 0 & 1 \\ 3 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \end{array}_{4\times4}$

Ethene (C_2H_4) (Alkene)			Edge Cut-sets of Ethene are $C_1=\{e_1\}$, $C_2=\{e_2\}$, $C_3=\{e_3\}$, $C_4=\{e_4\}$ and $C_5=\{e_5,e_6\}$ So, the Edge Cut Set matrix pf methane is of order 5×6 is $C(G)=\begin{array}{c} \\ C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \end{array}\begin{array}{c} \begin{array}{cccccc} e_1 & e_2 & e_3 & e_4 & e_5 & e_6 \end{array} \\ \begin{bmatrix} 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}_{5\times 6} \end{array}$
Ethyne (C_2H_2) (Alkyne)			Edge Cut-sets of Ethyne are $C_1=\{e_1\}$, $C_2=\{e_2\}$, $C_3=\{e_3, e_4, e_5,e_6\}$ So, the Edge Cut Set matrix of methane is of order3×5 is $C(G)=\begin{array}{c} \\ C_1 \\ C_2 \\ C_3 \end{array}\begin{array}{c} \begin{array}{ccccc} e_1 & e_2 & e_3 & e_4 & e_5 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}_{3\times 5} \end{array}$

4.5. Cycle matrix

Table-4.5

Hydrocarbons	Structure	Structure into a graph	Adjacency Metrix
Methane (CH_4) (Alkane)			Alkanes does not exit cycle matrix.
Ethene (C_2H_4) (Alkene)			Ethene has one cycle $C_1=\{e_5,e_6\}$. In general alkenes has at least one cycle matrix. The cycle matrix of ethene is of order 1×4 as $B(G)=\begin{array}{c} \\ C_1 \end{array}\begin{array}{c} \begin{array}{cccccc} e_1 & e_2 & e_3 & e_4 & e_5 & e_6 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}_{1\times 6} \end{array}$
Ethyne (C_2H_2) (Alkyne)			Cycle of Ethyne are $C_1=\{e_1,e_2\}$, $C_2=\{e_4,e_5\}$ and $C_3=\{c_3,c_5\}$.The cycle matrix of the Ethyne is of order 3×5 as

			$B(G) = \begin{array}{c} \\ C_1 \\ C_2 \\ C_3 \end{array} \begin{array}{c} \begin{array}{ccccc} e_1 & e_2 & e_3 & e_4 & e_5 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array}_{3\times5}$

5. Conclusion

Group theory is used in the field of organic chemistry to model chemical compound in the form of graph where vertices represent the sequences in hydrocarbons and an edge will be drawn between two vertices. In this paper the major role of graph theoretic approach to find the matrix representation in hydrocarbons.

References

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