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Research Article

APPLICATION OF GRAPH THEORY IN CHEMISTRY

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ABSTRACT

Graph theory are branches of physics, chemistry, computer science, electrical and civil engineering, operations research, sociology, economics and so on. One of the important areas in mathematics is graph theory which is used in chemistry structural model, graph theory methods for finding all graph fulfilling certain mathematical condition followed by eliminating chemically impossible solution are equivalent to the molecular graph.

INTRODUCTION

In chemistry, constitutional isomers are substances with the same molecular formula, composed from the same kinds of atoms bonded differently such as butane and isobutene C_4H_{10}, the former has a linear chain of carbon atoms and the latter a branched chain. Each carbon atom is tetravalent and is symbolized by a vertex of degree 4 in the graph where all C and H atoms are displayed: Usually, however, organic chemists use hydrogen-depleted graph.

Chemical Enumeration: The structural formula for a chemical compound is essentially a graph in which the vertices are atoms and the edges correspond to the chemical bonds connecting them. That in chemical compounds there can be double or even triple bonds. But we shall not consider this possibility.

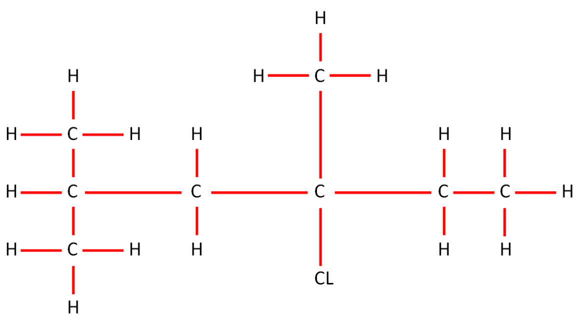

Fig 1

Such a formula is shows in figure (1), this particular formula is an example what are known as mono substituted alkenes, defined as follows. There are three type of atoms namely the carbon atom c with valiancy 4, hydrogen atom H with valiancy 1. and another atom X with valiancy 1, figure (1).

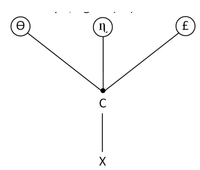

Fig 2

The atom X is taken to be a chlorine atom Cl there are no double or triple bonds. There facts induce that if there are P carbon atoms. Then there must be 2p+1 hydrogen atoms and thus C_pH_{2P+1} X is a recursive formula for a mono substituted alkanes.

Each of this part of the molecule is itself a mono substitute alkenes. That is we have three site Θ, and £ at each of which we place what is essentially a mono substituted alkenes. With the root carbon atom fig. (2) playing the role of X.

Enumeration of graph: in this section we will discuss about the main aim of this section the problem of enumeration unlabelled graphs. Since we now have the necessary apparatus to solve it, let us consider graphs with P vertices. We know that

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a pair of vertices may correspond to an edge of it may not. Thus we have $C = \frac{(P-1)}{2}$ possible pair of vertices. Which will be the sites for our problem and at each site we can place one of the two figures, edge or not-edge. If we give these figures content 1 and 0, respectively, then the content of the configuration is the number of the edges. Since the vertices are unlabelled. We can permute them by any permutations of the symmetric graph S_p of all permutations. Any permutation of vertices induces a permutation of the pairs of vertices. It is this set of permutations of the sites, denoted by S_p^2, that is relevant to this problem. We must therefore find its cycle index.

The case P = 4 provides some insight into what is involved. In this case we have 6 sites for possible edges. Permutations of the vertices having the same cycle type induce permutations of the site with the same cycle type. Even the converse is not true. Hence, we have to look at only one example of each cycle type. One such is the identity which leaves all the sites unmoved. So corresponding to the cycle type S_1^4 in Z (S_4), we have S_1^6 in Z (S_4^2), another type of permutation is one that interchanges just

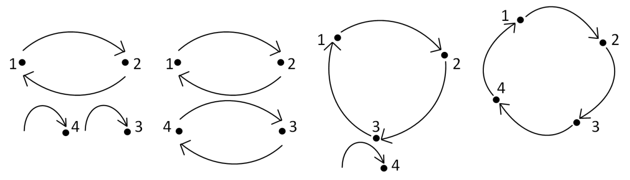

Fig 3

This maps the pair (1, 2) and (3, 4) on to themselves and it is easily verified that the other pairs interchange in two's. Hence the cycle type $S_1^2S_2$ in Z (S_4) gives rise to a term $S_1^2S_2^2$ in Z(S_4^2) proceeding like this with the three other types of permutations of four objects represented diagrammatically in fig. (3) we have the relations give in table.

In Z (S_4)	In Z (S_4^2)	Number
S_1^4	S_1^6	1
$S_1^2 S_2$	$S_1^2 S_2^2$	6
$S_1 S_3$	S_3^2	8
S_2^2	$S_1^2 S_2^2$	3
S_4	$S_2 S_4$	6

Graph Theory use Polya's theorem function in chemistry: Polya's theorem handles' this problem by using generating function to summarize the relevant information about the graph fig.

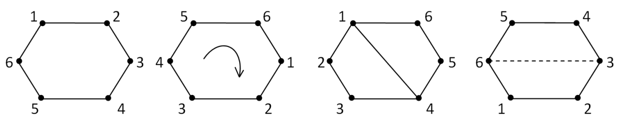

Fig 4

A generating function F(x) = $a_0 + a_1x + a_2x^2 + a_3x^3 +$ ……………………………where a_i is the number of figures with content i, this is known as the figure generating function. The answer to the problem then appears as a generating F(x) = $A_0 + A_1x + A_2x^2 + A_3x^3 +$………………where A_i is the number of configurations with content I, called as the configuration generating functions. Fig(4) ,suppose we number 6 sites around the necklace cycle 1, 2, 3, 4, 5, 6, in fig 4(a). Then the permutation corresponding to a clock wise rotation thought 120^0.

In fig 4(b) is

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 3 & 4 & 5 & 6 & 1 & 2 \end{pmatrix}$$

In this permutation 1 maps onto 3, 3 onto 5 and 5 onto 1, completing a cycle of length 3, which we write (1, 3 ,5). The remaining elements from another cycle of length 3, viz (2 4 6).

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 3 & 4 & 5 & 6 & 1 & 2 \end{pmatrix} = (1\ 3\ 5)(2\ 4\ 6)$$

And this permutation splits into two cycles of length 3, we know that any permutation can be expressed uniquely as a product of disjoint cycles apart from their order. With each permutation we associate a monomial say S_1^{j1} S_2^{j2} S_3^{j3}……………………………..and so on which the S_i^1 S are in determinates and J_i denoted the number of cycles of length I, we call this monomial the cycle type of permutation. For the permutation just considered with two cycle of length 3, the cycle type is S_2^2 for the permutation obtained flipping the necklace about a line joining sites 1 and 4 in fig 4(c). we have (1) (2 6) (3 5) (4) and the corresponding cycle type is $S_1^2s_2^2$, polya defined the cycle Indian of a group A to the average of all the cycle type for the elements of A, we calculate the cycle type of each element of A, add these together and divide by the number of elements. The cycle index of A is denoted by Z (A : S_1, S_2, S_3…………) now

CONCLUSION

The main aim of this paper is to present the importance of graph theoretical idea in chemistry. Researcher may set some information related to graph theory and chemistry and can get some ideas related to their field of research.

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