Discovery of many new compounds

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Abstract- Graph enumeration is the most important work in graph theory. Author's technique in graph enumeration is able to draw all types of graphs. All non-isomorphic structures of a compound has been possible to draw by this technique. By drawing all structures of all compounds and considering physical factors light, sound, temperature etc. on them it is possible to get the theory of evolution of matters.The number of possible connected non-isomorphic graphs having a fixed number of vertices and edges was possible to count by polya's method. This was the base of graph theory. But this method did not consider parallel edges (edges joining the same two vertices) and by this method the graphical pictures of the non-isomorphic graphs were not possible to obtain. All these limitations are removed in Roy's graph technique . For this reason, it is possible to draw all possible connected non-isomorphic structures of all compounds.In these way many new compounds are discovered. By drawing all structures of all compounds and considering physical factors light, sound, temperature etc. on them it is possible to get the theory of evolution of matters.

Technique:

Suppose one wants to draw all non-isomorphic connected graphs having n vertices and e edges (including parallel edges). n vertices can be connected minimally by (n-1) i.e. N(say) edges. Maximum number of degree of incidences for any vertex is k (say).

1. Find all non-isomorphic simple (excluding parallel edges) graphs having n vertices and N edges. These G_1 (say) graphs can be obtained by partition theory i.e. by n partition of the number 2 N.

2. Then find all non-isomorphic simple graphs having n vertices and (N+1) edges. Since (N+1) edges have totally 2(N+1) degree of incidence, these G_2 (say) graphs can be obtained by partition theory i.e. by n partition of the number 2(N+1).

3. Then find all non-isomorphic simple graphs having n vertices and (N+2) edges. Since (N+2) edges have totally 2(N+2) degree of incidence, these G_3 (say) graphs can be obtained by partition theory i.e. by n partition of the number 2(N+2).

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(k) In this way find all non-isomorphic simple graphs having n vertices and e edges. Since e edges have 2e degree of incidence. These G (say) graphs can be obtained by partition theory i.e. by n partition of the number 2e.

(I) Now for (1) to get e edges we have to add e-N edges to each of the G_1 graphs. For this, find all partitions (remembering no number is greater than or equal to k) of the number e-N. If there are r_1 elements in any one of this partition. Then these e-N edges can be added in N places in Nc_{r1} ways. In this way find Nc_{r2}, Nc_{r3}.....ways for other partitions having r2, r3,...... etc. elements. Then for (1) we shall get Nc_{r1} + Nc_{r2} + ...)G_1 connected graphs having n vertices and e edges.

(2) For (2) to get e edges we have to add e-(N+1) edges to each of the graphs. For this find all partitions (remembering no number is greater than or equal to k) of the number e-N-1. Find N+1Cm1, N+1Cm2 .....etc. ways for partitions having m1, m2......etc. elements respectively. Then for (2) we shall get (N+1Cm1 +N+1Cm2 +.........) G_2 connected graphs) having n vertices and e edges.

In this way add edges to edges to all graphs in (1), (2), ...k) to get e edges in all cases. Remember that for all graphs in (k) no edge is to be added. In this way we are getting.

(NCr2 +NCr2 + ...G1 + (N+1Cm1 +N+1Cm2.......)G2+....+G i.e. T_1 (say) connected graphs having n vertices and e edges (including parallel edges). Some of these graphs are again isomorphic. Find all non-isomorphic possible T_2 graphs among these T_1 graphs. Find all non-isomorphic possible (degree of incidence of no vertex is greater than or equal to k) T_3 graphs among these T_2 graphs. Then T_3 graphs will give all possible non-isomorphic connected graphs having n vertices and e edges (considering parallel edges). In this way we can show that total number of non-isomorphic connected graphs of C_6H_6 (benzene) is 3(5c2 +5c2+5c3+ +5c4)+4(6c1+6c2+6c3)+5(7c1+7c2)+6(8c1)+6=463(one hand of

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each carbon will be caught by one hydrogen. So we have considered the structure of six carbon considering their remaining three hands each).

All of these cmpounds are different in properties.But some of these compounds may be abolished after creation due to weak bonds between the molecules.In this way many new compounds are discovered.

REFERENCE:

Deo,N.- Graph theory