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CONSTRUCTION OF NEIGHBOURLY IRREGULAR CHEMICAL GRAPHS AMONG s-BLOCK AND p - BLOCK ELEMENTS COMBINATIONSAND ITS SIZE

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A B S T R A C T **RESEARCH ARTICLE**

A connected graph G is said to be neighbourly irregular, if no two adjacent vertices of G have the same degree. Given a positive integer n and a partition n with distinct parts. In this paper, we could derive some Neighbourly Irregular Chemical Graph (NICG) of molecular structure which is derived from the s-block elements and p-block elements combinations in the area of Inorganic Chemistry. Considering the atom as vertices, covalent bond as edges, and valence as degree of vertices. Also I have derived the size of such Neighbourly Irregular Chemical Graph (NICG).

Keywords:

Regular graph, irregular graph, Highly Irregular Graphs, Neighbourly irregular graph, Neighbourly irregular chemical graph, Molecular structure, Atoms, Valence of Atoms and Covalent Bond.

Introduction

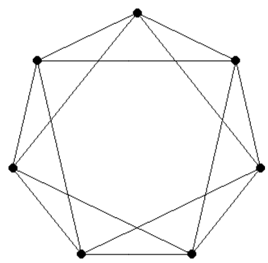
By a graph G we mean a finite undirected, connected graph without loops or multiple edges. In graph theory, regular graphs are those graph for which each vertex has the same degree. There are plenty of regular graphs, for example, complete graph. The problem arises when a graph is not regular. If it is irregular, how much of irregularity is thrust upon its vertices? A connected graph G is said to be highly irregular if each neighbour of any vertex has different degree. A connected graph G is said to be a k-neighbourhood regular graph if each of its vertices is adjacent to exactly k vertices of the same degree (If k=1, it becomes a highly irregular graph)

Inspired by the work of Dr. S.GNANA BHRAGASAM, we define the concept of Neighbourly Irregular Chemical Graph abbreviated ad NIC Graphs.

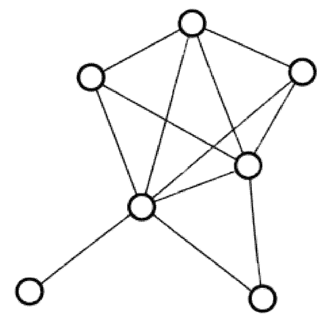
Chemical term	Mathematical (graph-theoretical) term
Atom	Vertex
Molecule	Molecular graph
Covalent bond	Edge
Acyclic hydrocarbon	Tree
Alternant structure	bipartite Graph
Valence of a atom	Vertex degree (number of lines at that vertex)
Skeletal structure	Hydrogen-depleted graph
Number of rings	Cyclamate number
[n] Annulene	n-vertex cycle
Huckel theory	Spectral theory
Topological matrix	Adjacency matrix
Energy level	Eigenvalue
Nonbonding level	Zero eigenvalue
Bonding level	Negative eigenvalue
Antibonding level	Positive eigenvalue
Secular polynomial	Characteristic polynomial
Kekule resonance formula	Perfect matching, 1- factor

Definitions

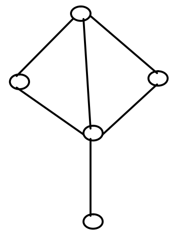
Regular Graphs: In a connected graph G is said to be regular graph for which each vertex has same degree.



Irregular Graphs: A graph G is called irregular graph, if there is a vertex which is adjacent only to vertices with distinct degrees.

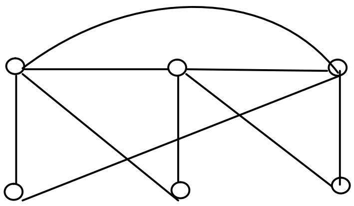


Neighbourly Irregular Graphs: A connected graph G is said to be neighbourly irregular Graph (NIG) if no two adjacent vertices of G have the same degree. NI graph where as it is not a k- neighbourhood regular graph.



k- neighbourhood

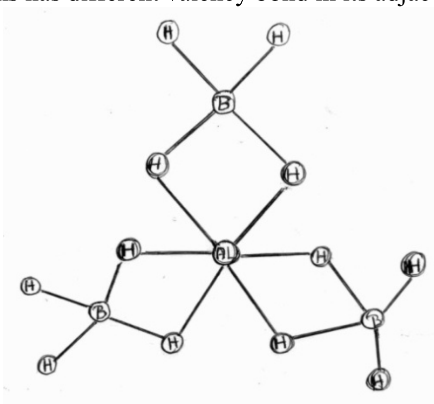
The graph is a 2-neighbourhood regular graph but not a NI graph



2-neighbourhood

Neighbourly Irregular Chemical Graphs (NICG): A graph is said to be a Neighbourly Irregular Chemical Graph (NICG) for the molecular structure of corresponding element of the atoms has different valency bond in its adjacent atoms.

Eg:



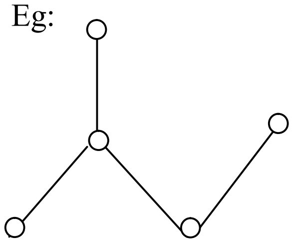
Aluminium Borohydride (AlB_3H_{12})

ACT-1: If v is a vertex of maximum degree in a NIC graph, then at least two of the adjacent vertices of v have the same degree.

Proof: Let v be a vertex of maximum degree Δ. Let v_1, v_2 ,………v_Δ be the vertices adjacent to V. If their degrees are distinct, then there is one vertex, v_i such that deg (v_i) = Δ=deg (v) which contradicts the neighbourly irregularness of the graph.

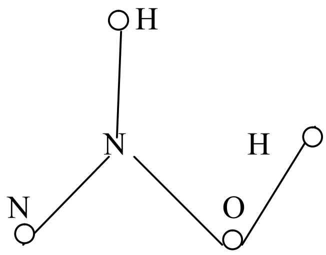
FACT-2: $K_{m,n}$ is NICG if and only if m≠n.

Eg:



m=5, n=4 ⇒ m≠n

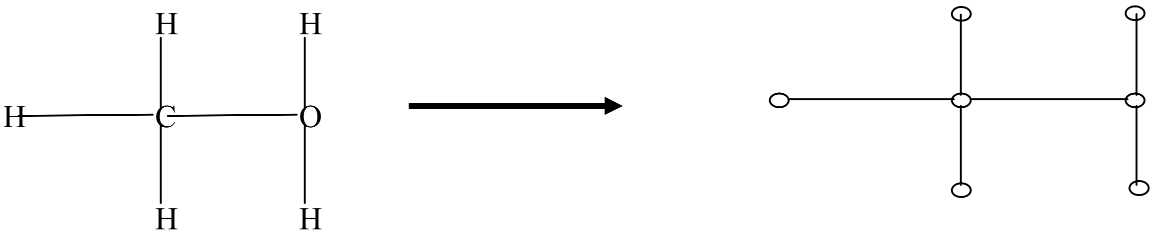
Derive from the molecular Structure of Hydroxylamine (NH $_3$O)



FACT-3: Let G be a NIC graph of order n. Then for any positive integer m<n, there exist at most m vertices of degree (n-m) for, if G has (m+1) vertices of degree (n-m), then due to their non adjacency nature, there must be at least m+1+n-m vertices that is (n+1) vertices contradicting the order of G.

Proof

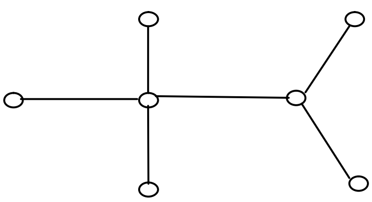
Let G be a NIC graph of order n=7, then any positive integer m<n



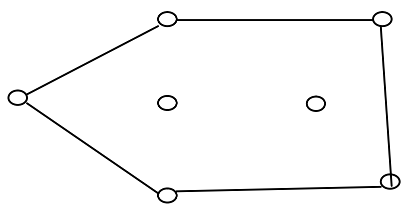
Methylamine (CH_5)

Fact-4: If a graph G is NIC, then G^C is not NIC

Proof: By fact -1 there are two nonadjacent vertices of same degree I in G. Those vertices are then adjacent vertices and also of same degree n-1-i in G^C



NIC



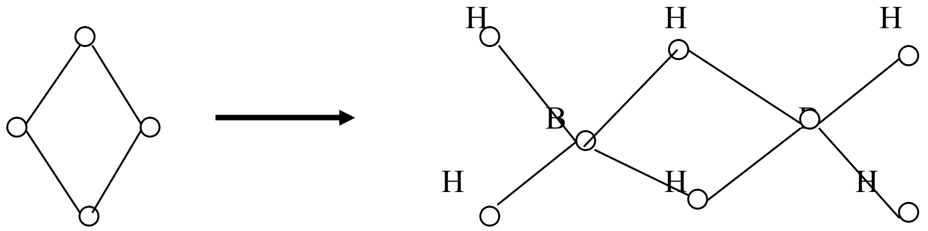
NIC^C

Theorem 1: Any graph of order n can be made to be an induced sub graph of a NIC graph of order at most $n+1C_2$

Proof: Choose any two adjacent vertices of G. If they are of same degree, introduce a new vertex. This process is repeated pairwise inductively till no two adjacent vertices are of same degree.

As it involves at most nC_2 steps only, the order of the induced NIC graph is $n+nC_2=n+1C_2$.

The induced NIC graph of K_4 are given below.



(Diborane B_2H_6)

Sum of NIC Graph of

K_4 is $n + nC_2 = (n+1)C_2$

$4 + 4C_2 = (4+1)\ C_2$

$4 + 6 = 10$

$10 = 10$

Theorem 2: Given a positive integer n and a partition $(n_1,n_2,\ldots\ldots.n_k)$ of n such that all n_is are distinct, there exists a NIC graph of order n and size

$$\frac{1}{2}\left\{n^2 - \left[n_1^2+n_2^2+\ldots\ldots\ldots n_k^2\right]\right\}$$

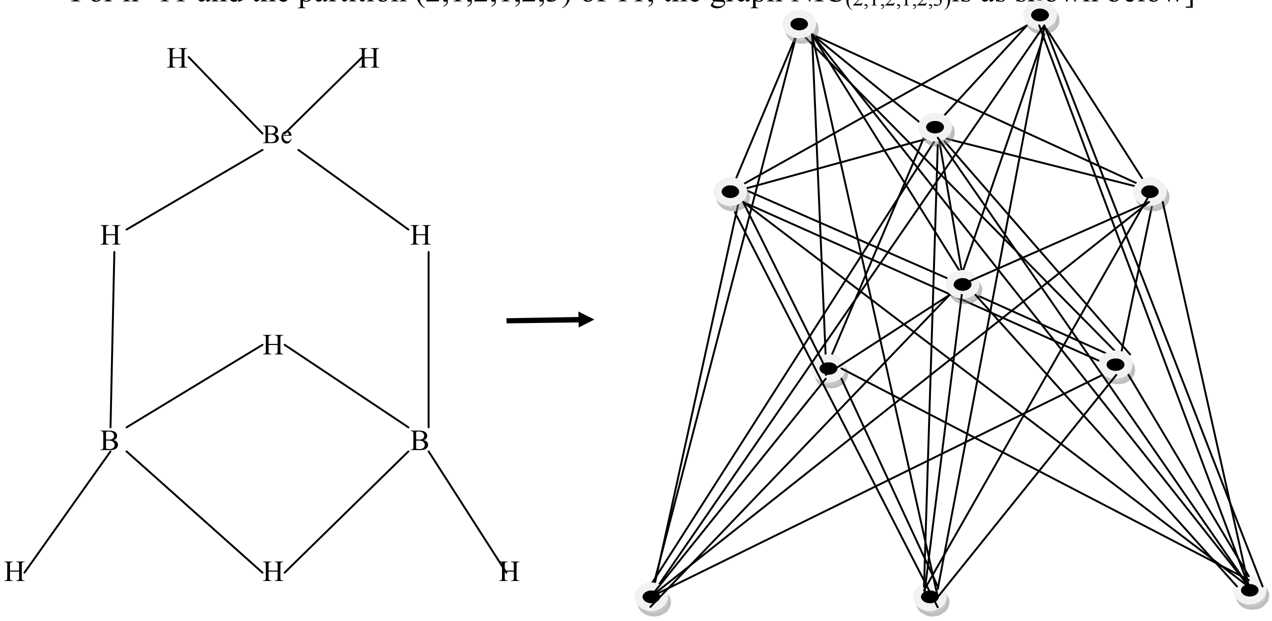
Proof: The required NIC graph is constructed follows. The n vertices are partitioned into k sets. The first set consists of n_1 vertices $u_1, u_2, \ldots\ldots\ldots u_{n1}$ the second consists of n_2 vertices $v_1,v_2,\ldots\ldots.v_{n2}$ and vertices $z_1,z_2,\ldots\ldots z_k$. Then every vertex in the first set is joined to all the other vertices in the remaining (k-1) sets. Similarly each vertex in the remaining set are joined set all those vertices in the other remaining sets. The vertices in the same set are non-adjacent. Therefore, degree of each vertex in the set in $n-n_j$. As all the n_i's are distinct, the connected graph so constructed is NIC and it is denoted by $NIC_{(n_1^2+n_2^2+\ldots\ldots\ldots n_k^2)}$.

The size of the graph $= \frac{1}{2}\sum \deg v$

$$=\frac{1}{2}\sum_{j=1}^{k} ni\ (n-n_i) = \frac{1}{2}[n^2-(n^2_1+n_2^2+\ldots\ldots\ldots\ldots n^2_k)]$$

Eg:

For n=11 and the partition (2,1,2,1,2,3) of 11, the graph $NIC_{(2,1,2,1,2,3)}$is as shown below]



Berlium borohydride ($Be(BH_4)_2$)

Size of graph

The maximum size of such a NIC graph of order 11 is

$= \frac{1}{2}[n^2-(n^2_1+n_2{}^2+\ldots\ldots\ldots\ldots+n^2_k)]$
$= \frac{1}{2}[11^2-(2^2+1^2+2^2+1^2+2^2+3^2)]$
$= \frac{1}{2}(121-23)$
$= \frac{1}{2}x98$
$= 49$

The minimum size of NIC Graph of order 11 in.
$= n_1{}^2+n^2{}_2+\ldots\ldots..+n_k{}^2$ is minimum
$= 2^2+1^2+2^2+1^2+2^2+3^2$
$=23$ is minimum

Lemma1.1

If $(m_1, m_2,\ldots., m_r)$ and $(n_1,n_2,\ldots..,n_k)$ are two partitions of a positive integer n with $r < k$, then $m_1{}^2+m_2{}^2+\ldots..+m_r{}^2 > n^2{}_1+n_2{}^2+\ldots\ldots\ldots\ldots+n^2{}_{k.}$

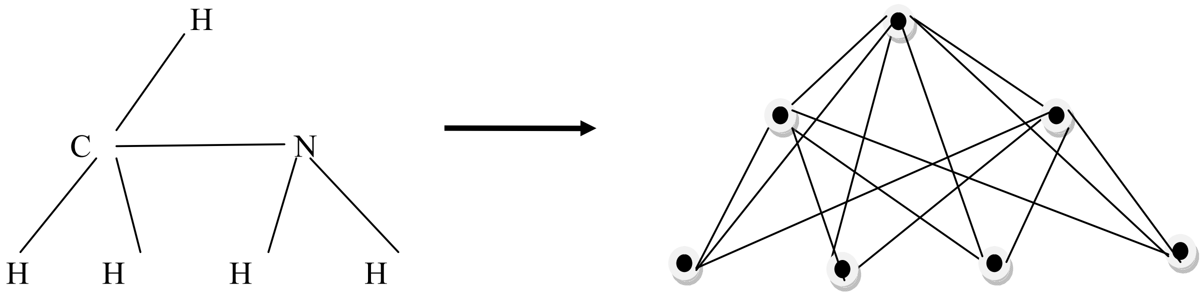
Proof : This is proved by induction on n. Assuming up to n, take two partitions $(m_1,m_2,\ldots.,m_r)$ and $(n_1,n_2,\ldots..,n_r)$ of the positive integer (n+1).

i.e., $m_1 +m_2+\ldots\ldots+m_r =n+1= n_1 +n_2+\ldots..,+n_k$

Let i and j be the first indices of m_i's and n_j's and respectively such that $m_i \geq n_j$. Now, If $(m_1,m_2,\ldots.,m_i-1,\ldots m_r)$ and $(n_1,n_2,\ldots.n_{j-1,\ldots}..,n_k)$ are two partitions of n with $r < k$. Applying the induction, we have
$m_1{}^2+m_2{}^2+\ldots\ldots+ (m_i{}^2-1)^2\ldots...+m_r{}^2$
$> n^2{}_1+n_2{}^2+\ldots\ldots..(n_j-1)^2\ldots\ldots+n^2{}_{k.}$
(i.e.) $m_1{}^2+m_2{}^2+\ldots\ldots+m_i{}^2\ldots...+m_r{}^2 - 2m_i$
$> n^2{}_1+n_2{}^2+\ldots\ldots..+ n_k{}^2+\ldots\ldots+n^2{}_{k.}-2n_j$
(i.e) $m_1{}^2+m_2{}^2+\ldots\ldots+m_i{}^2 > n^2{}_1+n_2{}^2+\ldots\ldots..+ n_k{}^2 + 2(m_i - n_j) > n^2{}_1+n_2{}^2+\ldots\ldots..+ n_k{}^2$ as $m_i > n_j$
This proves the lemma.

Corollary: Actual partition of n for which $NIC_{(}n_1+n_2+\ldots\ldots\ldots n_{K)}$ is of maximum size is given by { 2,3,2,,,,,r-,r+1,….k} where k is the least positive integer such that $\frac{k(k+1)}{2}$>n and r = $\frac{k(k+1)}{2}$-n.

Proof: If there exists a least positive integer k such that n= $\frac{k(k+1)}{2}$ then (1, 2,…… r-1,r+1,…..n) {where r= $\frac{k(k+1)}{2}$-n} is the partition of n of maximum number of parts and so the results is true by lemma Illustrations – for n =7 the partition (2, 3, 2) gives the maximum size and the NIC $_{(2,3,2)}$ graph is



(Methlamine CH_5)

Size $= \frac{1}{2} [7^2-(1^2+2^2+4^2)]$
$= \frac{1}{2}x28$
$=14$

Conclusion

In this paper we have constructer Neighbourly Irregular Chemical Graph(NICG) amongs-block elements and p- block elements combinations and its size in inorganic chemistry.

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