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CONSTRUCTION OF NEIGHBOURLY IRREGULAR CHEMICAL GRAPHS AMONG P-BLOCK ELEMENTS AND IT'S 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 of n with distinct parts. In this paper, we could derive some Neighbourly Irregular Chemical Graphs (NICG) of molecular structure which is derived from the p-block elements in the area of Inorganic Chemistry. Considering the atoms as vertices, covalent bond as edges, and valency as degree of vertices. Also I have derived the size of such Neighbourly Irregular Chemical Graphs.

Keywords:

Regular Graphs; Irregular Graphs; Highly Irregular Graphs; Neighbourly Irregular Graphs; Neighbourly irregular chemical graphs; Molecular Structure; Valence and Covalent Bond.

1. Introduction

By a graph G we mean a finite undirected, connected graph without loops or multiple edges. In graph theory, Regular graphs are those graphs where each vertex has same number of neighbours degree. For example, complete bipartite graph. Here the problem arises when a graph is not regular. If it is irregular, how much of irregularity is deducted 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 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.GNAANA BHRAGAASAM, we define the concept of Neighbourly Irregular Chemical graphs abbreviated as NIC Graphs.

Chemical term	Mathematical (graph-theoretical)term
Atom	Vertex
Molecule	Molecular graph
Covalent bond	Edge
Valence of an atom	Vertex degree (number of lines at that vertex)

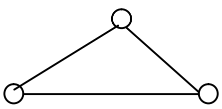
Definitions

1.Graph

A Graph G = (V (G), E(G)) consists of two finite sets;
V (G), the vertex set of the graph, often denoted by just V, which is a nonempty set of elements called vertices and E (G), the edge set of the graph, often denoted by just E, which is a possibly empty set of elements called edges.

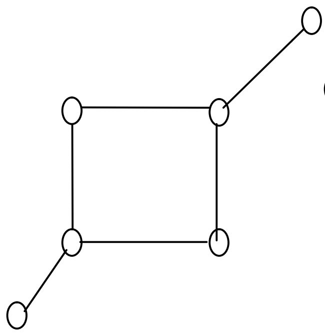
2.Regular Graphs

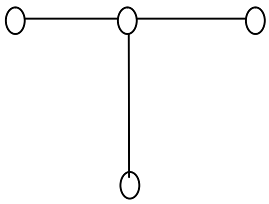
In a connected graph G is said to be regular graph for which each vertex has same degree.



3. Irregular Graphs

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

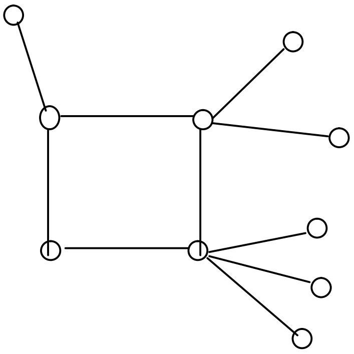




4. Neighbourly Irregular Graph

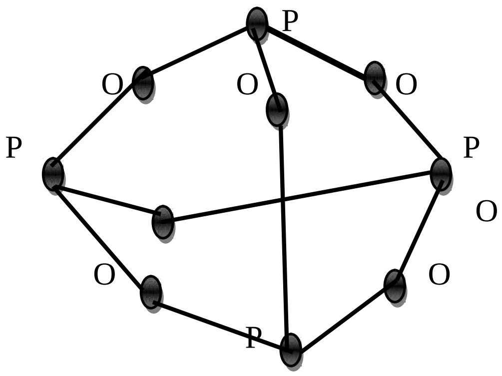
A graph G is said to be a Neighbourly Irregular Graph (NI graph) if every pair of its adjacent vertices have distinct degree.

Eg:1



$G_1$is a NI graph where as it is not a k-neighbourhood regular graph.

Eg:



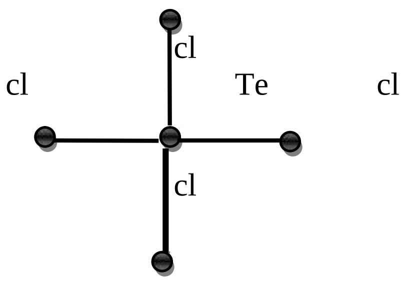
$P_4\,O_6$ (Tetra phosphorus Hexaoxide)

Fact:1--- If V is a atom of maximum degree in NIC graph, then at least two of the adjacent atoms of v have the same number of valence.

Proof: Let v be an atom of maximum valence Δ. Let $v_{1,}$ $v_{2.....}v_{\Delta}$ be the atoms adjacent to v. If there is the number of valence are distinct, then there is one atom v_i such that deg(v_i) = Δ = deg (v) which contradicts the neighbourly irregularness of the graph.

Fact:2- Let G be a NIC graph of order n. Then for any positive integer m<n, there exist atmost m atoms of the number of valency bond (n-m). For if G has (m+1) atoms of the number of valence bond (n-m), then due to their nonadjacency nature, there must be atleast m+1+n-m valency bond that is n+1 vertices contradiction the order of G.

Eg:

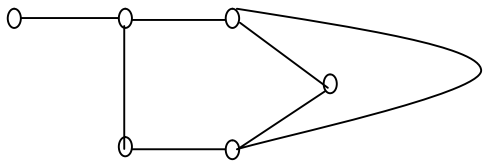


Tecl$_4$(Tellurium Tetrachloride)

Fact:3-If a graph G is Neighbourly Irregular Chemical Graph , then G^c is not Neighbourly Irregular Chemical Graphs.

BY the fact1, there are two nonadjacent atoms of same valence i in G. those atoms are adjacents and also of same number of valence n-1-I in G^c.

Eg:2

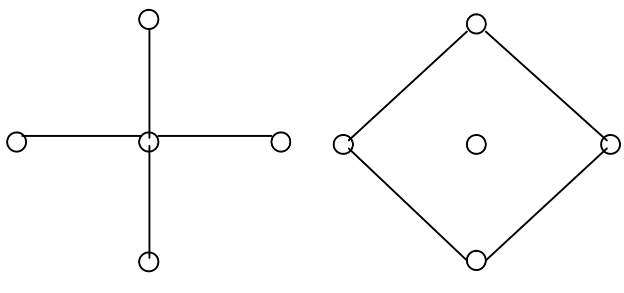


G_2 as shown below 2-neighbourhood regular graph but not a NI graph.

5.Neighbourly Irregular Chemical Graphs

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

Eg:



NIC NIC^c

Theorem:1

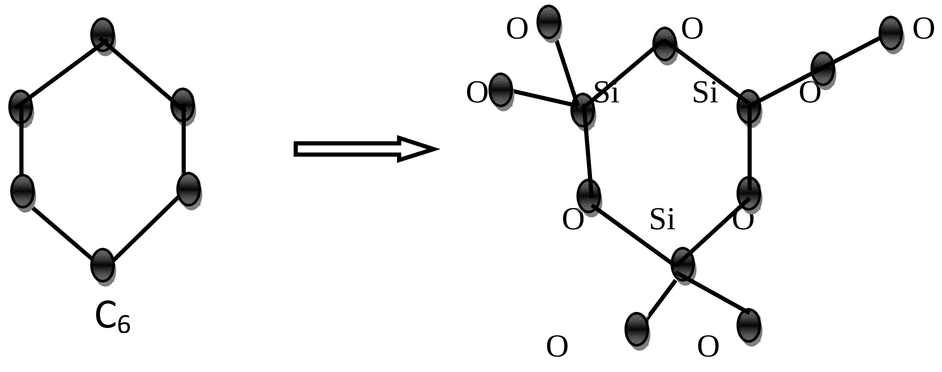
Any graph of order n can be made to be an induced subgraph of a NIC graph of order atmost n+1$C_{2.}$

Proof:

Choose any two adjacent atoms o G. If they are of same valence, indroduce a new vertex and join this to exactly one of these adjacent atoms. This process is repeatly pairwise inductively till no two adjacent atoms are of the same valency bond.

As it involves atmost nC_2 steps only, the order of the induced NIC graph is n + nC_2 = (n+1)C_2

The induced NIC grpah of C_6 is given below



Si_3O_{10}(Crystal structure)

Induced NIC graph of

C_6 is $n + nC_2 = (n+1)C_2$
$12 + 12C_2 = (12+1)C_2$
$12 + 66 = 78$
$78 = 78$

Theorem: 2

Given a positive integer n and a partition $(n_1, n_2, n_3, \ldots, n_k)$ of order n such that all n_i's are distinct, there exists a NIC graph of order n and size.

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

Proof: The required NIC graph is constructed as follows. The n atoms are partitioned into k sets. The first set consists of n_1 atoms $u_1, u_2, \ldots u_{n1}$; The second consists of n_2 atoms $v_1, v_2, \ldots, v_{n2}$ and finally the k'th set consists of n_k atoms $z_1, z_2, \ldots, z_{nk}$. then every atoms in the first set is joined to all the other atoms in the remaining sets. The vertices in the same set are non-adjacent. Therefore, valence bond of each atomd in the ith set is $n - n_i$.

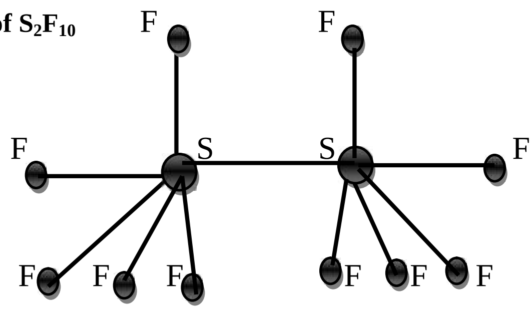
As all the n_i's are distinct, the connected graph so constructed is NIC and it is denoted by
$N(n_1, n_2, n_3, \ldots, n_k)$

The size of this graph

$$= \frac{1}{2} \Sigma \text{ valency bond V}$$
$$= \frac{1}{2} \Sigma\; n_i (n - n_i)$$
$$= \frac{1}{2} [n^2 - (n_1^2 + n_2^2 + \ldots + n_k^2)]$$

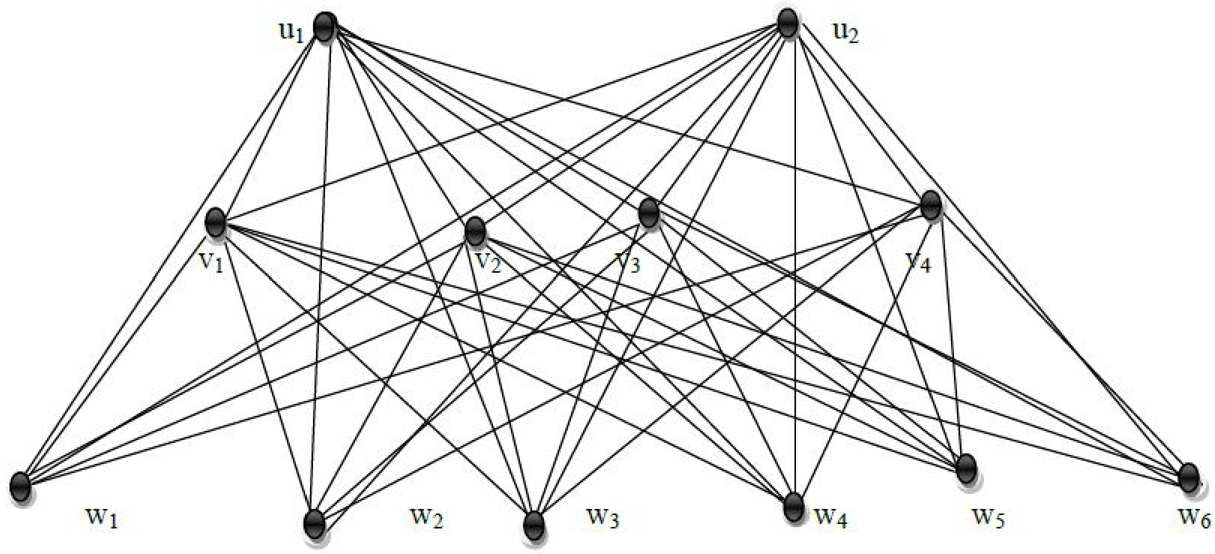
Example of S_2F_{10} --- For n = 12 and the partition (2,4,6) of 12, the graph $NI_{(2,4,6)}$ is as shown

Molecular structure of S_2F_{10}



S_2F_{10} (Disulfur Decafluoride)

Structure of Size of Graph



Size of the graph $= \frac{1}{2}\ \{ 12^2 - [2^2+4^2+6^2] \}$

$= \frac{1}{2}\ \{ 144 - 56 \}$

$= \frac{1}{2}\ \{ 88 \}$

$= 44$

Conclusion

we have constructed Neighbourly Irregular Chemical Graph from p-block elements and also its size.

References

[1] S.Arumugam and C. Pakkiam, Indian J.Pure appl. Math., 20(4) (1989), 330-33.

[2] R.Balakrishnan and A. Selvam, k-neighbourhood regular graphs, Procedings of the National Seminar on Graph Theory, 1996, pp.35-45.

[3] Devadoss Acharya and E. Sampathkumar, Indian J. Pure appl. Maths., 18(10) (1987), 882-90.

[4] Gary Wulfsberg, Inorganic Chemistr (417-433)

[5] Dr.S.Gnaana Bhragaasam and S. K.Ayyaswamy, Indian J.pure appl. Maths., 35(3): 389 -399, March 2004.

[6] James E.Huheey, Ellen.A.Keiter, Richard L.Keiter, Inorganic Chemistry Principles of Structure and Reactivity.(10 - 203)

[7] K.R. Parthasarathy, Basic Graph Theory, Tata McGraw Hill Publishing Company Ltd., New Delhi, 1994.

[8] Puri, Sharma, Kalia, Principles of Inorganic Chemistry (138-201) and (416-447).

[9] Yousef Alavi, Gary Chartrand, F.R.K.Chang, Paul Erdos, H.L. Graham and O.R. Oellermann, *J.Graph Theory*. 11(1987),235-49.

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