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.

### 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: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:

P_4O_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. Let v_1, v_2, ..., v 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) = 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 valency 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' is not Neighbourly Irregular Chemical Graphs.

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

Theorem: 1

Any graph of order n can be made to be an induced subgraph of a NIC graph of order atmost n+1C_2.

Proof:

Choose any two adjacent atoms o G. If they are of same valence, introduce a new vertex and join this to exactly one of these adjacent atoms. This process is repeatedly 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 graph of C_6 is given below.
Induced NIC graph of

\[ C_6 = n + nC_2 = (n+1)C_2 \]
\[ 12 + 12C_2 = (12+1)C_2 \]
\[ 12 + 66 = 78 \]
\[ 78 = 78 \]

**Theorem:** 2

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

\[ \frac{1}{2} \left( n^2 - \sum n_i^2 \right) \]

**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 \( u_1, u_2, ..., u_{n_1} \); the second consists of \( n_2 \) atoms \( v_1, v_2, ..., v_{n_2} \), and finally the \( k \)'th set consists of \( n_k \) atoms \( z_1, z_2, ..., z_{n_k} \), then every atom 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 atom in the \( i \)th 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 \( N(n_1,n_2,n_3,...,n_k) \).

The size of this graph

\[ \frac{1}{2} \left( n^2 - \sum n_i^2 \right) \]

**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 \( S_2F_{10} \)**

\[ S_2F_{10} \text{ (Disulfur Decafluoride)} \]
Structure of Size of Graph

\[ \text{Size of the graph} = \frac{1}{2} \left( 12^2 - \left( 2^2 + 4^2 + 6^2 \right) \right) \]
\[ = \frac{1}{2} \left( 144 - 56 \right) \]
\[ = \frac{1}{2} \left( 88 \right) \]
\[ = 44 \]

**Conclusion**

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

**References**

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

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