IRREGULAR COLOURING OF NEIGHBOURLY IRREGULAR CHEMICAL GRAPHS AMONG s- BLOCK AND p- BLOCK ELEMENTS

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Abstract: In any Neighbourly Irregular Chemical Graphs (NICG), if distinct atoms have distinct color codes and colouring is defined as irregular colouring. In this paper, we establish Irregular Colouring and also discussed about the Chromatic number $\chi(G)$ and Irregular Chromatic number $\chi_{ir}(G)$ of some classes of NIC graphs.

Keywords: NICG, Irregular colouring of NICG, Irregular chromatic number of NICG.

I. Introduction

An assingnment of k -colours to the vertices of graph G which is undirected and loopless, is said to be colouring, if no two distinct adjacent vertices have the same colour. The Chromatic number $\chi(G)$ is the minimum number of colours used in the graph. Inspired by the work of Mary Radcliffe and Ping Zhang [3], we define a Irregular Colouring $\chi_{ir}(G)$ in a Neighbourly Irregular Chemical Graphs among some classes of s- block and p- block elements and it should satisfy the condition as $\chi(G) \leq \chi_{ir}(G)$

Basic Definitions:

Definition 1.1

A *k-colouring* of a graph G = (V, E) is a function $c: V \rightarrow C$ where |c| = k having the property that $c(u) \neq c(v)$ for every pair(u ,v) of adjacent vertices of G, where C is the set of positive integers. The *Chromatic number* $\chi(G)$ of G is the minimum positive integer k for which there is a k- colouring of G .

Definition 1.2

For a positive integer k and a proper colouring $c: V(G) \rightarrow \{1,2,.....k\}$ of the vertices of a graph G, the *color code* of a vertex v of G is the ordered (k+1) – tuple code $_c(v) = (a_0,a_1,......a_k)$, where a_0 is the color assigned to v and for $1 \leq i \leq k$, a_i is the number of vertices adjacent to v that are colored i.

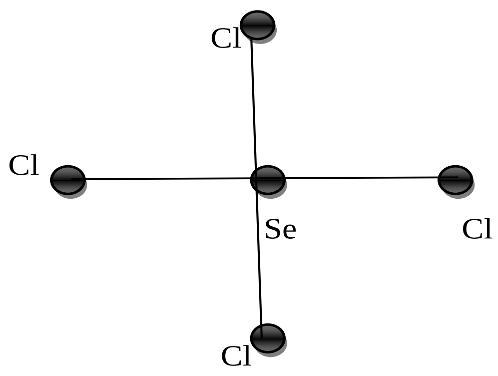
Definition 1.3

The colouring c is called *irregular* if distinct vertices have distinct color codes and the *irregular chromatic number* $\chi_{ir}(G)$ of G is the minimum positive integer k for which G has an irregular k- colouring. An irregular k- colouring with $\chi_{ir}(G)$ = k is a *minimum irregular colouring*. Since every irregular colouring of a graph G is a colouring of G, it follows that $\chi(G) \leq \chi_{ir}(G)$

Definition 1.4

A graph is said to be a *Neighbourly Irregular Chemical Graph* (NICG) for the molecular structure of corresponding element of the atoms have distinct color codes and different valency bond in its adjacent atoms.[1]

Example



Selenium tetrachloride ($SeCl_3$)

$$\chi(G) = \chi_{ir}(G) = 2$$

2.Irregular Colouring of NIC graph

Theorem 2.1

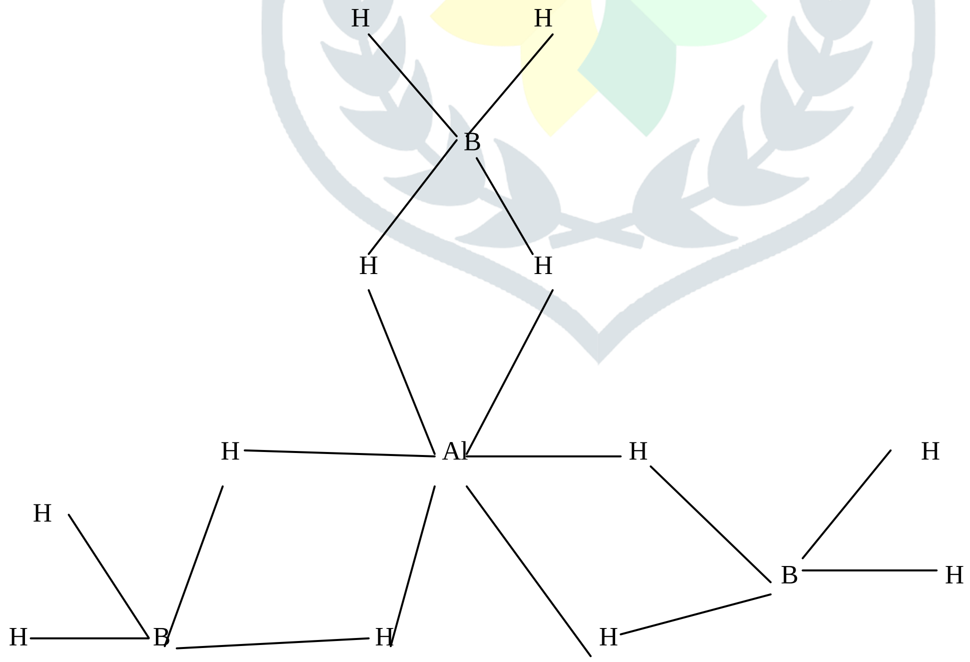
Let G be an Neighbourly Irregular Chemical Graph(NICG) for $3 \le n \le 21$ and if valency of any atom is less than or equal to 6, then $\chi_{ir}(G) = 2.$

Proof :

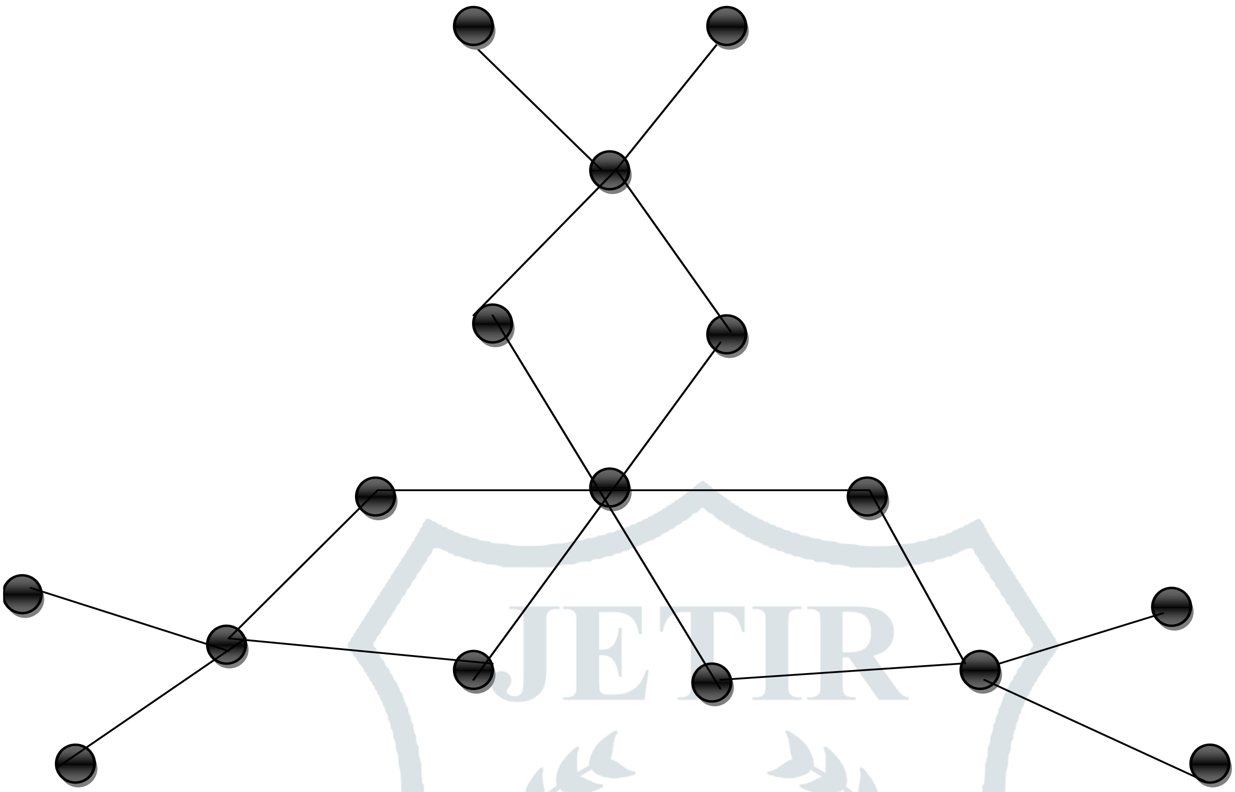
The Neighbourly Irregular Chemical graph contains atmost 16 atoms for which maximum valency is 6.
And c is an irregular 2- colouring .

The Irregular Chromatic number of this graph is denoted by $\chi_{ir}(G) = 2.$
Moreover , if c is an irregular 2- colouring of NIC graph for which maximum number of atoms is 21 and maximum valency is 4.
Hence , Chromatic number for this graph also same as 2 .
Hence, valency of an atom is less than or equal to 6, then Chromatic number of NIC graph is equal to 2.(n = 3,4,….21).

Example :1



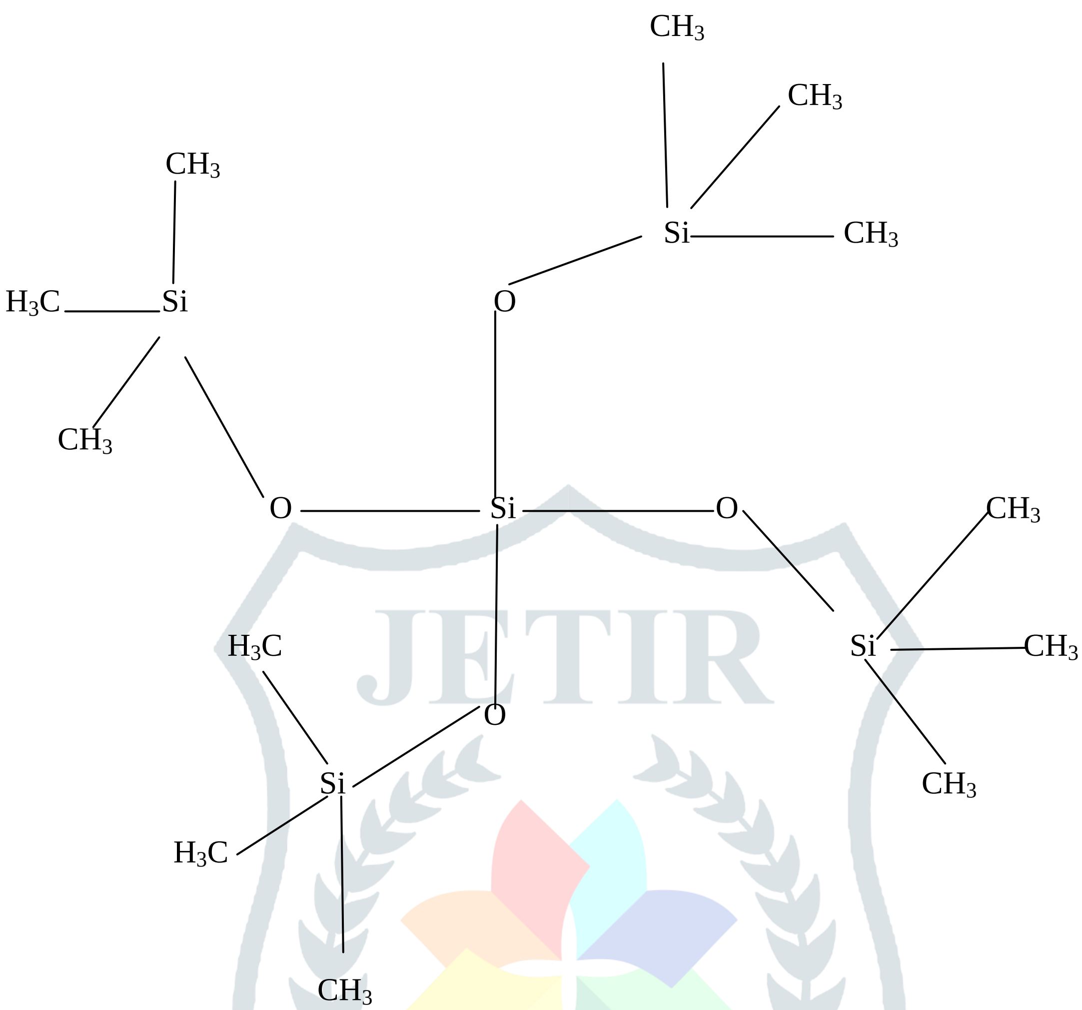
Aluminium borohydride $Al(BH_4)_3$



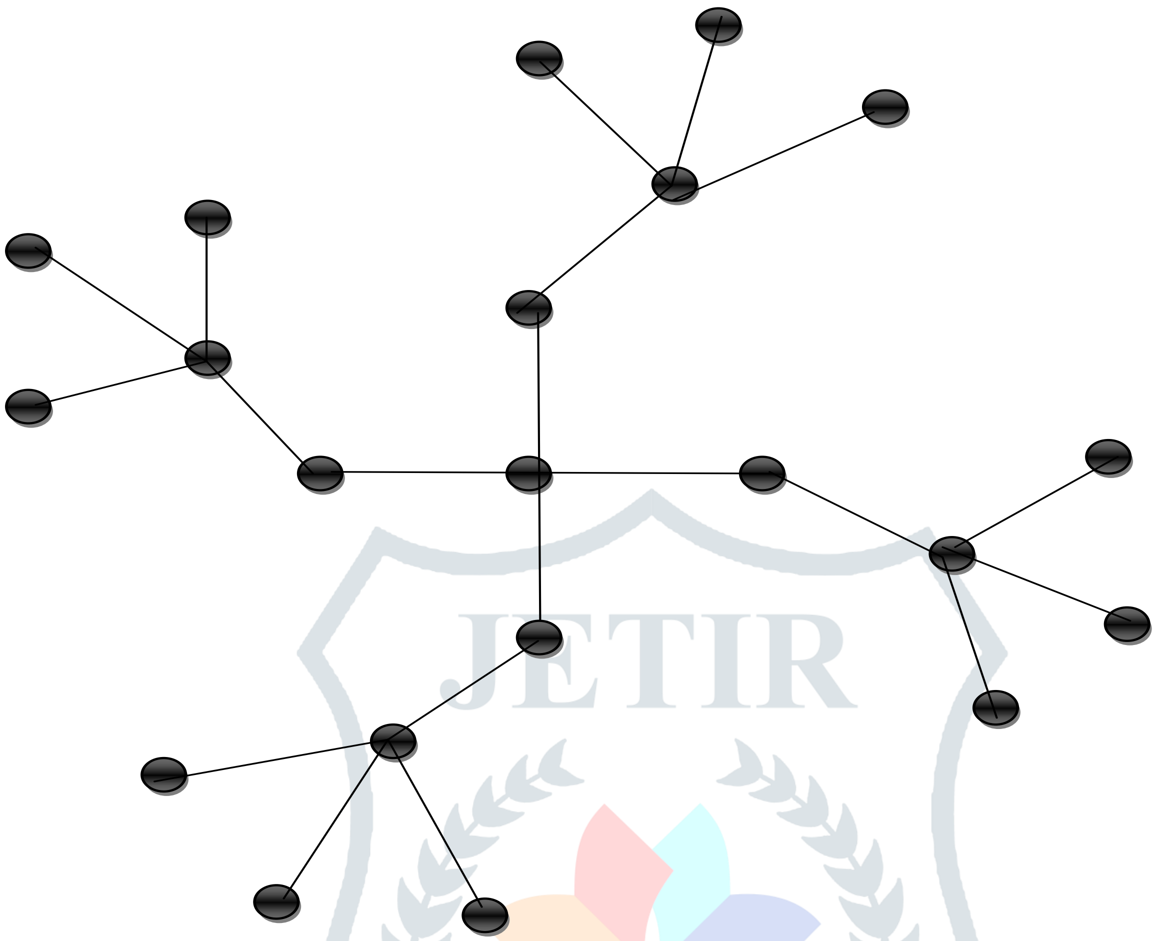
$\chi_{ir}(G) = 2.$

An irregular 2- colouring of NIC graph of order 16.

Example :2



Trimethylsiloxysilane ($C_{12}H_{36}O_4Si_5$)



$\chi_{ir}(G) = 2.$

An irregular 2- colouring of NIC graph of order 21.

Theorem 2.2

For any Chemical graph (NICG) , $\chi_{ir}(G) = 2$ if and only if G is Neighbourly Irregular Chemical Graph.

Proof :

If $\chi_{ir}(G) = 2$

To show that G is Neighbourly Irregular Chemical Graph.

A colouring of NIC graph is $\chi(G)$ = 2.

By definition of irregular colouring , $\chi(G) \leq \chi_{ir}(G)$

Let c be an 2- irregular colouring of graph and coding of any two adjacent atoms is not same.

code (u) = (1, k, 0)

code (v) = (1, 0, k) for some positive integer k = 0,1,2..

$code(u) \neq code(v) \qquad and$

i.e) $c(u) \neq c(v)$

Therefore , no two adjacent atoms have same colouring and codes, so that G is a Neighbourly Irregular Chemical Graph.

Conversely, if G is a Neighbourly Irregular Chemical Graph.

Maximum number of colourings c used in this graph is either 1 or 2, because of non- adjacent atoms.

Hence , $\chi_{ir}(G) = 2$

Theorem 2.3

If G_1, G_2,…….G_k are distinct NIC k graphs which are connected, then

$$\chi_{ir}(G_1 \cup G_2 \cup .....G_k) \le \left(\sum_{i=1}^{k} \chi_{ir}(G_i) \right) - k + 1.$$

Proof:

If k = 1 for NIC graph without isolated atoms then the result is obvious.
Thus assume that k = 2 for neighbourly irregular chemical graphs.

Let G_1 and G_2 be two NIC graphs, $\chi_{ir}(G)$ for both graph is 2, because distinct atoms having different colourings.
By using theorem 2.1,

We have $\chi_{ir}(G) = 2$

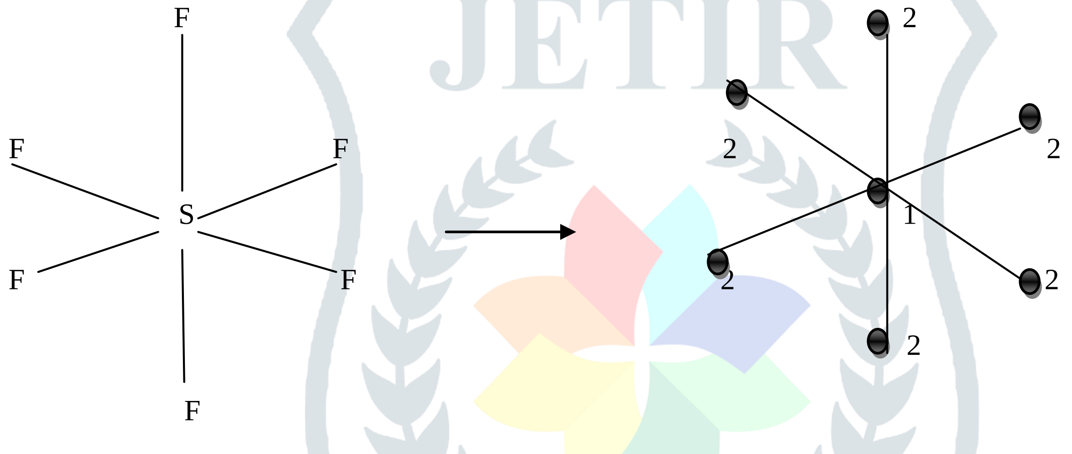
c_1 is an irregular k_1 – colouring of Neighbourly Irregular Chemical Graph G_1 and using colors in this graph is 1 and 2.
c_2 is an irregular k_2 – colouring of another Neighbourly Irregular Chemical Graph G_2.
Here , also using colors namely 1 and 2.

Assuming that $x \in V(G_1)$ and $y \in V(G_2)$ and coding for each atom in both graphs are different.

i.e)., $code(x) \ne code(y)$

So ,the result is true for k = 2.
By induction method it is true for k = n-1.
Hence the proof is completed.

Example :3



$\chi_{ir}(G) = 2$

Sulfur hexafluoride (SF_6)

Let G_1 be the NIC graph and $\chi_{ir}(G) = 2$

As stated in the above theorem,

$\chi_{ir}(G) \le \sum \chi_{ir}(G_1) - k + 1$ (k = number of graphs)

$2 \le 2 - 1 + 1$

$2 \le 2$

Theorem 2.4

For Neighbourly Irregular Chemical Complete Bipartite Graph $K_{m,n}$, (m = 1, n = 2,3,4,….7) then $\chi_{ir}(G) = 2$

Proof :

For m = 1, n =2, the Tellurium Dibromide ($TeBr_2$) is NIC Complete Bipartite Graph.
Let v_1, v_2, v_3, be an atoms of complete bipartite NIC graph for $K_{1,2}$.
It can be classified into two sets V_1 and V_2 , every atoms in V_1 is adjacent to V_2 as viceversa.

$V_1 = \{ v_1 \}$

$V_2 = \{ v_2, v_3 \}$

Color coding for each atom is

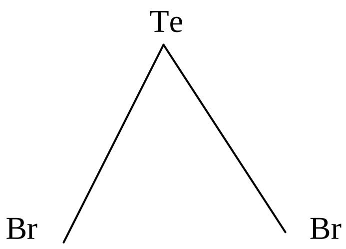
$v_1 = 102$,

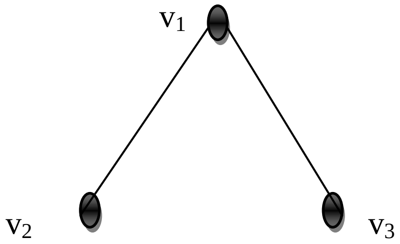
$v_2 = 210$ and

$v_3 = 210$

$\chi_{ir}(G) = 2$

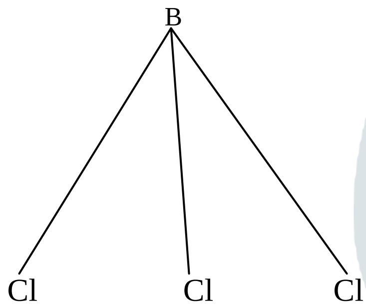
And satisfy the condition that adjacent atoms not have same color codes.

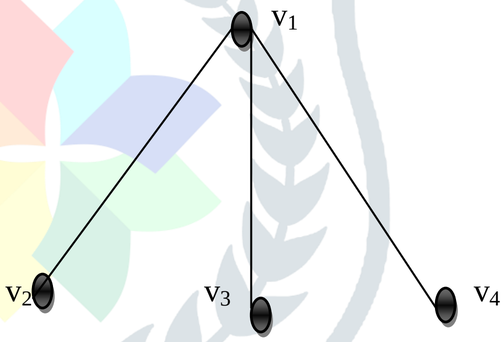




Tellurium Dibromide ($TeBr_2$) **$K_{1,2}$**

For m = 1, n = 3, the Boron trichloride (BCl_3) is NIC complete bipartite graph
Let v_1, v_2, v_3,v_4 be an atoms of complete bipartite NIC graph for $K_{1,3}$.
It can be classified into two sets V_1 and V_2 , every atoms in V_1 is adjacent to V_2 as viceversa.
$V_1 = \{ v_1\}$
$V_2 = \{ v_2, v_3, v_4\}$
Color coding for each atom is
v_1 = 103,
v_2 = 210,
v_3 = 210 and
v_4 = 210
$\chi_{ir}(G) = 2$
And satisfy the condition that adjacent atoms not have same color codes.

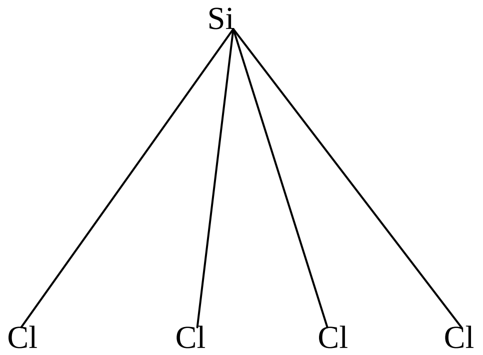




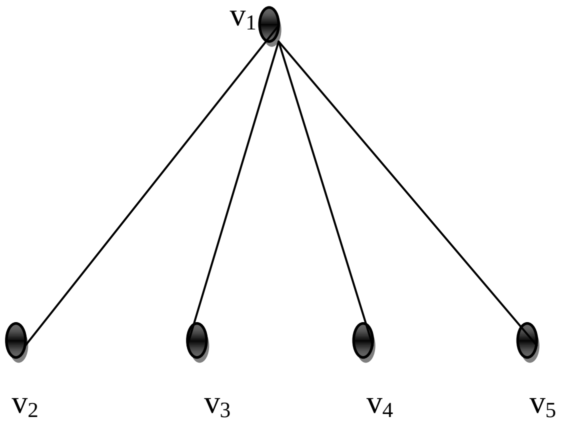
Boron trichloride (BCl_3) **$K_{1,3}$**

For m =1,n = 4, the Silicon tetrachloride ($SiCl_4$) is NIC complete bipartite graph
Let v_1, v_2, v_3,v_4, v_5 be an atoms of $K_{1,4}$ graph.
It can be classified into two sets
$V_1 = \{ v_1\}$ and
$V_2 = \{ v_2, v_3, v_4, v_5\}$
Color coding for each atom is
v_1 = 104,
v_2 = 210,
v_3 = 210 ,
v_4 = 210 and
v_5 = 210

The Irregular Chromatic number for this graph is 2 and have distinct codes for adjacent atoms.



Silicon trichloride($SiCl_3$)



$K_{1,4}$

Hence it is true for n = 5,6,7

$\therefore$ $\chi_{ir}(G)$ of $K_{m,n}$ graph is 2. (m = 1, n =2,3,4,….7).

Observation:

- $K_{1,2}$, $K_{1,3}$, $K_{1,4}$, $K_{1,5}$, $K_{1,6}$ and $K_{1,7}$ are only NIC Complete Bipartite Graph among s- block and p- block elements.
- For Neighbourly Irregular Chemical Complete Bipartite Graph $K_{m,n}$, (m = 1, n = 2,3,4,….7) its $\chi_{ir}(G)$ = 2 then $\chi_{ir}(\overline{G}) \neq 2$, because which is disconnected into two componenets.

Problem

Let G be the NIC graph of Dimethyl Sulfoxide $\chi_{ir}(G) = 2$, then its chromatic number of complement of NIC graph $\overline{G}$ is not equal to two.

Solution :

The Chromatic number of Dimethyl Sulfoxide (C_2H_6OS) graph, is 2 as and Chromatic number for Complement of Dimethyl Sulfoxide (C_2H_6OS) graph is not equal to 2 .

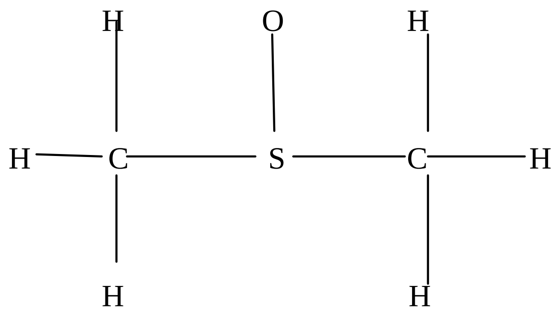
Codes for complement graph $\overline{G}$ is

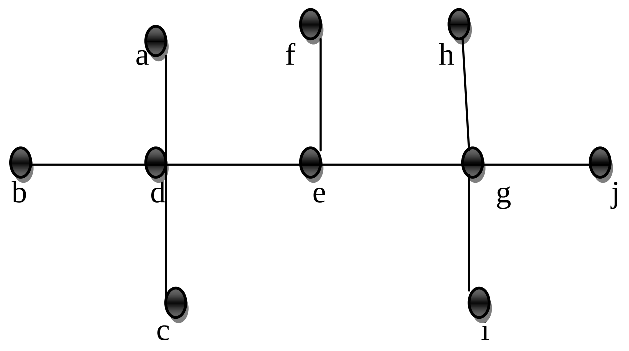
c(a) = 10112211
c(b) = 21012211
c(c) = 31102211
c(d) = 20001211
c(e) = 41110111
c(f) = 41210211
c(g) = 51211000
c(h) = 51212011
c(i) = 61212101
c(j) = 71212110

The irregular chromatic number of complement of dimethyl sulfoxide is 7.

$\therefore$ $\chi_{ir}(G) \neq \chi_{ir}(\overline{G})$.

Example:4

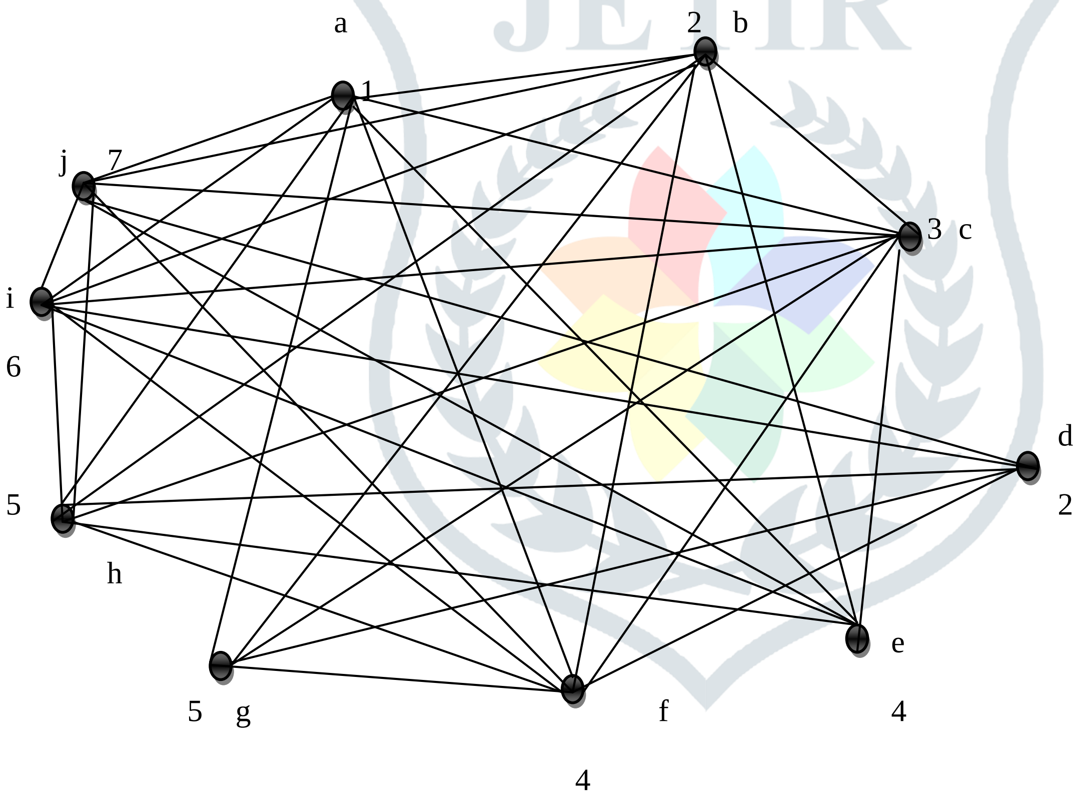




Dimethyl Sulfoxide (C_2H_6OS)

$$\chi_{ir}(G) = 2.$$

Example: 5



Complement of Dimethyl Sulfoxide (C_2H_6OS)

Conclusion

Here ,we applied the Irregular Colouring for Neighbourly Irregular Chemical Graph (NICG) and the NIC Complete bipartite graph Km,n . And find the Irregular Chromatic number for such graphs and its corresponding complement graph $\overline{G}$ also.

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