Irregular Chromatic number of Line graph of Neighbourly Irregular Chemical Graph among s-block and p-block elements

J.Arockia Aruldoss[1], U.Gogulalakshmi[2]

Assistant Professor[1], Research Scholar[2],

PG and Research Department of Mathematics,

St.Joseph's College of Arts and Science (Autonomous), Cuddalore-1

Abstract

Let G be a Neighbourly Irregular Chemical Graph(NICG) . We obtain the Line graph L(G) from the graph G for some chemical graph, in which each atoms of L(G) represents an covalent bonds of G. In this paper, finding the Irregular Chromatic Number $\chi_{ir}(G)$ of Line Graph by using different codes and colors. And also, discuss about some examples of Line graph L(G) and Complete bipartite $K_{1,n}$(G) of NIC graph.

Keywords: Irregular colouring, line graph , complete bipartite graph.

1. Introduction

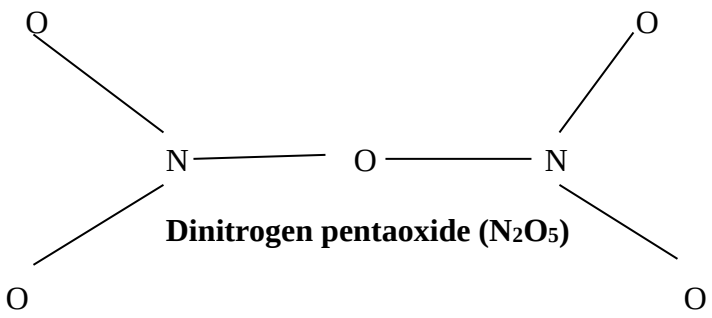
In a graph G = (V,E) considered as a pair of vertices and edges. Here ,we consider the V as atoms and E be an covalent bond in chemical term of molecular structure of the Neighbourly Irregular Chemical Graph (NICG) which is finite, undirected, and without loop and isolated atom[1]. Mary Radcliffe and Ping Zhang [2], introduce the concept of irregular colouring of graphs. In 1932, H.Whitney invented the line graph [3]. In this paper, we define the concept of Irregular Chromatic number of line graph of graph (NICG).

2.Basic Definitons:

Definition 2.1

For the molecular structure of chemical graph corresponding element of the atoms has different valency in its adjacent atoms is said to be a Neighbourly Irregular Chemical Graph (NICG).

Example: 2.1.1



Dinitrogen pentaoxide (N_2O_5)

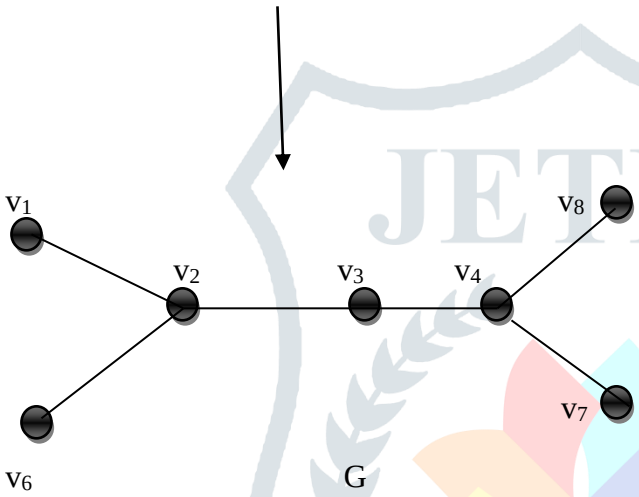


Figure 2.1

Definition 2.2

Let G be a graph and let V(G) be the set of all vertices of G and let {1,2,….k} be denote the set of all colours which are assigned to each vertex of G. A proper vertex colouring of a graph G is a mapping c: V(G) $\rightarrow$ {1,2,….k} such that $c(u) \neq c(v)$ for all arbitrary adjacent vertices $u,v \in V(G)$.

Definition 2.3

If distinct vertices have distinct color codes and the colouring c is called irregular colouring.

Definition 2. 4

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 coloring.

Definition 2.5

Let G = (V, X) be a graph. The Complement $\overline{G}$ of G is defined to be the graph which has V as its set of points and two points are adjacent in $\overline{G}$ if and only if they are not adjacent in G.

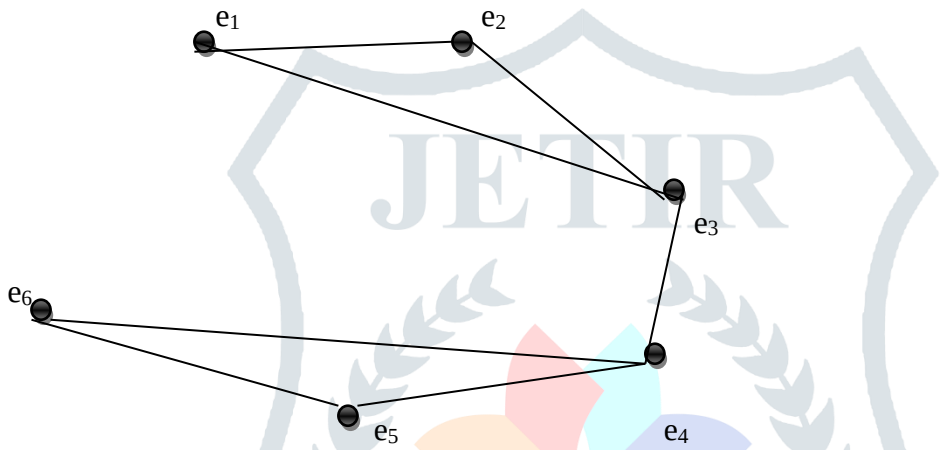
Definition 2.6

A graph G is called a bigraph or bipartite graph if V can be partitioned into two disjoint subsets V_1 and V_2 such that every line of G joins a point of V_1 to a point V_2. (V_1, V_2) is called a bipartition of G. If further G contains every line joining the points V_1 to the points of V_2 then G is called a complete bigraph.$K_{1,m}$ is called a star for $m \geq 1$.

Definition 2. 7

A line graph L(G) (also called an adjoint,covering) of a simple graph G such that each vertex of L(G) represents an edge of G and two vertices of L(G) are adjacent iff their corresponding edges are incident in G

Example: 2.1.2



L(G) of Dinitrogen Pentaoxide

Figure 2.2

3.Irregular Chromatic Number of Line graph of NICG:

Theorem 3.1

For some line graph of Neighbourly Irregular Chemical Graph its chromtic number $\chi_{ir}(L(G))$ is either 3 or 4 for $n \geq 4$ atoms of molecular structure.

Proof:

Let $\{v_1, v_2, v_3, \ldots\ldots v_9\}$ be the maximum number of atoms of molecular structure of NIC graph G of order 9.

And $\{e_1, e_2, e_3, \ldots\ldots e_8\}$ be an covalent bond of graph

Here , covalent bond is considered as atoms of line graph which shown in fig 3.2

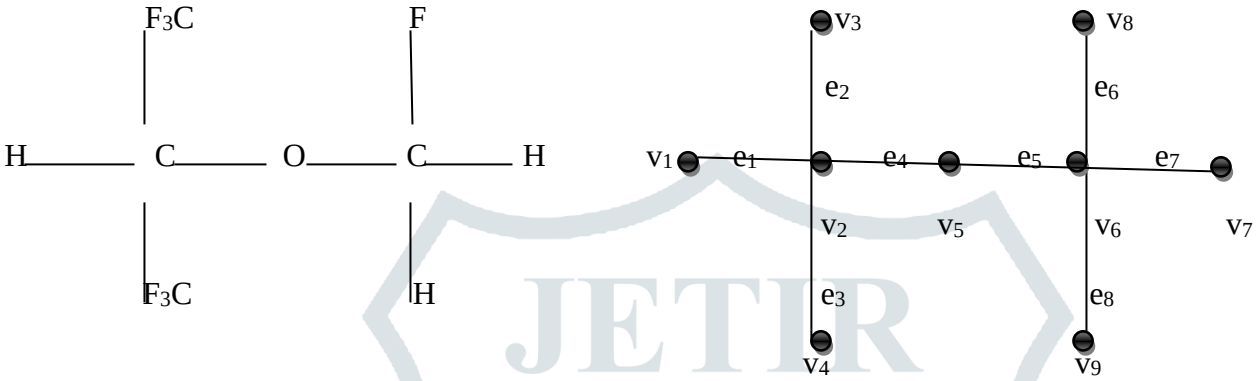
$\therefore$ Irregular chromatic number for line graph $\chi_{ir}(L(G)) = 4$.

Moreover , $\{v_1, v_2, v_3, \ldots\ldots v_{10}\}$ be an atom of NIC graph of maximum order 10.

Covalent bond for line graph is $\{e_1, e_2, e_3, \ldots\ldots e_{12}\}$

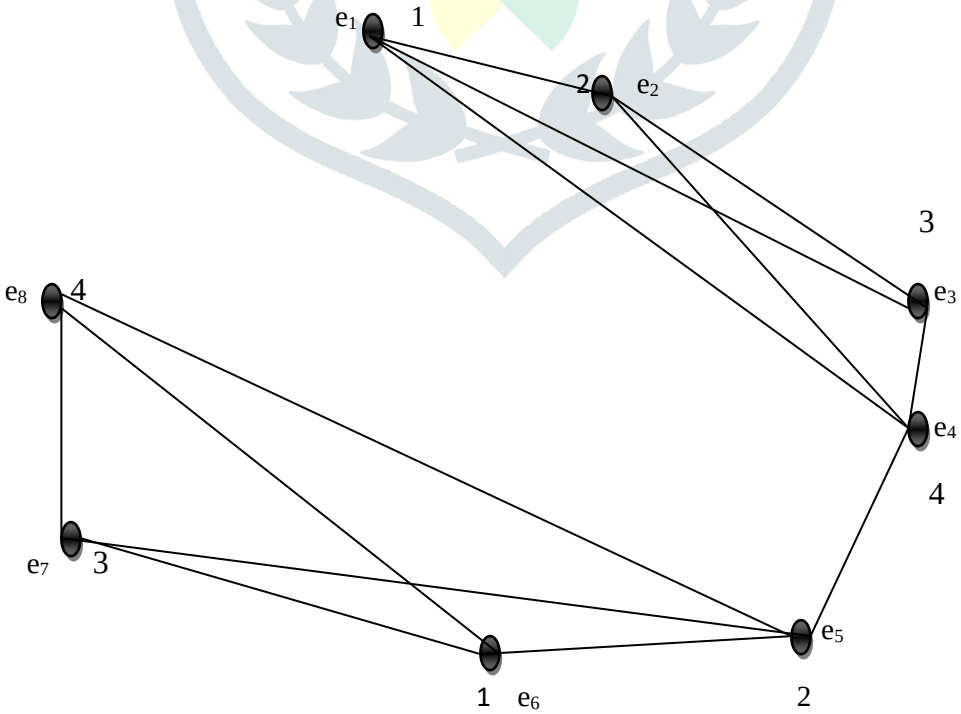
Here the same process followed as above and shown in fig 3.4

$\therefore \chi_{ir}(L(G)) = 4.$



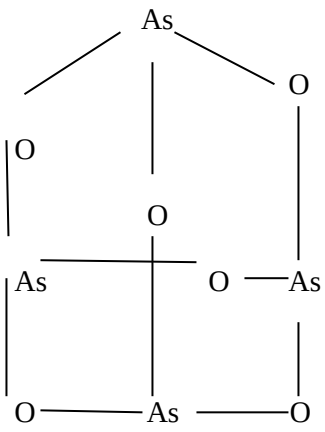
Sevoflurane($C_4H_3F_7O$) G

Figure 3.1



L(G) of Sevoflurane($C_4H_3F_7O$)

Figure 3.2



Arsenic Trioxide (As_4O_6)

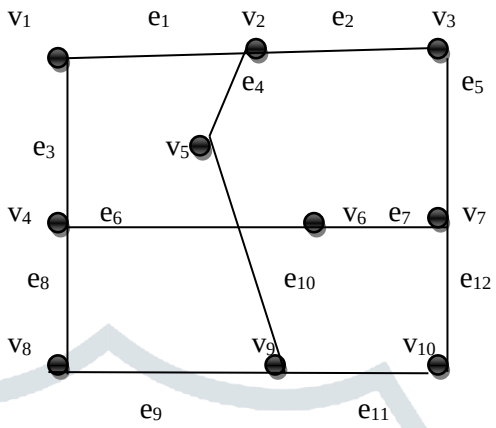


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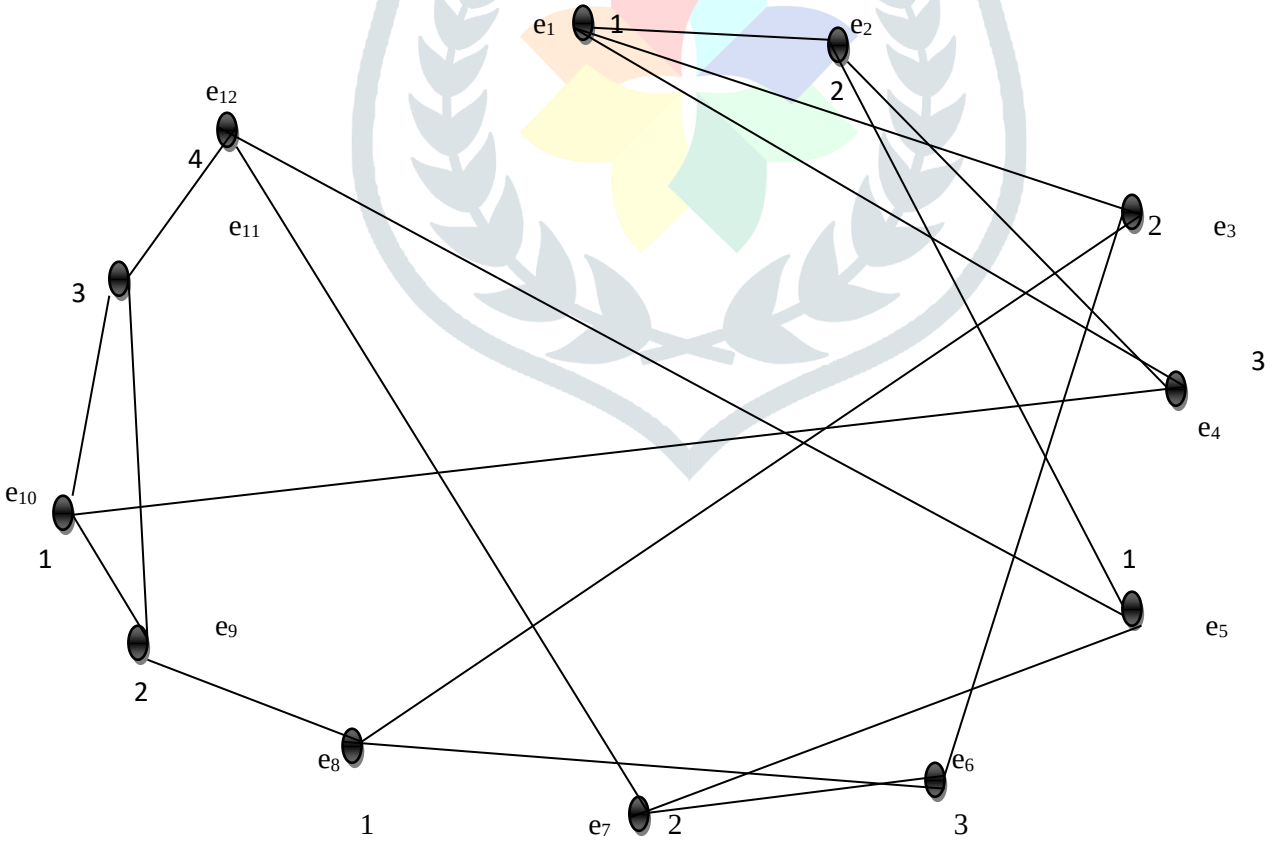
Figure 3.3



L(G) of Arsenic Trioxide (As_4O_6)

Figure 3.4

3.2 Irregular Chromatic Number of Line graph of Complete bipartite NICG

Theorem 3.2

For every line graph L(G) of Complete bipartite NIC graph G of order n, then $\chi_{ir}\left(L\left(K_{1,m}\right)\right)=m$ $\forall m \geq 3$

Proof:

Let $\{v_1, v_2, v_3, \ldots\ldots v_n\}$ be an atom of Complete bipartite NIC graph $K_{1,n}$ and $\{e_1, e_2, e_3, \ldots\ldots e_n\}$ be an covalent bond of such graph.

This covalent bond are considered as atoms of line graph of Complete bipartite graph $L(K_{1,m})$.

For m = 3 atom,

$\chi_{ir}\left(L\left(K_{1,3}\right)\right) = 3$

For m = 4 atom,

$\chi_{ir}\left(L\left(K_{1,4}\right)\right) = 4$

For m = 5 atom,

$\chi_{ir}\left(L\left(K_{1,5}\right)\right) = 5$

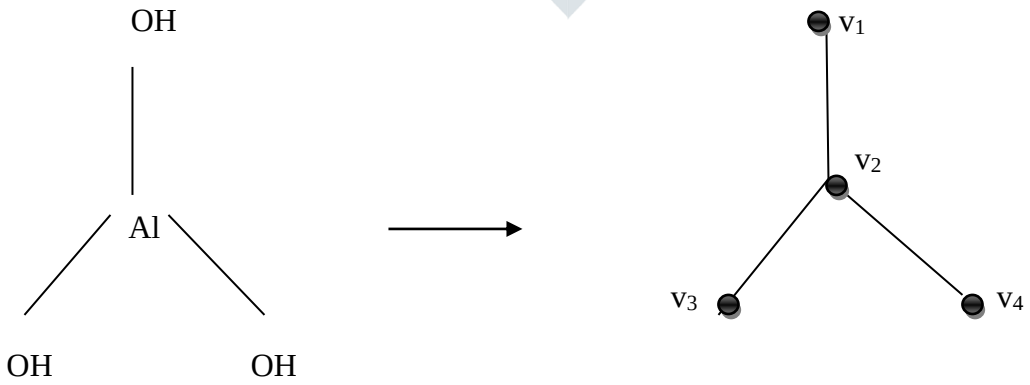
It is true for m = 4,5,6 atom, and by induction method

Hence the result is true for m -1.

Therefore $\chi_{ir}\left(L\left(K_{1,m}\right)\right)=m$

Example:3.2.1

Consider the line graph L(G) of complete bipartite graph $K_{1,3}$ of Aluminium hydroxide $(Al(OH)_3)$



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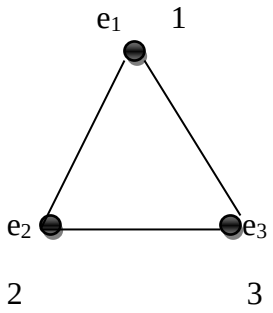
Aluminium hydroxide $(Al(OH)_3)$

Figure 3.5

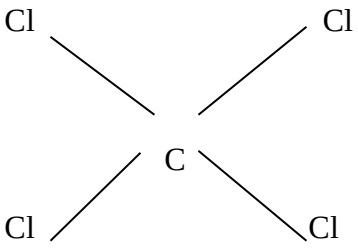


$$\chi_{ir}\left(L\left(K_{1,3}\right)\right)=3$$

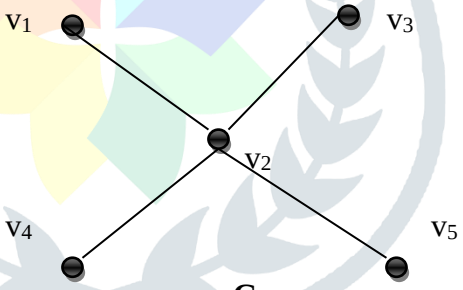
Figure 3.6

Example:3.2.2

Consider the line graph L(G) of Complete bipartite graph $K_{1,4}$ of Carbon tetrachloride (CCl_4)



Carbon tetrachloride (CCl_4)



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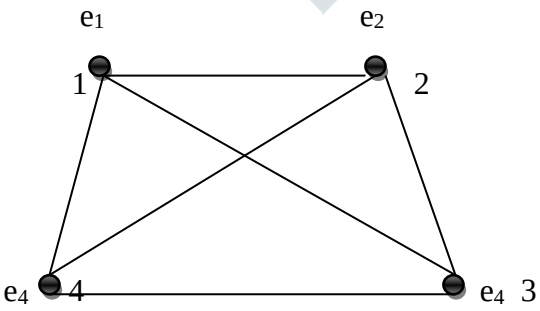
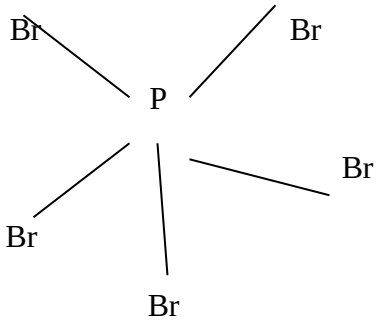


$$\chi_{ir}\left(L\left(K_{1,4}\right)\right)=4$$

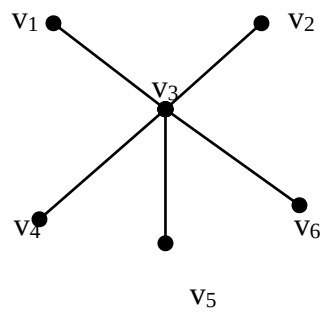
Figure 3.7

Example:3.2.3

Consider the line graph L(G) of complete bipartite graph $K_{1,5}$ of Phosphorous pentabromide (PBr_5)



Phosphorous pentabromide (PBr_5)



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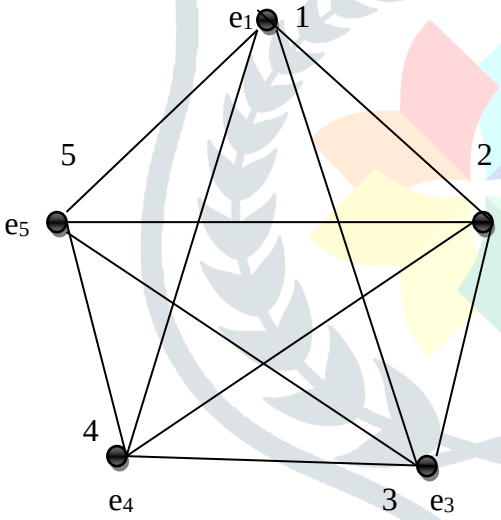


$$\chi_{ir}\left(L\left(K_{1,5}\right)\right)=5$$

Figure 3.8

Problem :3.3

If L(G) and $L(\overline{G})$ are line graph and its Complement of NIC graph G , which is molecular structure of Arsenic trioxide (As_4O_6) , both graph has same irregular chromatic number.

Solution :

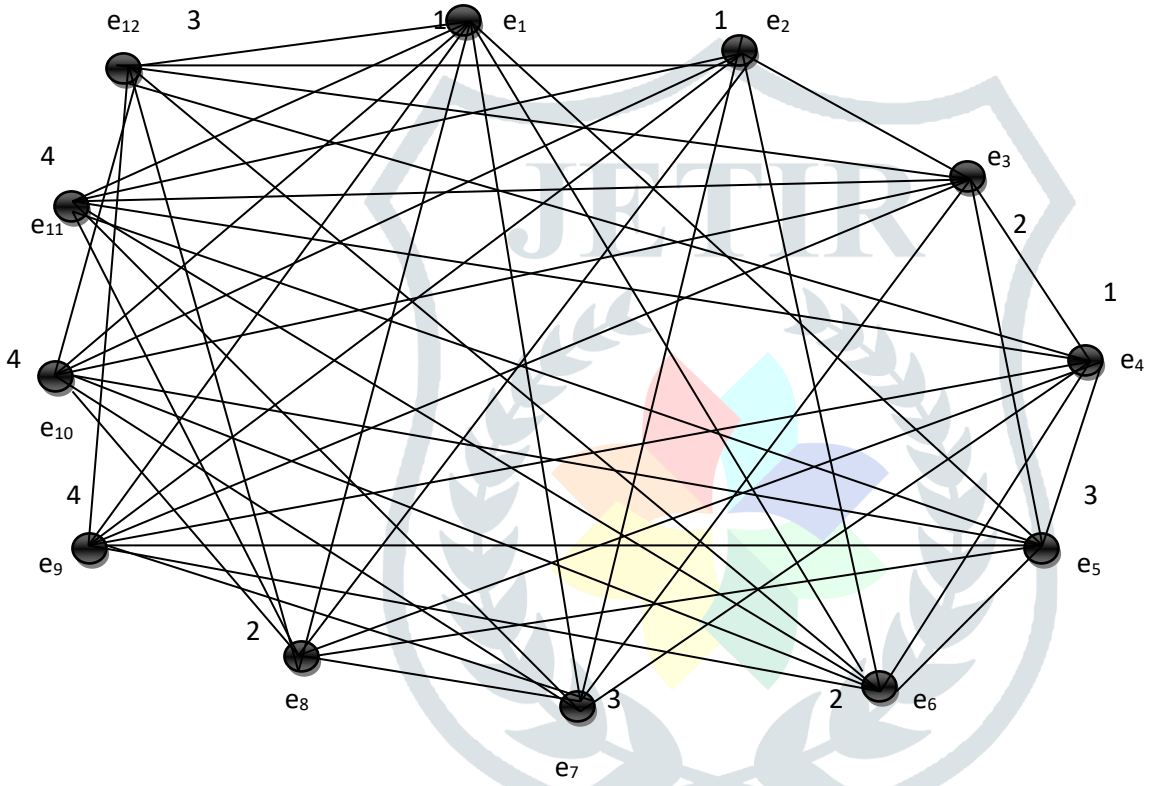
Let G be an arsenic trioxide which is Neighbourly Irregular Chemical Graph as shown in figure 3.3

Its irregular chromatic number is 2.

The irregular chromatic number for line graph of arsenic trioxide is 4 as shown in figure 3.4

And Complement of L(G) graph of arsenic trioxide is shown figure 3.9 in have valency bond 8 .

$\chi_{ir}\left(L\left(\overline{G}\right)\right)=4$



Complement of L(G) graph of Arsenic trioxide

Figure 3.9

Colour codes for Line graph and it's Complement graph:

Colour codes for each atoms	Line Graph of Arsenic Trioxide	Complement of Line graph of Arsenic Trioxide
$c(e_1)$	10210	10233
$c(e_2)$	22010	10323
$c(e_3)$	22010	22033
$c(e_4)$	32100	10332
$c(e_5)$	10201	32303
$c(e_6)$	31200	23023
$c(e_7)$	21011	33203

$c(e_8)$	10210	23032
$c(e_9)$	22010	43230
$c(e_{10})$	10120	42330
$c(e_{11})$	31101	43320
$c(e_{12})$	41110	33302

Adjacent atom for Line graph and it's Complement graph has distinct codes.

But they has same chromatic number

i.e.) $\chi_{ir}(L(G)) = 4$.

$\chi_{ir}(L(\overline{G})) = 4$

$\chi_{ir}(L(G)) = \chi_{ir}(L(\overline{G}))$

Observation: 3.4

Number of atoms of NICG	$\chi_{ir}(L(G))$	**Molecular structure name**
4	3	Arsenic chloride ($Ascl_3$)
5	3	Pentaborane (B_5H_9)
6	4	Disulfur tetrafluoride (F_4S_2)
7	3	Dinitrogen pentaoxide (N_2O_5)
8	4	Diborane (B_2H_6)
9	4	Sevoflurane ($C_4H_3F_7O$)
10	4	Arsenic trioxide (As_4O_6)
11	3	Beryllium borohydride ($Be(BH_4)_2$)

4. Conclusion

In this paper , we consider the Line Graph of Neighbourly Irregular Chemical Graph. Further constructing the Irregular Chromatic number for line graph and its Complement graph of NICG.

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