Chapter 5

COLOR ENERGY OF A SEMIGRAPH

5.1 Introduction

In chemical literature graphs are used to represent different chemical objects like molecules, reactions etc. It depicted a chemical system whose vertices are atoms, electrons, molecules, groups of atoms etc. and edges are bound between molecules, bounded and non-bonded interactions, elementary reaction steps etc. Molecular graphs are a special type of chemical graphs in which vertices are considered as individual atoms and edges as chemical bonds between them. Graph energy was first introduced by Serbian chemist and mathematician Ivan Gutman [22] in 1978 to approximate the total π-electron energy of a conjugate hydrocarbon as calculated by the Huckel molecular orbital (HMO) method in quantum chemistry.

Adiga *et al.* [6] introduced the concept of graph coloring, color matrix, and its energy defined as follows:

Let *G* be a vertex-colored graph of order *n*. Then the color matrix of *G* is the matrix $A_c(G) = (a_{ij})_{n\times n}$ for which

$a_{ij}(v_i, v_j)$ = 1 if v_i and v_j are adjacent,

= -1 if v_i and v_j are non-adjacent with $c(v_i) = c(v_j)$,

= 0, otherwise.

Where $c(v_i)$ is the color of the vertex v_i in *G*. The vertices of the graph *G* are colored so that two adjacent vertices always have different colors.

The color energy of a graph *G* with respect to a given coloring is the sum of the absolute values of eigenvalues of the color matrix $A_c(G)$.

Further Joshi and Joseph [34, 35] established some new bounds for the color energy of graphs. Motivated by the above-mentioned works, we got interested to develop the concepts on color energy of semigraphs.

A coloring of a semigraph $G(V,E)$ is an assignment of colors to its vertices, such that not all vertices in an edge are equally colored. A strong coloring of G is a coloring of vertices such that no two adjacent vertices are equally colored, whereas an e-coloring is a coloring of vertices such that no two adjacent end vertices of an edge are equally colored. As r-coloring (r-strong coloring, r-e-coloring) uses r colors, and partitions V into r respective color classes, each class consisting of vertices with the same color. The chromatic number $\chi = \chi(G)$ of G is the minimum number of colors needed in any coloring of G. Similarly, we defined the strong chromatic number $\chi_s = \chi_s(G)$, and the e-chromatic number $\chi_e = \chi_e(G)$ of G. Clearly, a strong coloring is an e-coloring and an e-coloring is a coloring.

5.2 Color matrix and color energy of semigraphs

Definition 5.1 Color matrix and energy of a semigraph

If $G(V,E)$ be a vertex-colored semigraph order n and size m where not all the vertices in an edge are colored equally. Denote by $c(v_i)$ the color of the vertex v_i. Then the color matrix of the semigraph $A_c(G) = (a_{ij})_{n\times n}$ is defined as

$a_{ij}(v_i, v_j)$ = 1 if v_i and v_j are adjacent.

= -1 if v_i and v_j are non-adjacent with $c(v_i) = c(v_j)$.

= 0, otherwise.

If $A_c(G)$ be color matrix of a colored semigraph G. Then its eigenvalues $\xi_1, \xi_2, \ldots, \xi_n$ are called color eigenvalues. The color matrix $A_c(G)$ is symmetric and hence all of color eigenvalues are real. If the distinct color eigenvalues of $A_c(G)$ are $\xi_1 > \xi_2 > \ldots > \xi_r$, $r \le n$ with their multiplicities $m_1, m_2, \ldots, m_r$ then we have

$$Spec_c G = \begin{pmatrix} \xi_1 & \xi_2 & \cdots & \xi_r \\ m_1 & m_2 & \cdots & m_r \end{pmatrix}$$

called the color spectrum of a semigraph. The color energy of semigraph G is defined as $E_c(G) = \sum_{i=1}^{n} |\xi_i|$.

This definition parallels the definition of the ordinary graph energy [22], and also of the color energy of a simple graph [6]. For a symmetric matrix, singular values are same as their eigenvalues. Therefore, the present definition of color energy $E_c(G)$ of semigraph is consistent with the energy of a semigraph [64], as well as with the definition of distance matrix and energy of a semigraph [51].

Example 5.1 $G(V, X)$ be a connected semigraph as shown in **Figure 5.1,** having vertex set $V = \{1,2,3,4,5,6,7,8\}$ with the minimum colors C1, C1, C2, C1, C2, C2, C1 and C2 respectively and edge set $X = \{(1,2,3), (3,4), (4,5,6), (6,7,3), (7,8)\}$.

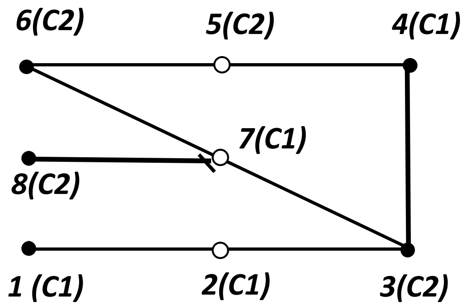

Figure 5.1

Then, color matrix $A_c(G)$ of the semigraph $G(V, X)$ is

$$A_c(G) = \begin{bmatrix} 0 & 1 & 1 & -1 & 0 & 0 & -1 & 0 \\ 1 & 0 & 1 & -1 & 0 & 0 & -1 & 0 \\ 1 & 1 & 0 & 1 & -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 0 & 1 & 1 & -1 & 0 \\ 0 & 0 & -1 & 1 & 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & 1 & 1 & 0 & 1 & -1 \\ -1 & -1 & 1 & -1 & 0 & 1 & 0 & 1 \\ 0 & 0 & -1 & 0 & -1 & -1 & 1 & 0 \end{bmatrix}$$

5.3 Fundamental properties of color energy of semigraphs:

Suppose that $G(V, E)$ is a vertex-colored semigraph of order n, and having m edges. Let $A_c(G)$ be the adjacency matrix with respect to a given coloring of $G(V, E)$. Consider the characteristic polynomial of $A_c(G)$,

$$P_c(G, \xi) = det(\xi I - A_c(G)) = a_0\xi^n + a_1\xi^{n-1} + a_2\xi^{n-2} + \ldots\ldots + a_n.$$

Theorem 5.1 Using the notations given above, we have

(a) $\quad a_0 = 1$

(b) $\quad a_1 = 0$

$(c)\quad \boldsymbol{a_2} = -\sum_{\mathbf{i=1}}^{\mathbf{m}} \binom{|\mathrm{e_i}|}{\mathbf{2}} -$ (Number of pairs of non − adjacent vertices receiving the same color in G)

$(d)\quad a_3 = -2\{$(Number of triangles of G) + (No of triplet of which two adjacent vertices with same color) – (No of triplet of which two non-adjacent vertices with same color) – (Number of non-adjacent triplet having same color in G)$\}$.

Proof: (a) It is clear from the definition of the characteristic polynomial of $A_c(G)$.

i.e. $\quad P_c(G,\xi) = det(\xi I - A_c(G))$, that $a_0 = 1$

(b) Since the diagonal elements of $A_c(G)$ are all zeros, $a_1 = 0$

(c) $(-1)^2 a_2$ = Sum of all the 2×2 principal minors of $A_c(G)$

$$= \sum_{1\le i<j\le n} \begin{vmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{vmatrix} = \sum_{1\le i<j\le n} \left(a_{ii}a_{jj} - a_{ij}a_{ji}\right) = -\sum_{1\le i<j\le n} a^2{}_{ij}$$

$\boldsymbol{i.e.}\quad \boldsymbol{a_2} = -\sum_{\boldsymbol{i=1}}^{\boldsymbol{m}} \binom{|e_i|}{\mathbf{2}} -$ Number of pairs of non − adjacent vertices receiving the same color in G.

(d) $a_3 = (-1)^3$ Sum of all the 3×3 principal minors of $A_c(G)$

$$= (-1)^3 \sum_{1\le i<j<k\le n} \begin{vmatrix} a_{ii} & a_{ij} & a_{ik} \\ a_{ji} & a_{jj} & a_{jk} \\ a_{ki} & a_{kj} & a_{kk} \end{vmatrix} = -2\sum a_{ij}\, a_{jk}\, a_{ki}$$

$= -2\{$(Number of triangles of G) + (No of triplet of which two adjacent vertices with same color) – (No of triplet of which two non-adjacent vertices with same color) – (Number of non-adjacent triplet having same color in G)}

Lemma 5.1 If $\xi_1, \xi_2, \xi_3, \ldots, \xi_n$ are the eigenvalues of the color matrix $A_c(G)$ of a semigraph $G(V,E)$ of order n, having m edges, then

$$\sum_{\boldsymbol{i=1}}^{\boldsymbol{n}} \boldsymbol{\xi_i^2} = \mathbf{2}\left[\sum_{\boldsymbol{i=1}}^{\boldsymbol{m}} \binom{|e_i|}{\mathbf{2}} + \boldsymbol{m'_c}\right]$$

where m'_c is the number of pairs of non-adjacent vertices receiving the same color and $|e_i|$ is the number of vertices in the edge $e_i \in E$.

Proof: Consider

$$\sum_{i=1}^{n} \xi_i^2 = \sum_{i=1}^{n} \left(A_c{}^2\right)_{ii} = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}\, a_{ji}$$

As $A_c(G)$ is a symmetric matrix

$$\sum_{i=1}^{n} \xi_i^2 = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}{}^2$$

$i.e.$

$$= 2\sum_{i<j} \left(a_{ij}\right)^2 + \sum_{i=1}^{n} (a_{ii})^2$$

$$= 2\left[\sum_{i-1}^{m} \binom{|e_i|}{2} + m'_c\right] \qquad Since, \quad \sum_{i=1}^{n} (a_{ii})^2 = 0$$

Lemma 5.2 Let $G(V,E)$ be a colored semigraph having *n* vertices and *m* edges. If $|e_i|$ is the number of vertices in the edge $e_i \in E$, then

$$\left(\sum_{i=1}^{m} \binom{|e_i|}{2} + m'_c\right) \geq m\,.$$

Equality holds when *G* is a graph.

Proof: Clearly, for a connected semigraph, $|e_i| \geq 2$

Thus $\binom{|e_i|}{2} \geq 1$

$i.e.$ $\sum_{i=1}^{m} \binom{|e_i|}{2} \geq m$

Hence $\sum_{i=1}^{m} \binom{|e_i|}{2} + m'_c \geq m$

Lemma 5.3 Let $G(V,E)$ be a connected semigraph having *n* vertices and *m* edges. If $|e_i|$ is the number of vertices in the edge $e_i \in E$, then

$$n \leq 2\sum_{i=1}^{m} \binom{|e_i|}{2}$$

Proof: Clearly

$$n \leq \sum_{i=1}^{n} deg_e\, v_i = \sum_{i=1}^{m} |e_i| \leq 2\sum_{i=1}^{m} \binom{|e_i|}{2}$$

Theorem 5.2 If the energy of a colored semigraph is a rational number, then it must be an even positive integer.

Proof: (Following **Theorem 2.12** in [7])

If $\xi_1, \xi_2, \xi_3, \dots\dots, \xi_n$ are color eigenvalues of $A_c(G)$, the adjacency matrix of a semigraph $G(V, E)$ of order *n* then,

$$Trace\ of\ |A_c(G)| = 0 = \sum_{i=1}^{n} \xi_i$$

of these eigenvalues, $\xi_1, \xi_2, \xi_3, \dots\dots, \xi_r$ are positive and the rest non-positive.
Thus, we have

$$\begin{aligned} E_c(G) &= \sum_{i=1}^{n} |\xi_i| \\ &= (\xi_1 + \xi_2 + \dots\dots + \xi_r) - (\xi_{r+1} + \xi_{r+2} + \dots\dots + \xi_n) \\ &= 2(\xi_1 + \xi_2 + \dots\dots + \xi_r) \end{aligned}$$

The sum $\xi_1 + \xi_2 + \xi_3 + \dots + \xi_r$ is an algebraic integer as ξ_1, ξ_2, $\xi_3, \dots, \xi_r$ are algebraic integers. Hence $2(\xi_1 + \xi_2 + \dots + \xi_r)$ must be an even positive integer if $E_c(G)$ is rational.

5.4 Bounds for color energy of a semigraph:

Theorem 5.3 Let $G(V, E)$ be a colored semigraph having *n* vertices and *m* edges. Then

$$E_c(G) \leq \sqrt{2n\left(\sum_{i=1}^{m} \binom{|e_i|}{2} + m'_c\right)}$$

where m'_c is the number of pairs of non-adjacent vertices in *G* receiving the same color.

Proof: The color matrix of a semigraph $A_c(G)$ is symmetric and hence its color eigenvalues are real and can be ordered as $\xi_1 \geq \xi_2 \geq \xi_3 \geq \dots \geq \xi_n$. Appling the Cauchy-Schwarz inequality, we have

$$\left(\sum_{i=1}^{n} u_i v_i\right)^2 \leq \left(\sum_{i=1}^{n} u_i\right)^2 \left(\sum_{i=1}^{n} v_i\right)^2$$

Substituting $u_i = 1$, $v_i = |\xi_i|$ in the above inequality and by **Lemma 5.1**, we have

$$[E_c(G)]^2 = \left(\sum_{i=1}^{n} |\xi_i|\right)^2 \leq n\left(\sum_{i=1}^{n} |\xi_i|^2\right) = n\sum_{i=1}^{n} \xi_i^2 = 2n\left(\sum_{i=1}^{m} \binom{|e_i|}{2} + m'_c\right)$$

Hence,
$$E_c(G) \leq \sqrt{2n\left(\sum_{i=1}^{m} \binom{|e_i|}{2} + m'_c\right)}.$$

Theorem 5.4 Let $G(V,E)$ be a colored semigraph having *n* vertices and *m* edges, and let m'_c be the number of pairs of non-adjacent vertices receiving the same color. Then

$$E_c(G) \geq \sqrt{2\left(\sum_{i=1}^{m} \binom{|e_i|}{2} + m'_c\right) + n(n-1)\Delta^{2/n}} \qquad where\ \ \Delta = |detA_c(G)|.$$

Proof: In view of **Definition 5.1** and **Lemma 5.1** we have,

$$[E_c(G)]^2 = \left(\sum_{i=1}^{n} |\xi_i|\right)^2$$

$$= \sum_{i=1}^{n} \xi_i^2 + \sum_{i \neq j} |\xi_i|\,|\xi_j|$$

By applying $AM \geq GM$, we have

$$\frac{1}{n(n-1)}\sum_{i \neq j} |\xi_i|\,|\xi_j| \geq \left(\prod_{i \neq j} |\xi_i||\xi_j|\right)^{1/n(n-1)}$$

$$= \left(\prod_{i \neq j} |\xi_i|^{2(n-1)}\right)^{1/n(n-1)}$$

$$= \left(\prod_{i \neq j} |\xi_i|\right)^{2/n}$$

$$= \Delta^{2/n}$$

$$i.e. \qquad \sum_{i\neq j} |\xi_i|\,|\xi_j| \geq n(n-1)\Delta^{2/n}$$

Thus, $$[E_c(G)]^2 \geq \sum_{i=1}^{n} \xi_i^2 + n(n-1)\Delta^{2/n}$$

$$= 2\left(\sum_{i=1}^{m} \binom{|e_i|}{2} + m'_c\right) + n(n-1)\Delta^{2/n}$$

Therefore $$E_c(G) \geq \sqrt{2\left(\sum_{i=1}^{m} \binom{|e_i|}{2} + m'_c\right) + n(n-1)\Delta^{2/n}}$$

Theorem 5.5 Let $G(V,E)$ be a colored semigraph of order *n* and size *m*. Let the color eigenvalues of $A_c(G)$ be $\xi_1 \geq \xi_2 \geq \xi_3 \geq \ldots\ldots \geq \xi_n$. Then

$$E_c(G) \leq |\xi_1| + \sqrt{(n-1)\left[2\left(\sum_{i=1}^{m} \binom{|e_i|}{2} + m'_c\right) - \xi_1^2\right]}$$

where m'_c is the number of pairs of non-adjacent vertices in *G* receiving the same color.

Proof: Let $\xi_1 \geq \xi_2 \geq \xi_3 \geq \ldots\ldots \geq \xi_n$ be the color eigenvalues of $A_C(G)$. Appling the Cauchy-Schwarz inequality on to vectors $(|\xi_2|, |\xi_3|, \ldots, |\xi_n|)$ and $(1,1,\ldots,1)$ with $n-1$ entries,

$$\left(\sum_{i=2}^{n} |\xi_i|\right)^2 \leq (n-1)\left(\sum_{i=2}^{n} |\xi_i|^2\right)$$

i. e. $$\left(\sum_{i=2}^{n} |\xi_i|\right) \leq \sqrt{(n-1)\left(\sum_{i=2}^{n} |\xi_i|^2\right)}$$

i. e. $$\sum_{i=1}^{n} |\xi_i| - |\xi_1| \leq \sqrt{(n-1)\left(\sum_{i=2}^{n} {\xi_i}^2\right)}$$

By **Definition 5.1** and **Lemma 5.1.,** we have

$$E_c(G) \le |\xi_1| + \sqrt{(n-1)\left[2\left(\sum_{i=1}^{m}\binom{|e_i|}{2} + m'_c\right) - \xi_1^2\right]}$$

Theorem 5.6 Let $G(V, E)$ be a colored semigraph of order *n* and size m. Let ξ_{max} be the largest absolute value of a color eigenvalue. Then

$$\boldsymbol{E_c(G)} \ge \frac{2\left[\sum_{i=1}^{m}\binom{|e_i|}{2} + m'_c\right]}{\xi_{max}}$$

where m'_c is the number of pairs of non-adjacent vertices in *G* receiving the same color.

Proof: Let ξ_{max} be the largest absolute value of the color eigenvalue of $A_c(G)$. Then

$$\xi_{max}|\xi_i| \ge \xi_i^2$$

Thus,

$$\sum_{i=1}^{n} \xi_{max}|\xi_i| \ge \sum_{i=1}^{n} \xi_i^2$$

By **Lemma 5.1** we get,

$$\xi_{max}\sum_{i=1}^{n}|\xi_i| \ge 2\left[\sum_{i=1}^{m}\binom{|e_i|}{2} + m'_c\right]$$

Hence,

$$\boldsymbol{E_c(G)} \ge \frac{2\left[\sum_{i=1}^{m}\binom{|e_i|}{2} + m'_c\right]}{\xi_{max}}$$

Theorem 5.7 Let $G(V, E)$ be a colored semigraph of order *n*, size *m*, and m'_c be the number of pairs of non-adjacent vertices in *G* receiving the same color. Then

$$2\sqrt{\left(\sum_{i=1}^{m}\binom{|e_i|}{2} + m'_c\right)} \le E_c(G) \le 2\left(\sum_{i=1}^{m}\binom{|e_i|}{2} + m'_c\right)$$

Proof: Consider

$$[E_c(G)]^2 = \left(\sum_{i=1}^{n}|\xi_i|\right)^2$$

$$= \sum_{i=1}^{n} |\xi_i|^2 + \sum_{i \neq j} |\xi_i| \, |\xi_j|$$

$$= \sum_{i=1}^{n} |\xi_i|^2 + 2 \sum_{i<j} |\xi_i| \, |\xi_j| \qquad (5.1)$$

By **Lemma 4.3** we have,

$a_2 = (-1)^2 \times$ Sum of all the 2×2 principal minors of $A_c(G)$

$$= \sum_{1 \leq i<j \leq n} \xi_i \xi_j$$

Therefore,

$$\sum_{1 \leq i<j \leq n} \xi_i \xi_j = \sum_{1 \leq i<j \leq n} \begin{vmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{vmatrix}$$

$$= \sum_{1 \leq i<j \leq n} \left(a_{ii} a_{jj} - a_{ij} a_{ji} \right)$$

As color matrix $A_c(G)$ is symmetric, $a_{ij} = a_{ji}$ and $a_{ii} = 0 \ \ \forall \, i$ Thus,

$$\sum_{1 \leq i<j \leq n} \xi_i \xi_j = - \sum_{1 \leq i<j \leq n} a_{ij} a_{ji} = - \sum_{1 \leq i<j \leq n} \left(a_{ij} \right)^2$$

$$= - \left[\sum_{i=1}^{m} \binom{|e_i|}{2} + m'_c \right]$$

We know that,

$$\sum_{i<j} |\xi_i| \, |\xi_j| \geq | \sum_{i<j} \xi_i \xi_j |$$

Thus

$$\sum_{i<j} |\xi_i| \, |\xi_j| \geq | \sum_{i=1}^{m} \binom{|e_i|}{2} + m'_c | \qquad (5.2)$$

Using equation (5.1) and (5.2) and **Lemma 5.1**, we get

$$[E_c(G)]^2 \geq 4 | \sum_{i=1}^{m} \binom{|e_i|}{2} + m'_c |$$

Taking positive square-root, we get

$$E_c(G) \geq 2 \sqrt{\sum_{i=1}^{m} \binom{|e_i|}{2} + m'_c} \qquad (5.3)$$

By **Lemma 5.3** we have,

$$\boldsymbol{n} \le \mathbf{2}\sum_{i=1}^{m}\binom{|e_i|}{\mathbf{2}} \le \mathbf{2}\left[\sum_{i=1}^{m}\binom{|e_i|}{\mathbf{2}} + \boldsymbol{m}'_{\boldsymbol{c}}\right]$$

Thus
$$2\boldsymbol{n}\left[\sum_{i=1}^{m}\binom{|e_i|}{\mathbf{2}} + \boldsymbol{m}'_{\boldsymbol{c}}\right] \le \mathbf{4}\left[\sum_{i=1}^{m}\binom{|e_i|}{\mathbf{2}} + \boldsymbol{m}'_{\boldsymbol{c}}\right]^{2}$$

Taking positive square-root, we get

$$\sqrt{\mathbf{2}\boldsymbol{n}\left[\sum_{i=1}^{m}\binom{|e_i|}{\mathbf{2}} + \boldsymbol{m}'\right]} \le \mathbf{2}\left[\sum_{i=1}^{m}\binom{|e_i|}{\mathbf{2}} + \boldsymbol{m}'_{\boldsymbol{c}}\right]$$

Thus by using **Theorem 5.3**

$$\boldsymbol{E_c}(\boldsymbol{G}) \le \mathbf{2}\left[\sum_{i=1}^{m}\binom{|e_i|}{\mathbf{2}} + \boldsymbol{m}'_{\boldsymbol{c}}\right] \qquad (\mathbf{5.4})$$

Hence, from (5.3) and (5.4) we have

$$\mathbf{2}\sqrt{\sum_{i=1}^{m}\binom{|e_i|}{\mathbf{2}} + \boldsymbol{m}'_{\boldsymbol{c}}} \le \boldsymbol{E}_c(\boldsymbol{G}) \le \mathbf{2}\left[\sum_{i=1}^{m}\binom{|e_i|}{\mathbf{2}} + \boldsymbol{m}'_{\boldsymbol{c}}\right]$$

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