$\mathbf{RANDI}\acute{C}$ TYPE HADI ENERGY OF A GRAPH

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Abstract: Randić index is one of the most famous topological graph indices. The energy of a graph was defined more than four decades ago for its molecular applications. The classical energy of a graph modelling a molecule is defined as the sum of absolute values of all the eigenvalues of the adjacency matrix corresponding to the modelling graph. There are several other versions of the energy notion obtained using other types of graph matrices. In this paper, we are introducing and investigating the Randić type hadi energy RHE(G) of a graph G, determine several properties of it and calculate RHE(G) for several interesting graphs.

Key Words: Randić type hadi index, Randić type hadi eigenvalues, Randić type hadi energy, k-complement, splitting graph

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1. INTRODUCTION

SIGNIFICANCE OF THE WORK

Graph energy is one of the popular and important research areas in graph theory due to its applications. Frequently used energy types are the adjacency, incidency and Laplacian energy. In this work, the Randić type Hadi energy is introduced and some results are obtained. Some bounds on eigenvalues are obtained and the Randić type Hadi energy is calculated for several graph classes.

2. INTRODUCTION

Let G be a simple graph and let $\{v_1, v_2, \dots, v_n\}$ be the set of its vertices. Let $i, j \in \{1, 2, \dots, n\}$. If two vertices v_i and v_j of G are adjacent, then we use the notation

 $v_i \sim v_j$. For a vertex $v_i \in V(G)$, the degree of v_i will be denoted by $d(v_i)$ or briefly by d_i .

Energy of a graph is used to approximate the total π -electron energy of the molecule. For some studies on energy, see [1, 3, 4, 6, 7, 9, 11]. Conjugated hydrocarbons can be represented by means of a graph called as molecular graph. We can represent the atoms by vertices and the edges between the atoms by edges to form the molecular graph. Topological indices are numerical quantities which are very significant in QSPR and QSAR studies in chemistry. Many physical properties and chemical reactivity can be predicted by these molecular descriptors. There is a large number of topological indices such as Randić index [8], sum-connectivity index, atom bond connectivity index, Zagreb indices, etc. One of those numerical descriptors, the Randić type hadi index of a graph G is proven to be the best predictor of density and of molar volume for octane isomers. It is defined by

$$\sum_{i \sim j} \frac{1}{2^{d_i + d_j}}.$$

The concept of the Randić type hadi index motivates one to associate a symmetric square matrix RH(G) to a graph G. The Randić type hadi matrix $RH(G) = (S_{ij})_{n \times n}$ is, by this reason, defined as

$$S_{ij} = \begin{cases} \frac{1}{2^{d_i + d_j}} & \text{if } v_i \sim v_j, \\ 0 & otherwise. \end{cases}$$

3. The Randić type hadi energy of a graph

Let G be a simple, finite, undirected graph. The classical energy E(G) is defined as the sum of the absolute values of the eigenvalues of its adjacency matrix. For more details on energy of a graph, see [3, 4].

Let RH(G) be the Randić type hadi matrix. The characteristic polynomial of RH(G)will be denoted by $\phi_{RH}(G, \lambda)$ and defined as

$$\phi_{RH}(G,\lambda) = det(\lambda I - RH(G)).$$

Since the Randić type hadi matrix is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The Randić type hadi energy of G is similarly defined by

(3.1)
$$RHE(G) = \sum_{i=1}^{n} |\lambda_i|.$$

This paper is organized as follows: In Section 3, we give some basic properties of Randić type hadi energy of a graph. In Section 4, Randić type hadi energy of some standard graphs are obtained. In Section 5, we find Randić type hadi energy of some complements of some specific graphs. In Section 6, the Randić type hadi energy for splitting graphs are calculated.

Let us define a number ${\cal H}$ as

$$H = \sum_{i < j} \left(\frac{1}{2^{d_i + d_j}} \right)^2.$$

Then we can calculate the first three coefficients of the Randi \dot{c} type hadi characteristic polynomial:

Proposition 4.1. The first three coefficients of the Randić type hadi polynomial $\phi_{RH}(G, \lambda)$ are as follows:

(*i*) $a_0 = 1$, (*ii*) $a_1 = 0$,

(*iii*) $a_2 = -H$.

Proof. (i) By the definition of $\phi_{RH}(G,\lambda) = det[\lambda I - RH(G)]$, we get $a_0 = 1$.

(ii) The sum of the determinants of all 1×1 principal submatrices of RH(G) is equal to the trace of RH(G) implying that

$$a_1 = (-1)^1 \times \text{the trace of } RH(G)$$

= 0.

(iii) By the definition, we have

$$(-1)^{2}a_{2} = \sum_{1 \leq i < j \leq n} a_{ii}a_{jj} - a_{ji}a_{ij}$$
$$= \sum_{1 \leq i < j \leq n} a_{ii}a_{jj} - \sum_{1 \leq i < j \leq n} a_{ji}a_{ij}$$
$$= -H.$$

Proposition 4.2. If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the Randić type hadi eigenvalues of RH(G), then

$$\sum_{i=1}^{n} \lambda_i^2 = 2H.$$

Proof. It follows as

$$\sum_{i=1}^{n} \lambda_{i}^{2} = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} a_{ji}$$
$$= 2 \sum_{i < j} a_{ij}^{2} + \sum_{i=1}^{n} a_{ii}^{2}$$
$$= 2 \sum_{i < j} a_{ij}^{2}$$
$$= 2H.$$

Using this result, we now obtain lower and upper bounds for the Randić type hadi energy of a graph:

Theorem 4.1. Let G be a graph with n vertices. Then

 $RHE(G) \le \sqrt{2nH}.$

Proof. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of RH(G). By the Cauchy-Schwartz inequality, we have

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \le \left(\sum_{i=1}^{n} a_i^2\right) \left(\sum_{i=1}^{n} b_i^2\right).$$

Let $a_i = 1, b_i = |\lambda_i|$. Then

$$\left(\sum_{i=1}^{n} |\lambda_i|\right)^2 \le \sum_{i=1}^{n} 1 \sum_{i=1}^{n} |\lambda_i|^2$$

implying that

$$[RHE(G)]^2 \le n \cdot 2H$$

and hence we get

$$[RHE(G)] \le \sqrt{2nH}$$

as an upper bound.

Next we give a lower bound for RHE(G):

Theorem 4.2. Let G be a graph with n vertices. If $R = \det RH(G)$, then

$$RHE(G) \ge \sqrt{2H + n(n-1)R^{\frac{2}{n}}}.$$

Proof. By definition, we have

$$(RHE(G))^{2} = \left(\sum_{i=1}^{n} |\lambda_{i}|\right)^{2}$$
$$= \sum_{i=1}^{n} |\lambda_{i}| \sum_{j=1}^{n} |\lambda_{j}|$$
$$= \sum_{i=1}^{n} |\lambda_{i}|^{2} + \sum_{i \neq j} |\lambda_{i}|| \lambda_{j}|.$$

Using arithmetic-geometric mean inequality, we have

$$\frac{1}{n(n-1)}\sum_{i\neq j}|\lambda_i||\lambda_j| \geq \left(\prod_{i\neq j}|\lambda_i||\lambda_j|\right)^{\frac{1}{n(n-1)}}.$$

Therefore,

$$[RH(G)]^{2} \geq \sum_{i=1}^{n} |\lambda_{i}|^{2} + n(n-1) \left(\prod_{i \neq j} |\lambda_{i}| |\lambda_{j}|\right)^{\frac{1}{n(n-1)}}$$

$$\geq \sum_{i=1}^{n} |\lambda_{i}|^{2} + n(n-1) \left(\prod_{i=1}^{n} |\lambda_{i}|^{2(n-1)}\right)^{\frac{1}{n(n-1)}}$$

$$= \sum_{i=1}^{n} |\lambda_{i}|^{2} + n(n-1)R^{\frac{2}{n}}$$

$$= 2H + n(n-1)R^{\frac{2}{n}}.$$

Thus,

$$RHE(G) \ge \sqrt{2H + n(n-1)R^{\frac{2}{n}}}.$$

Let λ_n and λ_1 be the minimum and maximum values of all $\lambda'_i s$, respectively. Then the following results can easily be proven by means of the above results:

Theorem 4.3. For a graph G of order n, we have

$$RHE(G) \ge \sqrt{2nH - \frac{n^2}{4}(\lambda_1 - \lambda_n)^2}$$

Theorem 4.4. For a graph G of order n with non-zero eigenvalues, we have

$$RHE(G) \ge \frac{2\sqrt{2n\lambda_1\lambda_nH}}{(\lambda_1 + \lambda_n)^2}.$$

Theorem 4.5. Let G be a graph of order n. Let $\lambda_1 \ge \lambda_2 \ge \lambda_3 \ge \cdots \ge \lambda_n$ be the eigenvalues in increasing order. Then

$$RHE(G) \ge \frac{|\lambda_1||\lambda_n|n+2H}{|\lambda_1|+|\lambda_n|}.$$

Theorem 4.6. For a graph G, $RHE(G) = \frac{E(\hat{G})}{2^n}$ in which \hat{G} is the bipartite graph with adjacency matrix

$$\left(\begin{array}{cc} 0 & RH(G) \\ RH(G)^T & 0 \end{array}\right).$$

5. Randić type hadi energy of some standard graphs

In this section, we obtain the Randić type hadi energy for some standard graphs such as complete graph, star graph, crown graph, cocktail party graph, double star graph and complete bipartite graph.

Theorem 5.1. The Randić type hadi energy of a complete graph K_n is

$$RHE(K_n) = 2^{3-2n}(n-1).$$

Proof. Let K_n be the complete graph with vertex set $V = \{v_1, v_2, \dots, v_n\}$. The Randić type hadi matrix is

$$RH(K_n) = \left(\begin{array}{c} \frac{1}{2^{2(n-1)}} (J-I) \end{array} \right).$$

Then the characteristic equation is

$$\left(\lambda + \frac{1}{2^{2(n-1)}}\right)^{n-1} \left(\lambda - \frac{2(n-1)}{2^{2(n-1)}}\right) = 0$$

and the spectrum is $Spec_{RH}(K_n) = \left(\begin{array}{cc} \frac{1}{2^{2(n-1)}} & \frac{2(n-1)}{2^{2(n-1)}}\\ n-1 & 1 \end{array}\right)$. Therefore, $RHE(K_n) = 2^{3-2n}(n-1)$.
1).

Theorem 5.2. The Randić type hadi energy of the star graph $K_{1,n-1}$ is

$$RHE(K_{1,n-1}) = \frac{\sqrt{n-1}}{2^{n-1}}.$$

Proof. Let $K_{1,n-1}$ be the star graph with vertex set $V = \{v_0, v_1, \dots, v_{n-1}\}$ with v_0 denoting the central vertex. The Randić type hadi matrix is

$$RH(K_{1,n-1}) = \frac{1}{2^n} \begin{pmatrix} 0_{1\times 1} & J_{1\times n-1} \\ J_{n-1\times 1} & 0_{n-1\times n-1} \end{pmatrix}.$$

Clearly, the characteristic equation is $\lambda^{n-2}(\lambda + \frac{\sqrt{n-1}}{2^n})(\lambda - \frac{\sqrt{n-1}}{2^n}) = 0$. Therefore, the spectrum would be

$$Spec_{RH}(K_{1,n-1}) = \begin{pmatrix} \frac{\sqrt{n-1}}{2^n} & \frac{-\sqrt{n-1}}{2^n} & 0\\ 1 & 1 & n-2 \end{pmatrix}.$$

Therefore,

$$RHE(K_{1,n-1}) = \frac{\sqrt{n-1}}{2^{n-1}}.$$

Theorem 5.3. The Randić type hadi energy of the cycle graph C_{2n} is

$$RHE(C_{2n}) = \frac{1}{4} + \frac{1}{8} \sum_{m=1, m \neq n}^{2n-1} |\cos \frac{\pi m}{n}|.$$

Proof. The Randić type hadi matrix corresponding to the cycle graph C_{2n} is a circulant matrix of order 2n. Its eigenvalues are

(5.1)
$$\lambda_m = \begin{cases} \frac{1}{8}, & \text{for } m = 0\\ -\frac{1}{8}, & \text{for } m = n\\ \frac{1}{8}\cos\frac{\pi m}{n}, & \text{for } 0 < m < n, \ n < m \le 2n - 1. \end{cases}$$

Therefore the Randić type hadi energy is

$$SDD(C_{2n}) = |-\frac{1}{8}| + |\frac{1}{8}| + \sum_{m=1, m \neq n}^{2n-1} |\frac{1}{8} \cos \frac{\pi m}{n}|$$

and finally we get

$$SDDE(C_{2n}) = \frac{1}{4} + \frac{1}{8} \sum_{m=1, m \neq n}^{2n-1} |\cos \frac{\pi m}{n}|.$$

Theorem 5.4. The Randić type hadi energy of the crown graph S_n^0 is

$$RHE(S_n^0) = 2^{4-2n}(n-1).$$

Proof. Let S_n^0 be the crown graph of order 2n with vertex set $\{u_1, u_2, \cdots, u_n, v_1, v_2, \cdots, v_n\}$. The Randić type hadi matrix is

$$RHE(S_n^0) = \frac{1}{2^{2(n-1)}} \left(\begin{array}{cc} 0_{n \times n} & (J-I)_{n \times n} \\ (J-I)_{n \times n} & 0_{n \times n} \end{array} \right).$$

Hence the characteristic equation is

$$\left(\lambda - \frac{1}{2^{2(n-1)}}\right)^{n-1} \left(\lambda + \frac{1}{2^{2(n-1)}}\right)^{n-1} \left(\lambda + \frac{n-1}{2^{2(n-1)}}\right) \left(\lambda - \frac{n-1}{2^{2(n-1)}}\right) = 0$$

and therefore, the spectrum is $Spec_{RH}(S_n^0) = \begin{pmatrix} \frac{n-1}{2^{2(n-1)}} & -\frac{n-1}{2^{2(n-1)}} & -\frac{1}{2^{2(n-1)}} \\ 1 & 1 & n-1 & n-1 \end{pmatrix}$. Therefore we get the result.

Theorem 5.5. The Randić type hadi energy of the double star graph $S_{n,n}$ is

$$RHE(S_{n,n}) = \frac{\sqrt{1 + (n-1)2^{2n}}}{2^{2n-1}}.$$

Proof. The characteristic equation is obtained in a classical way as

$$(\lambda)^{2n-4} \left(\lambda^2 + \frac{1}{2^{2n}}\lambda - \frac{n-1}{2^{2n+2}}\right) \left(\lambda^2 - \frac{1}{2^{2n}}\lambda - \frac{n-1}{2^{2n+2}}\right) = 0.$$

Hence, the spectrum is

$$\begin{pmatrix} 0 & \frac{1+\sqrt{1+(n-1)2^{2n}}}{2^{2n+1}} & \frac{-1+\sqrt{1+(n-1)2^{2n}}}{2^{2n+1}} & \frac{-1-\sqrt{1+(n-1)2^{2n}}}{2^{2n+1}} & \frac{1-\sqrt{1+(n-1)2^{2n}}}{2^{2n+1}} \\ 2n-4 & 1 & 1 & 1 & 1 \end{pmatrix}.$$

Therefore the result is obtained.

Theorem 5.6. The Randić type hadi energy of the cocktail party graph $K_{n\times 2}$ is

$$RHE(K_{n \times 2}) = 2^{6-4n}(n-1).$$

Proof. Let $K_{n\times 2}$ be the cocktail party graph of order 2n. Let the vertex set of it be $\{u_1, u_2, \dots, u_n, v_1, v_2, \dots, v_n\}$. The Randić type hadi matrix is

$$RH(K_{n\times 2}) = \frac{1}{2^{4(n-1)}} \left(\begin{array}{cc} (J-I)_{n\times n} & (J-I)_{n\times n} \\ (J-I)_{n\times n} & (J-I)_{n\times n} \end{array} \right)$$

giving the characteristic equation as

$$\lambda^{n}(\lambda + 2^{-(4n-5)})^{n-1}(\lambda - 2^{-(4n-5)}(n-1)) = 0$$

Hence the spectrum is

$$Spec_{RH}(K_{n\times 2}) = \begin{pmatrix} 2^{-(4n-5)}(n-1) & 0 & -2^{-(4n-5)} \\ 1 & n & n-1 \end{pmatrix}.$$

Therefore the result follows.

Theorem 5.7. The Randić type hadi energy of the complete bipartite graph $K_{m,n}$ is

$$RHE(K_{m,n}) = 2\frac{\sqrt{mn}}{2^{m+n}}.$$

Proof. $RH(K_{m,n}) = RH(K_{m,n}) = \frac{1}{2^{m+n}} \begin{pmatrix} 0_{m \times m} & J_{m \times n} \\ J_{n \times m} & 0_{n \times n} \end{pmatrix}$. Hence the characteristic equation will be

$$\lambda^{m+n-2} \left(\lambda + \frac{\sqrt{mn}}{2^{m+n}} \right) \left(\lambda - \frac{\sqrt{mn}}{2^{m+n}} \right) = 0$$

giving the spectrum as

$$Spec_{RH}(K_{m,n}) = \begin{pmatrix} 0 & \frac{\sqrt{mn}}{2^{m+n}} & -\frac{\sqrt{mn}}{2^{m+n}} \\ m+n-2 & 1 & 1 \end{pmatrix}.$$

This gives the result.

6. Randić type hadi energy of complements

In this section we calculated the energy for some complements and k-complements.

Definition 6.1. [10] Let G be a graph and $P_k = \{V_1, V_2, \dots, V_k\}$ be a partition of its vertex set V. Then the k-complement of G is obtained as follows: For all V_i and V_j in P_k , $i \neq j$, remove the edges between V_i and V_j and add the edges between the vertices of V_i and V_j which are not in G. It is denoted by $\overline{(G)_k}$.

Theorem 6.1. The Randić type hadi energy of the complement $\overline{K_n}$ of the complete graph K_n is

$$RHE(\overline{K_n}) = 0.$$

Proof. Let K_n be the complete graph with vertex set $V = \{v_1, v_2, \dots, v_n\}$. The Randić type hadi matrix of the complement of the complete graph K_n is

$$RHI(\overline{K_n}) = \left(\begin{array}{c} 0_{n \times n} \end{array} \right).$$

Hence the characteristic equation is $\lambda^n = 0$. Therefore, $RHE(\overline{K_n}) = 0$.

Theorem 6.2. The Randić type hadi energy of the complement $\overline{K_{1,n-1}}$ of the star graph $K_{1,n-1}$ is

$$RHE(\overline{K_{1,n-1}}) = \frac{2n-4}{2^{(2n-4)}}.$$

Proof. Let $\overline{(K_{1,n-1})}$ be the complement of the star graph with vertex set $V = \{v_0, v_1, \cdots, v_{n-1}\}$. The Randić type hadi matrix is

$$RH(\overline{K_{1,n-1}}) = \begin{pmatrix} 0_{n-1\times 1} & 0_{1\times n-1} \\ 0 & \frac{1}{2^{2n-4}}(J-I)_{n-1\times n-1} \end{pmatrix}.$$

Hence the characteristic equation would be

$$\lambda^{1} \left(\lambda - \frac{n-2}{2}\right)^{n-2} \left(\lambda - \frac{(n-2)^{2}}{2}\right) = 0$$

implying that the spectrum is $Spec_{RH}\overline{K_{1,n-1}} = \begin{pmatrix} \frac{n-2}{2^{(2n-4)}} & 0 & \frac{1}{2^{(2n-4)}} \\ 1 & 1 & n-2 \end{pmatrix}$. Therefore,

$$RHE(\overline{K_{1,n-1}}) = \frac{2n-4}{2^{(2n-4)}}.$$

Theorem 6.3. The Randić type hadi energy of the complement $\overline{K_{n\times 2}}$ of the cocktail party graph $K_{n\times 2}$ of order 2n is

$$RHE\overline{(K_{n\times 2})} = \frac{n}{2}.$$

Proof. Let $\overline{K_{n\times 2}}$ be the complement of the cocktail party graph of order 2n with vertex set $\{u_1, u_2, \dots, u_n, v_1, v_2, \dots, v_n\}$. The Randić type hadi matrix is

$$RH(\overline{K_{n\times 2}}) = \begin{pmatrix} 0_{n\times n} & \frac{1}{4}I_{n\times n} \\ \frac{1}{4}I_{n\times n} & 0_{n\times n} \end{pmatrix}.$$

Hence the characteristic equation would be

$$(\lambda + \frac{1}{4})^n (\lambda - \frac{1}{4})^n = 0$$

Hence, the spectrum is $Spec_{RH}(K_{n\times 2}) = \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \\ n & n \end{pmatrix}$. The result then follows. \Box

Theorem 6.4. The Randić type hadi energy of the 2-complement of the cocktail party graph $K_{n\times 2}$ is

$$RHE(\overline{(K_{n\times 2})_{(2)}}) = \frac{n-1}{2^{2(n-1)}}$$

Proof. Consider the 2-complement of the cocktail party graph $\overline{(K_{n\times 2})_{(2)}}$. The corresponding matrix is

$$RH(\overline{(K_{n\times 2})_{(2)}}) = \frac{1}{2^{2n}} \begin{pmatrix} (J-I)_{n\times n} & (J-I)_{n\times n} \\ (J-I)_{n\times n} & (J-I)_{n\times n} \end{pmatrix}.$$

Hence the characteristic polynomial will be $\lambda^{n-1} \left(\lambda + \frac{1}{2^{2n-1}}\right)^{n-1} \left(\lambda - \frac{n-2}{2^{2n}}\right) \left(\lambda - \frac{n}{2^{2n}}\right) = 0.$ Randić type hadi spectra is

$$Spec(\overline{(K_{n\times 2})_{(2)}}) = \begin{pmatrix} 0 & \frac{n-2}{2^{2n}} & \frac{n}{2^{2n}} & -\frac{1}{2^{2n-1}} \\ n-1 & 1 & 1 & n-1 \end{pmatrix}$$

The result then follows.

7. Randić type hadi energy of splitting graphs

Derived graphs are graphs obtained from a graph according to some rule. They are useful in finding some property of a graph in an indirect way. Some examples of derived graphs are studied in [2, 5, 7]. Recall that the splitting graph Sp(G) of a graph G is obtained by adding a new vertex u_i for each vertex v_i such that u_i is adjacent to every vertex that is adjacent to v_i in G. In Fig. 1, we see the splitting graph of the cycle graph C_3 .



Figure 1 The splitting graph $Sp(C_3)$

Now we give the relation between the Randić type hadi energy of the splitting graph of the cycle graphs and the Randić type hadi energy of the cycle graphs:

Theorem 7.1. $RHE[Sp(C_n)] = 1.988[RHE(C_n)].$

Proof. By direct comparison of Randić type hadi energies of the C_n and $Sp(C_n)$, one can easily get the required relation.

Finally, we determine the relation between the Randić type hadi energy of the splitting graph of the complete graphs and the Randić type hadi energy of the complete graphs:

Theorem 7.2. $RHE[Sp(K_n)] = 2^{n-2}[RHE(K_n)].$

Proof. The Randić type hadi matrix for $Sp(K_n)$ is

$$RH(Sp(K_n)) = \frac{1}{2^{2(n-1)}} \begin{pmatrix} \frac{1}{2^{4n-4}}(J-I)_{n \times n} & \frac{1}{2^{3n-3}}(J-I)_{n \times n} \\ \frac{1}{2^{4n-4}}(J-I)_{n \times n} & 0_{n \times n} \end{pmatrix}$$

By direct comparison of Randić type hadi energies of the K_n and $Sp(K_n)$, one can easily get the required relation.

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