

Computation of Misbalance Type Degree Indices of Certain Classes of Derived-Regular Graph

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Abstract: A topological index can be considered as transformation of chemical structure into real number which can be used for correlation with Physical properties in Quantitative Structure Activity Relationship (*QSAR*) and Quantitative Structure Property Relationship (*QSPR*) studies. Adriatic indices are part of topological indices they were scrutinized on the testing sets provided by the International Academy of Mathematical Chemistry (*IAMC*) and it has been shown that they have good predictive properties in many cases. In this article, we compute some Adriatic indices of certain classes of derived-regular graph.

Key Words: Topological indices, line graph, subdivision graph, edge-semi total graph, vertex-semi total graph, Smarandachely vertex-semi total graph, Smarandachely edge-semi total graph, total graph, jump graph and para-line graph.

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§1. Introduction

A molecular graph is a graph in which the vertices correspond to the atoms and the edges to the bonds of a molecule. A single number that can be computed from the molecular graph, and used to characterize some property of the underlying molecule is said to be a topological index or molecular structure descriptor. Numerous such descriptors have been considered in theoretical chemistry, and have found application in various areas of chemistry, physics, mathematics, informatics, biology. Recently [17], D. Vukicevic revealed the set of 148 discrete Adriatic indices. They ever analyzed on the testing sets provided by the International Academy of Mathematical Chemistry and it had been shown that they have good predictive properties in many cases.

The graphs considered here are finite, undirected, without loops and multiple edges. Let $G = (V, E)$ be a connected graph with $|V(G)| = n$ vertices and $|E(G)| = m$ edges. The degree d_u of a vertex u is the number of vertices adjacent to u . The edge connecting the vertices u

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and v will be denoted by uv . For other definitions and notations, the reader may refer to [3].

Definitions 1.1 Let $\alpha_m(G)$ be the misbalance type index where $m \in \{-\frac{1}{2}, \frac{1}{2}, -1, 1\}$, then it is defined as

$$\alpha_m(G) = \sum_{uv \in E(G)} |d_u^m - d_v^m|. \quad (1)$$

Now,

- The $m = -\frac{1}{2}$ corresponds to misbalnce irdeg index is defined as

$$\alpha_{-\frac{1}{2}}(G) = \sum_{uv \in E(G)} \left| \frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_v}} \right|. \quad (2)$$

- The $m = \frac{1}{2}$ corresponds to misbalnce rodeg index is defined by

$$\alpha_{\frac{1}{2}}(G) = \sum_{uv \in E(G)} \left| \sqrt{d_u} - \sqrt{d_v} \right|. \quad (3)$$

- The $m = -1$ corresponds to misbalnce indeg index is defined to be

$$\alpha_{-1}(G) = \sum_{uv \in E(G)} |d_u - d_v|. \quad (4)$$

- The $m = 1$ corresponds to misbalnce deg index defined by

$$\alpha_1(G) = \sum_{uv \in E(G)} |d_u - d_v|. \quad (5)$$

The misbalance haddeg index-MHD is defined by

$$MHD = \sum_{uv \in E(G)} \left| \frac{1}{2^{d_u}} - \frac{1}{2^{d_v}} \right|. \quad (6)$$

These are the significant predictor of enthalpy of vaporisation and of standard enthalpy of vaporisation for octane isomers for more information the reader can see [17]. In forthcoming sections, we established misbalance degree based adriatic indices of regular and complete bipartite graph using some operators such as line, subdivision, semi-total(vertex and edge) graph, total, jump and para-line graphs.

§2. Line Graph

In this section, we established misbalance type degree based adriatic indices of line graph of regular and complete bipartite graph.

The line graph $L(G)$ of a graph G is that graph whose vertices can be put in one-to-one correspondence with the edges of G in such a way that two vertices of $L(G)$ are adjacent

whenever the corresponding edges of G are adjacent. For more details, the reader refers to [1].

Corollary 2.1 *Let G be a r -regular graph with $n \geq 2$ vertices. Then, $\alpha_m(L(G)) = 0, \forall m \in \{-\frac{1}{2}, \frac{1}{2}, -1, 1\}$ iff the equality holds for $MHD(L(G))$.*

Corollary 2.2 *Let $K_{r,s}$ be a complete bipartite graph with $1 \leq r \leq s$ vertices. Then, $\alpha_m(L(K_{r,s})) = 0, \forall m \in \{-\frac{1}{2}, \frac{1}{2}, -1, 1\}$ iff the equality holds for $MHD(L(K_{r,s}))$.*

§3. Subdivision Graph

In this section, we established misbalance type degree based adriatic indices of subdivision graph of regular and complete bipartite graph.

The subdivision graph $S(G)$ is the graph obtained from G by replacing each of its edges by a path of length two, or equivalently, by inserting an additional vertex into each edge of G with vertex set $V(G) \cup E(G)$. For more details, refer to [10].

Theorem 3.1 *Let G be a r -regular graph with $n \geq 2$ vertices. Then*

$$\alpha_m(S(G)) = \begin{cases} nr \left| \frac{\sqrt{r}-\sqrt{2}}{\sqrt{2r}} \right| & \text{when } m = -\frac{1}{2}; \\ nr |\sqrt{2} - \sqrt{r}| & \text{when } m = \frac{1}{2}; \\ n \left| \frac{r-2}{2} \right| & \text{when } m = -1; \\ nr |2 - r| & \text{when } m = 1, \end{cases}$$

$$MHD(S(G)) = nr |2^{-2} - 2^{-r}|.$$

Proof Let G be a r -regular graph with $n \geq 2$ vertices. By algebraic method, the cardinality for vertex and edge set is $n + \frac{nr}{2}$ and nr respectively. The edge set as follows $E_1 = \{uv \in E(S(G)) : d_{S(G)}(u) = 2, d_{S(G)}(v) = r\}$; Then by deploying these cardinalities for the definition of misbalance type degree indices the required results are obtained. \square

Theorem 3.2 *Let $K_{r,s}$ be a complete bipartite graph with $1 \leq r \leq s$ vertices. Then*

$$\alpha_m(S(K_{r,s})) = \begin{cases} rs \left[\left| \frac{\sqrt{r}-\sqrt{2}}{\sqrt{2r}} \right| + \left| \frac{\sqrt{s}-\sqrt{2}}{\sqrt{2s}} \right| \right] & \text{when } m = -\frac{1}{2}; \\ rs [|\sqrt{2} - \sqrt{r}| + |\sqrt{2} - \sqrt{s}|] & \text{when } m = \frac{1}{2}; \\ rs \left[\left| \frac{r-2}{2r} \right| + \left| \frac{s-2}{2s} \right| \right] & \text{when } m = -1; \\ rs [|2 - r| + |2 - s|] & \text{when } m = 1; \end{cases}$$

$$MHD(S(K_{r,s})) = rs |2^{-2} - 2^{-r}| + |2^{-2} - 2^{-s}|.$$

Proof Let $K_{r,s}$ be complete bipartite graph with $(r + s)$ vertices. By algebraic method, the cardinality for vertex and edge set is $r + s + rs$ and $2rs$ respectively.

The two partitions of the edge set $E(S(K_{r,s}))$ as follows:

$$E_1 = \{uv \in E(S(K_{r,s})) : d_{S(K_{r,s})}(u) = 2, d_{S(K_{r,s})}(v) = r\},$$

$$E_2 = \{uv \in E(S(K_{r,s})) : d_{S(K_{r,s})}(u) = 2, d_{S(K_{r,s})}(v) = s\}.$$

The cardinality for edge set E_1 and E_2 is rs . Then by deploying these cardinalities for the definition of misbalance type degree indices the required results are obtained. \square

§4. Vertex-Semitotal Graph

In this section, we established misbalance type degree based adriatic indices of vertex-semitotal graph of regular and complete bipartite graph.

The vertex-semitotal graph $T_1(G)$ with vertex set $V(G) \cup E(G)$ and edge set $E(S(G)) \cup E(G)$ is the graph obtained from G by adding a new vertex corresponding to each edge of G and by joining each new vertex to the end vertices of the edge corresponding to it. Generally, a Smarandachely vertex-semitotal graph $T_{E_1}^{S_1}(G)$ on edge set $E_1 \subset E(G)$ is such a graph with vertex set $V(G) \cup E_1(G)$ and edge set $E_1(S(G)) \cup E(G)$. Clearly, $T_{E_1}^{S_1}(G) = T_1(G)$ if $E_1 = E(G)$.

Theorem 4.1 *Let G be a r -regular graph with $n \geq 2$ vertices. Then*

$$\alpha_m(T_1(G)) = \begin{cases} nr \left\lfloor \frac{\sqrt{r}-1}{\sqrt{2r}} \right\rfloor & \text{when } m = -\frac{1}{2}; \\ nr \left\lfloor \sqrt{2} [1 - \sqrt{r}] \right\rfloor & \text{when } m = \frac{1}{2}; \\ n \left\lfloor \frac{r-1}{r} \right\rfloor & \text{when } m = -1; \\ nr \lfloor 2[1-r] \rfloor & \text{when } m = 1, \end{cases}$$

$$MHD(T_1(G)) = nr |2^{-2} - 2^{-2r}|.$$

Proof Let G be a r -regular graph with $n \geq 2$ vertices. By algebraic method, the cardinality for vertex and edge set is $\frac{nr}{2} + n$ and $\frac{3nr}{2}$ respectively.

The two partitions of the edge set $E(T_1(G))$ as follows:

$$E_1 = \{uv \in E(T_1(G)) : d_{T_1(G)}(u) = 2, d_{T_1(G)}(v) = 2r\},$$

$$E_2 = \{uv \in E(T_1(G)) : d_{T_1(G)}(u) = d_{T_1(G)}(v) = 2r\}.$$

The cardinalities of edge sets E_1, E_2 are $nr, \frac{nr}{2}$, respectively. Then, by deploying these cardinalities for the definition of misbalance type indices the required results are obtained. \square

Theorem 4.2 *Let $K_{r,s}$ be a complete bipartite graph with $1 \leq r \leq s$ vertices. Then*

$$\alpha_m(T_1(K_{r,s})) = \begin{cases} rs \left[\left\lfloor \frac{1-\sqrt{r}}{\sqrt{2r}} \right\rfloor + \left\lfloor \frac{1-\sqrt{s}}{\sqrt{2s}} \right\rfloor \right] & \text{when } m = -\frac{1}{2}; \\ rs \left[\left\lfloor \sqrt{2} [\sqrt{r} - 1] \right\rfloor + \left\lfloor \sqrt{2} [\sqrt{s} - 1] \right\rfloor \right] & \text{when } m = \frac{1}{2}; \\ rs \left[\left\lfloor \frac{1-r}{2r} \right\rfloor + \left\lfloor \frac{1-s}{2s} \right\rfloor \right] & \text{when } m = -1 \\ rs \left[\lfloor 2[r-1] \rfloor + \lfloor 2[s-1] \rfloor \right] & \text{when } m = 1, \end{cases}$$

$$MHD(T_1(K_{r,s})) = rs \left[|2^{-2r} - 2^{-2}| + |2^{-2s} - 2^{-2}| \right].$$

Proof If $K_{r,s}$ is a complete bipartite graph with $(r+s)$ - vertices and rs - edges, the

cardinality for vertex and edge set is $r + s + rs$ and $3rs$ respectively.

The three partitions of the edge set $E(T_1(K_{r,s}))$ as follows:

$$E_1 = \{uv \in E(T_1(K_{r,s})) : d_{T_1(K_{r,s})}(u) = 2r, d_{T_1(K_{r,s})}(v) = 2\},$$

$$E_2 = \{uv \in E(T_1(K_{r,s})) : d_{T_1(K_{r,s})}(u) = 2s, d_{T_1(K_{r,s})}(v) = 2\},$$

$$E_3 = \{uv \in E(T_1(K_{r,s})) : d_{T_1(K_{r,s})}(u) = 2r, d_{T_1(K_{r,s})}(v) = 2s\}.$$

The cardinalities of edge sets E_1 , E_2 and E_3 are rs . Then by deploying these cardinalities for the definition of misbalance type indices obtained the required results. \square

By above result with $r = s$, the complete regular bipartite graph $K_{r,r}$ with $r > 2$.

§5. Edge-Semitotal Graph

In this section, misbalance type degree based adriatic indices of edge-semitotal graph of regular and complete bipartite graph are studied.

An edge-semitotal graph $T_2(G)$ with vertex set $V(G) \cup E(G)$ and edge set $E(S(G)) \cup E(L(G))$ is the graph obtained from G by inserting a new vertex into each edge of G and by joining with edges those pairs of these new vertices which lie on adjacent edges of G . Generally, a Smarandachely edge-semitotal graph $T_{E_1}^{S_2}(G)$ on edge set $E_1 \subset E(G)$ is such a graph with vertex set $V(G) \cup E_1(G)$ and edge set $E_1(S(G)) \cup E(E_1 \cap L(G))$. Clearly, $T_{E_1}^{S_2}(G) = T_2(G)$ if $E_1 = E(G)$.

Theorem 5.1 *Let G be a r -regular graph with $n \geq 2$ vertices. Then*

$$\alpha_m(T_2(G)) = \begin{cases} nr \left\lfloor \frac{\sqrt{2}-1}{\sqrt{2r}} \right\rfloor & \text{when } m = \frac{-1}{2}; \\ nr \left\lfloor \sqrt{r} [1 - \sqrt{2}] \right\rfloor & \text{when } m = \frac{1}{2}; \\ \frac{n}{2} & \text{when } m = -1; \\ r^2 & \text{when } m = 1, \end{cases}$$

$$MHD(T_2(G)) = r \left\lfloor 2^{-r} - 2^{-2r} \right\rfloor.$$

Proof Let G be a r -regular graph with $n \geq 2$ vertices. By algebraic method, the cardinality for vertex and edge set is $\frac{nr}{2} + n$ and $\frac{nr}{2}(r+1)$ respectively.

The two partitions of the edge set $E(T_2(G))$ as follows:

$$E_1 = \{uv \in E(T_2(G)) : d_{T_2(G)}(u) = r, d_{T_2(G)}(v) = 2r\},$$

$$E_2 = \{uv \in E(T_2(G)) : d_{T_2(G)}(u) = d_{T_2(G)}(v) = 2r\}.$$

Then, the cardinalities of edge sets E_1 and E_2 are rn and $\frac{rn}{2}(r-1)$ respectively. By deploying these cardinalities for the definition of misbalance type indices, obtained the required results. \square

Theorem 5.2 *Let $K_{r,s}$ be a complete bipartite graph with $1 \leq r \leq s$ vertices. Then*

$$\alpha_m(T_2(K_{r,s})) = \begin{cases} rs \left[\left| \frac{\sqrt{r+s}-\sqrt{r}}{\sqrt{r}(\sqrt{r+s})} \right| + \left| \frac{\sqrt{r+s}-\sqrt{s}}{\sqrt{s}(\sqrt{r+s})} \right| \right] & \text{when } m = \frac{-1}{2}; \\ rs \left[\left| \sqrt{r} - \sqrt{r+s} \right| + \left| \sqrt{s} - \sqrt{r+s} \right| \right] & \text{when } m = \frac{1}{2}; \\ rs \left[\left| \frac{s}{r(r+s)} \right| + \left| \frac{r}{s(r+s)} \right| \right] & \text{when } m = -1; \\ rs[s+r] & \text{when } m = 1, \end{cases}$$

$$MHD(T_2(K_{r,s})) = rs \left[\left| 2^{-r} - 2^{-(r+s)} \right| + \left| 2^{-s} - 2^{-(r+s)} \right| \right].$$

Proof Let $K_{r,s}$ be complete bipartite graph with $(r+s)$ vertices. By algebraic method, the cardinality for vertex and edge set is $r+s+rs$ and $sr[1 + \frac{1}{2}(r+s)]$ respectively.

The three partitions of the edge set $E(T_2(K_{r,s}))$ as follows:

$$E_1 = \{uv \in E(T_2(K_{r,s})) : d_{T_2(K_{r,s})}(u) = r, d_{T_2(K_{r,s})}(v) = r+s\},$$

$$E_2 = \{uv \in E(T_2(K_{r,s})) : d_{T_2(K_{r,s})}(u) = s, d_{T_2(K_{r,s})}(v) = r+s\},$$

$$E_3 = \{uv \in E(T_2(K_{r,s})) : d_{T_2(K_{r,s})}(u) = d_{T_2(K_{r,s})}(v) = r+s\}.$$

The cardinalities of edge sets E_1 and E_2 are rs and the cardinality for edge set E_3 is $\frac{1}{2}rs[r+s-2]$. Then by utilizing these cardinalities for the definition of misbalance type indices, obtained the required results. \square

By above result with $r = s$, the complete regular bipartite graph $K_{r,r}$ with $r > 1$.

§6. Total Graph

In this section, the misbalance type degree based adriatic indices of total graph of regular and complete bipartite graph are reckoned.

The total graph of a graph G is denoted by $T(G)$ with vertex set $V(G) \cup E(G)$ and any two vertices of $T(G)$ are adjacent if and only if they are either incident or adjacent in G . For more details, refer to [1].

Corollary 6.1 *Let G be a r -regular graph with $n \geq 2$ vertices. Then $\alpha_m(T(G)) = 0, \forall m \in \{-\frac{1}{2}, \frac{1}{2}, -1, 1\}$ iff the equality holds for $MHD(T(G))$.*

Theorem 6.2 *Let $K_{r,s}$ be a complete bipartite graph with $1 \leq r \leq s$ vertices. Then*

$$\alpha_m(T(K_{r,s})) = \begin{cases} rs \left[\left| \frac{\sqrt{2r}-\sqrt{2s}}{2\sqrt{rs}} \right| + \left| \frac{\sqrt{r+s}-\sqrt{2s}}{\sqrt{2s(r+s)}} \right| + \left| \frac{\sqrt{r+s}-\sqrt{2r}}{\sqrt{2r(r+s)}} \right| \right] & \text{when } m = -\frac{1}{2}; \\ rs \left[\left| \sqrt{2}[\sqrt{s}-\sqrt{r}] \right| + \left| \sqrt{2s}-\sqrt{r+s} \right| + \left| \sqrt{2r}-\sqrt{r+s} \right| \right] & \text{when } m = \frac{1}{2}; \\ rs \left[\left| \frac{r-2}{sr} \right| + \left| \frac{r-s}{2s(r+s)} \right| + \left| \frac{s-r}{2r(r+s)} \right| \right] & \text{when } m = -1; \\ rs[2(s-r) + |s-r| + |r-s|] & \text{when } m = 1, \end{cases}$$

$$MHD(T(K_{r,s})) = rs \left[\left| 2^{-2} - 2^{-2r} \right| + \left| 2^{-2s} - 2^{-(r+s)} \right| + \left| 2^{-2r} - 2^{-(r+s)} \right| \right].$$

Proof Let $K_{r,s}$ be complete bipartite graph with $(r + s)$ vertices. By algebraic method, the cardinality for vertex and edge set is $r + s + rs$ and $\frac{1}{2}rs(r + s - 2) + 3rs$ respectively. The four partitions of the edge set $E(T(K_{r,s}))$ as follows:

$$\begin{aligned} E_1 &= \{uv \in E(T(K_{r,s})) : d_{T(K_{r,s})}(u) = 2s, d_G(v) = 2r\}, \\ E_2 &= \{uv \in E(T(K_{r,s})) : d_{T(K_{r,s})}(u) = 2s, d_{T(K_{r,s})}(v) = r + s\}, \\ E_3 &= \{uv \in E(T(K_{r,s})) : d_{T(K_{r,s})}(u) = 2r, d_{T(K_{r,s})}(v) = r + s\}, \\ E_4 &= \{uv \in E(T(K_{r,s})) : d_{T(K_{r,s})}(u) = d_{T(K_{r,s})}(v) = r + s\}. \end{aligned}$$

Then, the cardinalities of edge sets E_1 , E_2 and E_3 are rs and the cardinality of edge set E_4 is $\frac{1}{2}rs(r + s - 2)$. Then by deploying these cardinalities for the definition of misbalance type indices, obtained the required results. \square

By above result with $r = s$, the complete regular bipartite graph $K_{r,r}$ with $r > 2$.

§7. Jump Graph

In this section, the misbalance type degree based adriatic indices of jump graph of regular and complete bipartite graph are studied.

The jump graph $J(G)$ of a graph G defined on $E(G)$ and in which two vertices are adjacent if and only if they are not adjacent in G .

Corollary 7.1 *Let G be a r - regular graph with $n \geq 2$ vertices. Then $\alpha_m(J(G)) = 0, \forall m \in \{-\frac{1}{2}, \frac{1}{2}, -1, 1\}$ iff the equality holds for $MHD(J(G))$.*

Corollary 7.2 *Let $K_{r,s}$ be a complete bipartite graph with $1 \leq r \leq s$ vertices. Then $\alpha_m(J(K_{r,s})) = 0, \forall m \in \{-\frac{1}{2}, \frac{1}{2}, -1, 1\}$ iff the equality holds for $MHD(J(K_{r,s}))$.*

§8. Para-Line Graph

In this section, the misbalance type degree based adriatic indices of para-line graph of regular and complete bipartite graph are reckoned.

Given a graph G , insert two vertices to each edge xy of G . Those two vertices will be denoted by (x, y) , (y, x) where (x, y) (*resp.* (y, x)) is the one incident to x (*resp.* y). The vertex set and the edge set as follows:

$$\begin{aligned} V(P(G)) &= (x, y) \in V(G) \times V(G); xy \in E(G), \\ E(P(G)) &= (((x, w), (x, z)); (x, w), (x, z) \in V(P(G)), w \neq z) \cup ((x, y), (y, x); xy \in E(G)). \end{aligned}$$

The resultant graph is called a para-line graph and denoted by $P(G)$.

Corollary 8.1 *Let G be a r - regular graph with $n \geq 2$ vertices. Then $\alpha_m(P(G)) = 0, \forall m \in \{-\frac{1}{2}, \frac{1}{2}, -1, 1\}$ iff the equality holds for $MHD(P(G))$.*

Theorem 8.2 Let $K_{r,s}$ be a complete bipartite graph with $1 \leq r \leq s$ vertices. Then,

$$\alpha_m(P(K_{r,s})) = \begin{cases} rs \left| \frac{\sqrt{-\sqrt{r}}}{\sqrt{rs}} \right| & \text{when } m = -\frac{1}{2}; \\ |\sqrt{r} - \sqrt{s}| & \text{when } m = \frac{1}{2}; \\ |s - r| & \text{when } m = -1 \\ rs|r - s| & \text{when } m = 1, \end{cases}$$

$$MHD(P(K_{r,s})) = rs |2^{-r} - 2^{-s}|$$

Proof Let $K_{r,s}$ be complete bipartite graph with $(r + s)$ vertices. By algebraic method, the cardinality for vertex and edge set is $2rs$ and $\frac{rs(r+s)}{2}$ respectively. The three partitions of the edge set $E(P(K_{r,s}))$ as follows:

$$\begin{aligned} E_1 &= \{uv \in E(P(K_{r,s})) : d_{P(K_{r,s})}(u) = r, d_G(v) = s\}, \\ E_2 &= \{uv \in E(P(K_{r,s})) : d_{P(K_{r,s})}(u) = s, d_{P(K_{r,s})}(v) = r\}, \\ E_3 &= \{uv \in E(P(K_{r,s})) : d_{P(K_{r,s})}(u) = d_{P(K_{r,s})}(v) = s\}. \end{aligned}$$

Then the cardinalities of edge sets E_1 , E_2 and E_3 are rs , $rs(\frac{r-1}{2})$ and $rs(\frac{s-1}{2})$, respectively. By deploying these cardinalities for the definition of misbalance type indices, the required results are obtained. \square

§9. Conclusion

In this paper we established misbalance degree based adriatic indices of regular and complete bipartite graph using some operators such as line, subdivision, semi total (vertex and edge) graph, total, jump and para-line graphs. In future we will pay attention to some new classes of operations on graphs and study their adriatic indices which will be practically helpful to identify underlying topologies.

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