

# Max-min Rodeg index of bridge graphs and fullerenes

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## Article history

Submitted 17 August 2017  
 Revised 22 October 2017  
 Accepted 6 December 2017  
 Published Online 8 Mac 2018

## Abstract

In this study, it is presented exact expressions for the Max-min rodeg index of bridge graphs. Moreover, the Max-min rodeg index of fullerenes and link of fullerenes is computed. The Max-min rodeg index (Mmsde) which is vertex degree-based topological index has attracted attention and gained popularity. This index is defined as  $\sum \max\{\sqrt{d_u}, \sqrt{d_v}\} / \min\{\sqrt{d_u}, \sqrt{d_v}\}$ . A fullerene graph is a cubic planar graph whose faces are pentagons and hexagons.

**Keywords:** Topological index, max-min Rodeg index, fullerenes, link of two graphs, bridge graphs

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## INTRODUCTION

Chemical graph theory is a branch of mathematical chemistry which deals with the nontrivial applications of graph theory to solve molecular problems. In general, a graph is used to represent a molecule by considering the atoms as the vertices of the graph and the molecular bonds as the edges. The main goal of chemical graph theory is to use algebraic invariants to reduce the topological structure of a molecule to a single number which characterizes either energy of the molecule as a whole or its orbital, its molecular branching, structural fragments, and its electronic structures, among others.

A molecular graph  $G=(V(G),E(G))$  is a simple graph having  $n=|V(G)|$  nodes and  $m=|E(G)|$  edges. The nodes  $v_i \in V(G)$  represent non-hydrogen atoms and the edges  $v_i v_j \in E(G)$  represent covalent bonds between the corresponding atoms. In particular, hydrocarbons are formed only by carbon and hydrogen atoms and their molecular graphs represent the carbon skeleton of the molecule. Note that hydrogen atoms are often omitted.

A graph-based molecular descriptor or graph invariant, commonly known as topological index, is a graph-theoretic invariant characterizing numerically the topological structure of a molecule (Gutman, 1990). These graph theoretic invariants are expected to correlate with physical observables measures by experiments in a way that theoretical predictions can be used to gain chemical insights even for not yet existing molecules.

Topological indices are used for studying the properties of molecules such as structure-property relationship (QSPR), structure-activity relationship (QSAR) and structural design in chemistry, nanotechnology

and pharmacology. Its main role is to work as a numerical molecular descriptor in QSAR/QSPR models (Shafiei, 2015; Vukičević, 2011).

The first topological index is the Wiener index which was introduced by Harold Wiener in 1947 and used it to determine physical properties of types of alkenes known as paraffin (Wiener, 1947). It was used for the correlation of measured properties of molecules with their structural features by H. Wiener.

In 2010, D. Vukicevic and M. Gasperov introduced Adriatic indices that obtained by the analyses well known indices such as Randić and Wiener index and QSAR and QSPR studies of them have been performed (Vukičević and Gašperov, 2010). It is defined three classes of Adriatic descriptors. One of these descriptors is the Discrete Adriatic descriptors which consist of 148 descriptors. They have very good predictive properties. So, many scientists studied these indexes. One of the Discrete Adriatic descriptors is max-min rodeg index. Max-min rodeg index is defined as

$$Mm_{sdc}(G) = \sum_{uv \in E(G)} \frac{\max\{\sqrt{d_u}, \sqrt{d_v}\}}{\min\{\sqrt{d_u}, \sqrt{d_v}\}} = \sum_{uv \in E(G)} \sqrt{\frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}}}$$

where  $d_u$  is denoted as the degree of vertex  $u$  (Vukičević, 2010; Vukičević and Gašperov, 2010). This index give the best predictor for enthalpy of vaporization and standard enthalpy of vaporization in the set of octane isomers and also for log water activity coefficient in the set of polychlorobiphenyles. We encourage reader to references (Azari *et al.*, 2013; De, 2017; Ghorbani and Hosseinzadeh, 2010; Ghorbani and Khaksari, 2017; Gutman, 1990; Iranmanesh and Zeraatkar, 2011; Kanna *et al.*, 2017; Mansour and Schork, 2009a, 2009b, 2010; Nazir *et al.*, 2017).

To be a closed shape, a fullerene should exactly have 12 pentagon sides, but the number of hexagon sides can be extremely variable. Fullerenes were discovered in 1985 by Kroto *et al.*, (1985) and are named after Richard Buckminster Fuller. Fullerenes are molecules in the form of cage-like polyhedra, consisting only of carbon atoms. Moreover, a fullerene graph is a cubic planar 3-regular graph whose faces are 12 pentagons only and  $F_6$  hexagons. Therefore the general formula for carbon fullerenes can be given  $C_{120+2F_6}$ . The general formula for carbon fullerenes is  $C_{120+2F_6}$  ( $F_6 \geq 0$  and  $F_6 \neq 1$ ) with the number of hexagonal faces  $F_6=20$  for  $C_{60}$ . The smallest possible fullerene is  $C_{20}$  ( $F_6=0$ ) and the most famous fullerene molecule is  $C_{60}$  with 12 pentagons and 20 hexagons. Suppose  $G$  is a fullerene

molecule containing n carbon atoms. This graphs have 12 pentagonals and (n/2-10) hexagonal faces where n≥20 and n≠22. The number of for details.

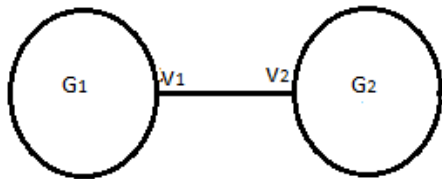
Schwerdtfeger *et al.* (2015) presented a general overview of recent topological and graph theoretical developments in fullerene research over the past two decades, describing both solved and open problems. A number of chemical properties of a fullerene can be derived from its graph structure.

There are infinitely many fullerenes in many different shapes depending on the distribution of the pentagons. Using experimental techniques, new fullerene with interesting chemical and physical applications is synthesized which require more information about their thermodynamic stability and electronic properties. It is quite difficult for quantum chemistry. But, fullerene graphs contain all the information we need, and we are able to sort out the millions of isomers, finding a few candidates for the most stable, by way of simple, easily computed topological indices. Topological index of fullerenes were studied by many scientists (Yaser Alizadeh *et al.*, 2014; Yaser Alizadeh *et al.*, 2012; Y Alizadeh *et al.*, 2009).

In this paper, we study recently defined the Max-min rodeg index. It is computed the Max-min rodeg index of link of any two graphs and bridge graphs. And also, it is presented exact expressions for the Max-min rodeg index of link of fullerenes.

**RESULTS AND DISCUSSION**

**Definition 1.** Let  $\{G_i\}_{i=1}^d$  be a set of finite pair wise disjoint molecular graphs with  $v_i \in V(G_i)$ . For given vertices  $v_1 \in V(G_1)$  and  $v_2 \in V(G_2)$ , a link or bridge of two graphs  $G_1$  and  $G_2$  is defined as the graph  $G_1 \sim G_2(v_1, v_2)$  obtained by joining  $v_1$  and  $v_2$  by an edge (see figure 1). For simply we show the bridge (link) of two graphs  $G_1$  and  $G_2$  by  $G_1 \sim G_2$ .

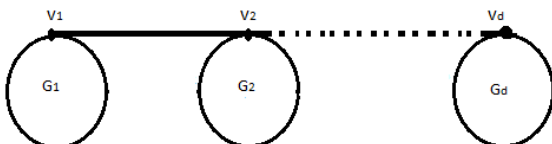


**Fig. 1** Bridge of two graphs

There are two types of bridge graphs.

**Definition 2.** The bridge of graphs  $G_1, G_2, \dots, G_d$  obtained joining a vertex of  $V(G_i)$  with a vertex of  $V(G_{i+1})$  and a vertex of  $V(G_{i+2})$  with same vertex of  $V(G_{i+1})$ ,  $i=1, \dots, d-2$  (fig. 2) is  $G_1 \sim G_2 \sim \dots \sim G_d$ .

If  $G_1 = G_2 = \dots = G_d = G$  then we use of the notation  $G \sim G$ .

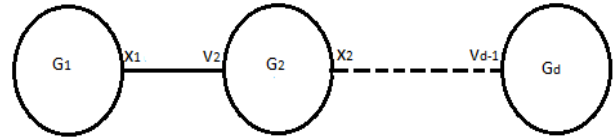


**Fig. 2** The bridge of graphs  $G_1, G_2, \dots, G_d$

**Definition 3.** The bridge of graphs  $G_1, G_2, \dots, G_d$  obtained joining a vertex of  $V(G_i)$  with a vertex of  $V(G_{i+1})$  ( $v_{i+1} \in V(G_{i+1})$ ) by an edge and different a vertex of  $V(G_{i+1})$  ( $v_{i+1} \neq x_{i+1}, x_{i+1} \in V(G_{i+1})$ )

edges of fullerene graph,  $|E(G)|$  are  $((3n)/2)$ , see (Ghorbani and Hosseinzadeh, 2010; Koorepazan-Moftakhar and Ashrafi, 2013)

with a vertex of  $V(G_{i+2})$  by an edge,  $i=1, \dots, d-2$  (fig. 3) is defined as the graph  $G_1 \sim G_2 \sim \dots \sim G_d$ . If  $G_1 = G_2 = \dots = G_d = G$  then we use of the notation  $G \sim G$ .



**Fig. 3** The bridge of graphs  $G_1, G_2, \dots, G_d$

We can write that the max-min Rodeg index of  $G$  as  $Mm_{sde}(G) = \sum_{uv \in E(G)} \gamma$  in which for the edge  $uv \in E(G)$ ,

$$\gamma = \gamma(d_u, d_v) = \sqrt{\frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}}}$$

**Theorem 1.** Let  $G$  be a fullerene graph. The Max-min Rodeg index of  $G$  is

$$Mm_{sde}(G) = \frac{3n}{2}$$

**Proof.** If  $G$  is a fullerene graph then for each edge  $uv$  of  $G$ ,  $\gamma(d_u, d_v) = \sqrt{\frac{\max\{3,3\}}{\min\{3,3\}}} = 1$  and  $|E(G)| = \frac{3n}{2}$ . From definition of max-min rodeg index, we obtain

$$Mm_{sde}(G) = \sum_{uv \in E(G)} \gamma(d_u, d_v) = \frac{3n}{2} \sqrt{\frac{\max\{3,3\}}{\min\{3,3\}}} = \frac{3n}{2}$$

**Theorem 2.** Consider the graph  $G_1$  and  $G_2$ . The Max-min rodeg index of  $G_1 \sim G_2$  is as follows:

$$Mm_{sde}(G_1 \sim G_2) = Mm_{sde}(G_1) + Mm_{sde}(G_2) + \gamma(d_{v_1} + 1, d_{v_2} + 1) + \sum_{u_i, v_i \in E(G_i)} (\gamma(d_{u_i}, d_{v_i} + 1) - \gamma(d_{u_i}, d_{v_i}))$$

where  $d_{v_i}$  denoted to the degree of vertex  $v_i \in V(G_i)$ ,  $i=1,2$ .

**Proof.** Let  $v_1 \in V(G_1)$  and  $v_2 \in V(G_2)$ . Then,

$$Mm_{sde}(G_1 \sim G_2) = \sum_{uv \in E(G_1)} \gamma + \sum_{uv \in E(G_2)} \gamma + \sum_{u_i, v_i \in E(G_i)} \gamma(d_{u_i}, d_{v_i} + 1) + \sum_{v_1, v_2} \gamma(d_{v_1} + 1, d_{v_2} + 1)$$

where  $E'$  is the set of edge joining  $v_1 \in V(G_1)$  with  $v_2 \in V(G_2)$  by an edge. From definition of the Max-min rodeg index, we obtain

$$Mm_{sde}(G_1 \sim G_2) = Mm_{sde}(G_1) - \sum_{u,v_1 \in E(G_1)} \gamma(d_{u_1}, d_{v_1}) + Mm_{sde}(G_2) - \sum_{u_2, v_2 \in E(G_2)} \gamma(d_{u_2}, d_{v_2}) + \sum_{u_i, v_i \in E(G_i)} \gamma(d_{u_i}, d_{v_i} + 1) + \gamma(d_{v_i} + 1, d_{v_i} + 1).$$

**Corollary 1.** Let  $G$  be a fullerene graph. The Max-min rodeg index of  $G \sim G$  is

$$Mm_{sde}(G \sim G) = 3n + \frac{4\sqrt{3}}{3} - 1.$$

**Proof.** By using Theorem 2, we have

$$Mm_{sde}(G \sim G) = 2Mm_{sde}(G) + 2 \sum_{uv \in E(G)} (\gamma(d_u, d_v + 1) - \gamma(d_u, d_v)) + \gamma(d_{v_1} + 1, d_{v_2} + 1)$$

and it is easy to see that

$$\gamma(d_u, d_v) = 1, \gamma(d_u, d_v + 1) = \sqrt{\frac{\max\{3, 4\}}{\min\{3, 4\}}} = \frac{2\sqrt{3}}{3},$$

$$\gamma(d_{v_1} + 1, d_{v_2} + 1) = \sqrt{\frac{\max\{4, 4\}}{\min\{4, 4\}}} = 1$$

Then, we obtain following equation:

$$Mm_{sde}(G \sim G) = 2Mm_{sde}(G) + 2\left(\frac{2\sqrt{3}}{3} - 1\right) + 1.$$

From Theorem 1, the proof is completed.

**Theorem 3.** Consider graphs  $G_1, G_2, \dots, G_d$  in figure 2. The Max-min rodeg index of  $G^* = G_1 \sim G_2 \sim \dots \sim G_d$  is

$$Mm_{sde}(G^*) = \sum_{i=1}^d Mm_{sde}(G_i) - \sum_{i=1}^d \sum_{uv_i \in E(G_i)} \gamma(d_u, d_{v_i}) + \sum_{i=2}^{d-1} \sum_{uv_i \in E(G_i)} \gamma(d_u, d_{v_i} + 2) + \sum_{uv_j \in E(G_j)} \gamma(d_u, d_{v_j} + 1) + \gamma(d_{v_1} + 1, d_{v_2} + 2) + \sum_{i=2}^{d-2} \sum_{v_i, v_{i+1} \in E(G_i)} \gamma(d_{v_i} + 2, d_{v_{i+1}} + 2) + \gamma(d_{v_{d-1}} + 2, d_{v_d} + 1).$$

where  $E'$  is the set of all edges joining  $v_i \in V(G_i)$  with  $v_{i+1} \in V(G_{i+1})$  by an edge,  $i=1, \dots, d-1$ .

**Proof.** In a similar way, we have

$$Mm_{sde}(G^*) = \sum_{i=1}^d \sum_{uv \in E(G_i)} \gamma + \sum_{i=2}^{d-1} \sum_{uv_i \in E(G_i)} \gamma(d_u, d_{v_i} + 2) + \sum_{uv_j \in E(G_j)} \gamma(d_u, d_{v_j} + 1) + \gamma(d_{v_1} + 1, d_{v_2} + 2) + \gamma(d_{v_{d-1}} + 2, d_{v_d} + 1) + \sum_{i=2}^{d-2} \sum_{v_i, v_{i+1} \in E(G_i)} \gamma(d_{v_i} + 2, d_{v_{i+1}} + 2).$$

From definition of the Max-min rodeg index, we can write

$$Mm_{sde}(G^*) = \sum_{i=1}^d Mm_{sde}(G_i) - \sum_{i=1}^d \gamma(d_u, d_{v_i}) + \gamma(d_{v_{d-1}} + 2, d_{v_d} + 1) + \sum_{i=2}^{d-1} \sum_{uv_i \in E(G_i)} \gamma(d_u, d_{v_i} + 2) + \sum_{uv_j \in E(G_j)} \gamma(d_u, d_{v_j} + 1) + \gamma(d_{v_1} + 1, d_{v_2} + 2) + \sum_{i=2}^{d-2} \sum_{v_i, v_{i+1} \in E(G_i)} \gamma(d_{v_i} + 2, d_{v_{i+1}} + 2).$$

**Corollary 2.** Let  $G$  be a fullerene. Then, the Max-min rodeg index of  $G \sim G$  is

$$Mm_{sde}(G \sim G) = d\left(\frac{3n}{2} + \sqrt{15} - 2\right) - 2\sqrt{15} + 4\sqrt{3} + \sqrt{5} - 3.$$

**Proof.** Let  $G^*$  be  $G \sim G$ . From Theorem 3, we get

$$Mm_{sde}(G^*) = \sum_{i=1}^d Mm_{sde}(G) - \sum_{i=1}^d \sum_{uv_i \in E(G)} \gamma(d_u, d_{v_i}) + \sum_{uv_j \in E(G)} \gamma(d_u, d_{v_j} + 1) + \sum_{i=2}^{d-1} \sum_{uv_i \in E(G)} \gamma(d_u, d_{v_i} + 2) + \gamma(d_{v_1} + 1, d_{v_2} + 2) + \sum_{i=2}^{d-2} \sum_{v_i, v_{i+1} \in E(G)} \gamma(d_{v_i} + 2, d_{v_{i+1}} + 2) + \gamma(d_{v_{d-1}} + 2, d_{v_d} + 1).$$

Note that  $d_u = 3$  and  $\gamma(d_u + 2, d_v + 2) = \gamma(d_u, d_v) = 1$ .

$$\gamma(d_u, d_v + 1) = \sqrt{\frac{\max\{3, 4\}}{\min\{3, 4\}}} = \frac{2\sqrt{3}}{3},$$

$$\gamma(d_u + 2, d_v + 1) = \gamma(d_u + 1, d_v + 2) = \sqrt{\frac{\max\{4, 5\}}{\min\{4, 5\}}} = \frac{\sqrt{5}}{2},$$

$$\gamma(d_u, d_v + 2) = \sqrt{\frac{\max\{3, 5\}}{\min\{3, 5\}}} = \frac{\sqrt{15}}{3}.$$

Then

$$Mm_{sde}(G^*) = \sum_{i=1}^d Mm_{sde}(G) - \sum_{i=1}^d \sum_{uv_i \in E(G)} \gamma(d_u, d_{v_i}) + \sum_{i=2}^{d-1} \sum_{uv_i \in E(G)} \gamma(d_u, d_{v_i} + 2) + \sum_{uv_j \in E(G)} \gamma(d_u, d_{v_j} + 1) + \gamma(d_{v_1} + 1, d_{v_2} + 2) + \sum_{i=2}^{d-2} \sum_{v_i, v_{i+1} \in E(G)} \gamma(d_{v_i} + 2, d_{v_{i+1}} + 2) + \gamma(d_{v_{d-1}} + 2, d_{v_d} + 1).$$

Or

$$Mm_{sde}(G^*) = \sum_{i=1}^d Mm_{sde}(G) - \sum_{i=1}^d 3.1 + \sum_{i=2}^{d-1} 3 \cdot \frac{\sqrt{15}}{3} + 3 \cdot \frac{2\sqrt{3}}{3} + 3 \cdot \frac{2\sqrt{3}}{3} + \frac{\sqrt{5}}{2} + \sum_{i=2}^{d-2} 1.1 + \frac{\sqrt{5}}{2}.$$

Or

$$Mm_{sde}(G^*) = dMm_{sde}(G) - 3d + (d-2)\sqrt{15} + 4\sqrt{3} + \sqrt{5} + (d-3).$$

By using Theorem 1, this proof is completed.

Now, we compute the Max-min rodeg index of bridge graphs for other type:

**Theorem 4.** Consider graphs  $G_1, G_2, \dots, G_d$  in figure 3. Let  $G^* = G_1 \overset{l}{\sim} G_2 \overset{l}{\sim} \dots \overset{l}{\sim} G_d$ . Then

$$Mm_{sde}(G^*) = \sum_{i=1}^{d-1} \left( \sum_{ux_i \in E(G_i)} \gamma(d_u, d_{x_i} + 1) + \sum_{x_i v_i \in E'} \gamma(d_{x_i} + 1, d_{v_i} + 1) \right) + \sum_{i=1}^d \left( Mm_{sde}(G_i) - \sum_{\substack{ux_i \in E(G_i) \\ u \neq v_{i-1}}} \gamma(d_u, d_{x_i}) - \sum_{\substack{uv_{i-1} \in E(G_i) \\ u \neq x_i}} \gamma(d_u, d_{v_{i-1}}) \right) + \sum_{i=2}^d \sum_{uv_{i-1} \in E(G_i)} \gamma(d_u, d_{v_{i-1}} + 1)$$

where  $E'$  is the set of all edges joining vertices of  $V(G_i)$  with vertices of  $V(G_{i+1})$ ,  $i=1, \dots, d-1$ .

**Proof.** Let

$$E' = \{x_i v_i \in E(G^*) \mid x_i \in V(G_i), v_i \in V(G_{i+1}), i = 1, \dots, d-1\}.$$

So, we have

$$Mm_{sde}(G^*) = \sum_{i=1}^d \sum_{uv \in E(G_i)} \gamma + \sum_{i=1}^{d-1} \sum_{x_i v_i \in E'} \gamma(d_u, d_{x_i} + 1) + \sum_{i=2}^d \sum_{uv_{i-1} \in E(G_i)} \gamma(d_u, d_{v_{i-1}} + 1) + \sum_{i=1}^{d-1} \sum_{x_i v_i \in E'} \gamma(d_{x_i} + 1, d_{v_i} + 1).$$

Or we get

$$Mm_{sde}(G^*) = \sum_{i=1}^{d-1} \left( \sum_{ux_i \in E(G_i)} \gamma(d_u, d_{x_i} + 1) + \sum_{x_i v_i \in E'} \gamma(d_{x_i} + 1, d_{v_i} + 1) \right) + \sum_{i=1}^d \left( Mm_{sde}(G_i) - \sum_{\substack{ux_i \in E(G_i) \\ u \neq v_{i-1}}} \gamma(d_u, d_{x_i}) - \sum_{\substack{uv_{i-1} \in E(G_i) \\ u \neq x_i}} \gamma(d_u, d_{v_{i-1}}) \right) + \sum_{i=2}^d \sum_{uv_{i-1} \in E(G_i)} \gamma(d_u, d_{v_{i-1}} + 1).$$

**Corollary 3.** Consider  $G$  fullerene graph. The Max-min rodeg index of  $G \sim G$  is

$$Mm_{sde}(G^*) = d \left( \frac{3n}{2} + 4\sqrt{3} - 5 \right) + 5 - 4\sqrt{3}.$$

**Proof.** Let  $G^*$  be  $G \sim G$ . From Theorem 4 and  $d_u = 3$  for  $u \in V(G)$  we can write

$$Mm_{sde}(G^*) = \sum_{i=1}^d \left( Mm_{sde}(G_i) - 3\gamma(d_u, d_{x_i}) - 3\gamma(d_u, d_{v_{i-1}}) \right) + \sum_{i=2}^d 3\gamma(d_u, d_{v_{i-1}} + 1) + \sum_{i=1}^{d-1} \left( 3\gamma(d_u, d_{x_i} + 1) + 1.\gamma(d_{x_i} + 1, d_{v_i} + 1) \right).$$

We known that  $x_d, v_0 \notin V(G^*)$  and  $\gamma(d_x, d_v + 1) = \frac{2\sqrt{3}}{3}$

$\gamma(d_x + 1, d_v + 1) = \gamma(d_x, d_v) = 1$ . Then,

$$Mm_{sde}(G^*) = \sum_{i=1}^d Mm_{sde}(G_i) - 3(d-1).1 - 3(d-1).1 + 3(d-1) \frac{2\sqrt{3}}{3} + (d-1) \left( 3 \frac{2\sqrt{3}}{3} + 1.1 \right)$$

or

$$Mm_{sde}(G^*) = d \frac{3n}{2} + (d-1)(4\sqrt{3} - 5).$$

## CONCLUSION

In this paper, exact computing formulae for the Max-min rodeg index which is vertex- degree based topological index of fullerene and of link of fullerene were obtained. Also, the Max-min rodeg index of bridge graphs was computed. There are infinitely many fullerenes in many different shapes depending on the distribution of the pentagons. We need more information about new fullerenes. This index give the best predictor for enthalpy of vaporization and standard enthalpy of vaporization in the set of octane isomers and also for log water activity coefficient in the set of polychlorobiphenyles. So, our results will help to predict certain physico-chemical properties such as standard enthalpy of vaporization, enthalpy of log water activity coefficient so on.

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