Innovative Edge-Centric Topological Measures for Enhanced Chemical Structure Characterization

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***Abstract*—In chemical graph theory, topological indices play a crucial role in correlating the structural properties of chemical compounds with their physicochemical characteristics and biological activities. In this study, we investigate the edge versions of several well-known degree-based topological invariants, including the Zagreb indices, Randic index, and atom-bond connectivity (ABC) index, for important chemical structures. The edge-based approach focuses on the relationships between adjacent edges, providing a refined mathematical framework that captures additional structural information often overlooked in vertex-based models. Exact analytical expressions for these edge invariants are derived, and comparative analyses are performed to explore their behavior across different molecular frameworks. The results demonstrate that edge versions of these indices offer deeper insights into molecular stability, branching, and resonance characteristics.**

***Index Terms*—QSPR, Topological Indices, Grid graph and descriptor.**

Subject Classification: 05C92

I. INTRODUCTION

Degree-based TIs are one of several types of TIs that have received a lot of attention since they are crucial for modeling the physical and chemical characteristics of molecules in QSPR/QSAR analyses. For several types of molecular networks, we investigate some of the edge versions of degree-based TIs in this chapter, including the geometric arithmetic descriptor, the atom-bond connectivity descriptor, and the Zagreb descriptor. Now we recall some definitions which are need to study this chapter. The Randi´c connectivity descriptor, defined as the sum of specific bond contributions determined from the vertex degree of the hydrogen suppressed molecular networks, is one of the most significant topological descriptors [1]. Inspired by the Randi´ c descriptor in a graph Λ, Vukicevi´c and Furtula [2] proposed a topological descriptor named the geometric-arithmetic descriptor GA as $GA(\Lambda) = \sum_{uv\epsilon E(\Lambda)} \frac{2\sqrt{\mu_\Lambda(u).\mu_\Lambda(v)}}{\mu_\Lambda(u)+\mu_\Lambda(v)}$. Certain mathematical properties of the GA descriptor have been studied by Yuan et al. [3]. Refer [4, 5, 6, 7] to recent research on degree-based topological descriptors and their uses.

The atom-bond connectivity descriptor, developed by Estrada et al. [8], is another crucial descriptor defined as $(\Lambda) = \sum_{uv\epsilon E(\Lambda)} \sqrt{\frac{\gamma_\Lambda(u)+\gamma_\Lambda(v)-2}{\gamma_\Lambda(u).\gamma_\Lambda(v)}}$. Estrada [8] offered a theoretical justification for his lucky ABC descriptor trait. Following the ABC descriptor's success, Furtula et al. [9] proposed the augmented Zagreb descriptor, another valency-based topological descriptor. It is defined for a connected graph Λ as have higher correlation coefficients. In Wang's et al. [10] study, the AZI descriptor was handled mathematically. See [11, 12, 13, 14, 15] for further information.

Based on the end-vertex degrees of edges in a line graph of Λ, the geometric arithmetic descriptor GAe was presented in [16]. It is a derived graph where two vertices of L(Λ) are adjacent if and only if their corresponding edges have a shared endpoint in Λ. It is defined as $GA_e(\Lambda) = \sum_{e=sf\epsilon E(L(\Lambda))} \frac{\sqrt{\gamma_s\cdot\gamma_f}}{\frac{1}{2}(\gamma_s+\gamma_r)} = \sum_{e=sf\epsilon E(L(\Lambda))} \frac{2\sqrt{\gamma_s\cdot\gamma_f}}{(\gamma_s+\gamma_r)}$, where γ_f denotes the vertex degree in L(Λ) or the degree of edge f in the original graph Λ. The equivalent definition of edge GA descriptor is $GA_e(\Lambda) = \sum_{i=1}^{|E(\Lambda)|} \xi_i$, where $\xi_i = \frac{2\sqrt{\gamma_s\cdot\gamma_f}}{(\gamma_s+\gamma_r)}$. If $e_i = u_iv_i\epsilon E(\Lambda)$, then we have $\gamma(e_i) = \gamma_{u_i} + \gamma_{v_i}$-2. Then the number of edges in a line graph L(Λ) is
$|E(L(\Lambda))| = \frac{1}{2}\sum_{e_i\epsilon V(L(\Lambda))} \gamma_{e_i} = \frac{1}{2}\sum_{e_i=u_iv_i\epsilon E(\Lambda)} (\gamma_{u_i} +$

$\gamma_{v_i} - 2) \times |E_i|$,

Where $|E_i| = |\{e_i | e_i \epsilon E(\Lambda), e_i = (\gamma_{u_i}, \gamma_{v_i})\}|$. In this sequence, the edge ABC descriptor and AZI descriptor are defined as $ABC_e(\Lambda) = \sum_{i=1}^{|E(\Lambda)|} \epsilon_i$, where $\epsilon_i = \frac{\sqrt{\gamma_s + \gamma_f - 2}}{(\gamma_s \cdot \gamma_r)}$ and

$AZI_e(\Lambda) = \sum_{i=1}^{|E(\Lambda)|} \eta_i$, where $\eta_i = \left(\frac{\gamma_s \cdot \gamma_f}{\gamma_s + \gamma_r - 2}\right)^3$, respectively.

Next we define a very general descriptor $I(\Lambda)$ based on degrees of the edges of a graph Λ,

that is, $I(\Lambda) = \sum_{ef \epsilon E(\Lambda)} t\left(\gamma_{L(\Lambda)}(e), \gamma_{L(\Lambda)}(f)\right)$, where $t\left(\gamma_{L(\Lambda)}(e), \gamma_{L(\Lambda)}(f)\right)$ is a real function of $\gamma_{L(\Lambda)}(e)$ and $\gamma_{L(\Lambda)}(f)$, and $t\left(\gamma_{L(\Lambda)}(e), \gamma_{L(\Lambda)}(f)\right) = t\left(\gamma_{L(\Lambda)}(f), \gamma_{L(\Lambda)}(e)\right)$.

If $t\left(\gamma_{L(\Lambda)}(e), \gamma_{L(\Lambda)}(f)\right) = \left(\gamma_{L(\Lambda)}(f), \gamma_{L(\Lambda)}(e)\right)^\alpha$ where $\alpha \neq 0$ is a real number,

then $I(\Lambda)$ is the general Randic descriptor of $e\Lambda$. Furthermore, $I(\Lambda)$ is the Randi´c

descriptor if $\alpha = -\frac{1}{2}$, the second Zagreb descriptor if $\alpha = 1$ and the second modified

Zagreb descriptor if $\alpha = -1$.

If $\left(\gamma_{L(\Lambda)}(e), \gamma_{L(\Lambda)}(f)\right) = \left(\gamma_{L(\Lambda)}(e) + \gamma_{L(\Lambda)}(t)\right)^\alpha$, then $I(\Lambda)$ is the general sum

connectivity descriptor of eG. Moreover, $I(\Lambda)$ is the sum-connectivity descriptor,

if $\alpha = -\frac{1}{2}$, the first Zagreb descriptor if $\alpha = 1$ and the second hyper Zagreb

descriptor if $\alpha = 2$.

If $t\left(\gamma_{L(\Lambda)}(e), \gamma_{L(\Lambda)}(f)\right) = \gamma_{L(\Lambda)}(e)^\alpha \gamma_{L(\Lambda)}(f)^\beta + \gamma_{L(\Lambda)}(f)^\alpha \gamma_{L(\Lambda)}(e)^\beta$, then $I(\Lambda)$ is

the generalized Zagreb descriptor of eG.

If $\left(\gamma_{L(\Lambda)}(e), \gamma_{L(\Lambda)}(f)\right) = \frac{2}{\gamma_{L(\Lambda)}(e) + \gamma_{L(\Lambda)}(f)}$, then $I(\Lambda)$ is the Harmonic descriptor

of $eH(\Lambda)$.

If $\left(\gamma_{L(\Lambda)}(e), \gamma_{L(\Lambda)}(f)\right) = \frac{\gamma_{L(\Lambda)}(e) \cdot \gamma_{L(\Lambda)}(f)}{\gamma_{L(\Lambda)}(e) + \gamma_{L(\Lambda)}(f)}$, then $I(\Lambda)$ is the inverse sum indeg descriptor

$eISI(\Lambda)$.

If $t\left(\gamma_{L(\Lambda)}(e), \gamma_{L(\Lambda)}(f)\right) = \frac{\gamma_{L(\Lambda)}(e)^2 \cdot \gamma_{L(\Lambda)}(f)^2}{\gamma_{L(\Lambda)}(e) \cdot \gamma_{L(\Lambda)}(f)}$, then $I(\Lambda)$ is the inverse symmetric division

deg descriptor $SDDe(\Lambda)$.

If $t\left(\gamma_{L(\Lambda)}(e), \gamma_{L(\Lambda)}(f)\right) = \frac{1}{\max\{\gamma_{L(\Lambda)}(e) + \gamma_{L(\Lambda)}(f)\}}$, then $I(\Lambda)$ is the variation of the Randi´c

descriptor $eR'(\Lambda)$.

Accurately predicting the physicochemical characteristics of different compounds is a challenging task in theoretical chemistry since chemical graphs may be used to describe chemical molecules. One of the key techniques in chemical graph theory is the topological index. It is a method of numerically representing a compound's molecular structure. As a result, a topological index is strongly tied to certain of a compound's physical and chemical characteristics. Although the molecular structure of various compounds has been studied, there hasn't been much study on degree-based topological indices for particular chemical structures. Researchers are therefore very interested in studying the topological index of the molecular structure of substances from a mathematical perspective. The objective of this study is to examine a variety of frequently used chemical structures' edge versions of degree-based topological indices. The use of these substances in the physical and chemical areas can be guided by these results in some way.

1. Grid graph

The Cartesian product of two path graphs given by $P_r \boxdot P_s$ is isomorphic to a two dimensional grid graph, also referred to as a rectangular grid graph. The mathematical characteristics and uses of grid graphs were examined in the works cited in [17,18,19,20,21]. We get certain edge version valency based topological indices of $P_r \boxdot P_s$, which are inspired by studies of grid graphs and their applications. Figures 1.1: and 1.2: respectively display the line graph and the graph of $P_4 \boxdot P_3$. By Figure 1.1: we get

$$\begin{aligned} |E(P_r \boxdot P_s)| &= |E(P_r)||V(P_s)| + |E(P_s)||V(P_r)| \\ &= (r-1)(s) + (s-1)(r) \\ &= 2rs - (r+s). \end{aligned}$$

Similarly, in Figure 1.2: the number of edges in the line graph of $P_r \boxdot P_s$ is

$$6rs - 6(r+s) + 4.$$

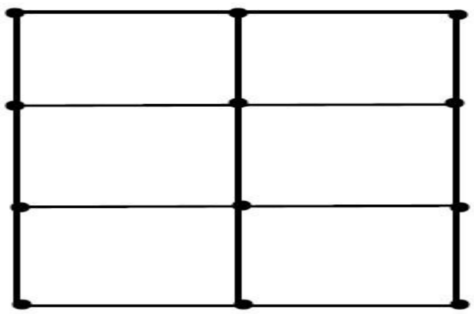

Figure-1.1: The graph $P_4 \boxdot P_3$

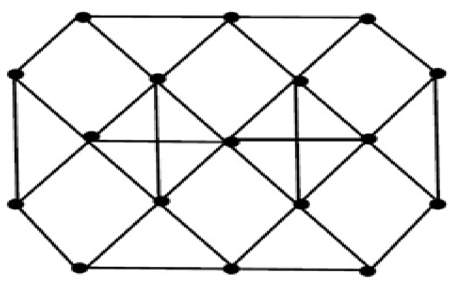

Figure-1.2: The graph $L(P_4 \boxdot P_3)$

Types of Edges	Number of Edges	ϵ_i	η_i
(3,3)	4	$\frac{2}{3}$	$\frac{729}{64}$
(3,4)	8	$\frac{1}{2}\sqrt{\frac{5}{3}}$	$\frac{1728}{125}$
(3,5)	8	$\sqrt{\frac{6}{15}}$	$\frac{3375}{216}$
(5,5)	4	$\frac{2\sqrt{2}}{5}$	$\frac{15625}{512}$
(4,4)	2r+2s-16	$\frac{\sqrt{6}}{4}$	$\frac{512}{27}$
(4,5)	4r+4s-24	$\frac{1}{2}\sqrt{\frac{7}{5}}$	$\frac{8000}{343}$
(5,6)	6r+8s-40	$\frac{3}{\sqrt{30}}$	$\frac{1000}{27}$
(6,6)	6rs-18r+20s+60	$\frac{\sqrt{10}}{6}$	$\frac{5832}{125}$

Table-1: Types of edges, their numbers and amount of ϵ_i and η_i of $L(P_r \boxdot P_s)$

Theorem: 1.1.

The edge ABC and AZI descriptor of $P_r \boxdot P_s$ are

(i) $ABC_e(P_r \boxdot P_s) = rs\sqrt{10} + r\left(\frac{\sqrt{6}}{2} + 2\sqrt{\frac{7}{5}} + \frac{24}{\sqrt{30}} - \frac{10\sqrt{10}}{10}\right) + s\left(\frac{\sqrt{6}}{2} + 2\sqrt{\frac{7}{5}} + \frac{18}{\sqrt{30}} - 3\sqrt{10}\right) + \frac{8}{3} + 4\sqrt{\frac{5}{3}} + 8\sqrt{\frac{6}{15}} + \frac{8\sqrt{2}}{5} - 4\sqrt{6} - 12\sqrt{\frac{7}{5}} - \frac{120}{\sqrt{30}} + 10\sqrt{10}$

(ii) $AZI_e(P_r \boxdot P_s) = (2r + 2s - 16)\frac{512}{27} + (4r + 4s - 24)\frac{8000}{343} + (6r + 8s - 40)\frac{1000}{27} + (6rs - 18r - 20s + 60)\frac{5832}{125} + \frac{729}{16} + \frac{13824}{125} + \frac{3375}{27} + \frac{15625}{128}$.

Proof:

From the structure of the graph $P_r \boxdot P_s$ and by Table 1.1, we obtain the required result.

We also arrive to the subsequent theorems.

Theorem: 1.2.

The edge GA descriptor of $P_r \boxdot P_s$ is

$GA_e(P_r \boxdot P_s) = 6rs + s\left(\frac{16\sqrt{5}}{9} + \frac{16\sqrt{30}}{11} - 18\right) + r\left(\frac{16\sqrt{5}}{9} + \frac{12\sqrt{30}}{11} - 16\right) - \frac{32\sqrt{5}}{3} - \frac{80\sqrt{30}}{11} + \frac{32\sqrt{3}}{7} + 2\sqrt{15} + 52.$

Next we obtain a general descriptor $I(\Lambda)$ based on degrees of the edges of a graph Λ.

Theorem: 1.3.

Let $\Lambda = P_r \boxdot P_s$. Then

$I(\Lambda) = 4t(3,3) + 8t(3,4) + 8t(3,5) + 4t(5,5) + (2r + 2s - 16)t(4,4) + (4r + 4s - 24)t(4,5) + (6r + 8s - 40)t(5,6) + (6rs - 18r - 20s + 60)t(6,6)$

Proof:

From the edge partition of Table 1.1, we have

$I(\Lambda) = \sum_{ef\epsilon E(\Lambda)} t\left(\gamma_{L(\Lambda)}(e), \gamma_{L(\Lambda)}(f)\right)$

$= \sum_{ef\epsilon E_1} t(3,3) + \sum_{ef\epsilon E_2} t(3,4) + \sum_{ef\epsilon E_3} t(3,5) + \sum_{ef\epsilon E_4} t(5,5) + \sum_{ef\epsilon E_5} t(4,4) + \sum_{ef\epsilon E_6} t(4,5) + \sum_{ef\epsilon E_7} t(5,6) + \sum_{ef\epsilon E_8} t(6,6)$

$$= 4t(3,3) + 8t(3,4) + 8t(3,5) + 4t(5,5) + (2r + 2s - 16)t(4,4) + (4r + 4s - 24)t(4,5) + (6r + 8s - 40)t(5,6) + (6rs - 18r - 20s + 60)t(6,6).$$

The exact values of the most well- known degree-based indices of $P_r \boxdot P_s$. are given below.

Corollary 1.4.

Let $\Lambda = P_r \boxdot P_s$. Then the general Randic´ descriptor of Λ,

$$eR_\alpha(\Lambda) = 4(9^\alpha + 2(12)^\alpha + 2(15)^\alpha + 25^\alpha + (r + s - 6)(20)^\alpha) + 2(r + s - 8)(16)^\alpha + (3r + 4s - 20)(30)^\alpha + (3rs - 9r - 10s + 30)(36)^\alpha,$$

the Randic´ descriptor

$$eR_{\frac{-1}{2}}(\Lambda) = rs - \frac{1}{6}(17s + 15r) + \frac{122}{15} + \frac{4}{\sqrt{3}} + \frac{8}{\sqrt{15}} + \frac{(2r + 2s - 12)}{\sqrt{5}} + \frac{(6r + 8s - 40)}{\sqrt{30}},$$

the second Zagreb descriptor

$$eR_1(\Lambda) = 216rs - 356r - 368s + 1656,$$

the second modified Zagreb descriptor

$$eR_{-1}(\Lambda) = \frac{rs}{6} + \frac{13}{360}s - \frac{99}{40}r + \frac{1950}{3375},$$

the general sum-connectivity descriptor

$$e\chi_\alpha(\Lambda) = 4(6)^\alpha + 8(7)^\alpha + 8(8)^\alpha + 4(10)^\alpha + (2r + 2s - 16)(8)^\alpha + (4r + 4s - 24)(9)^\alpha + (6r + 8s - 40)(11)^\alpha + (6rs - 18r - 20s + 60)(12)^\alpha,$$

the sum connectivity descriptor

$$e\chi_{\frac{-1}{2}}(\Lambda) = \frac{3rs}{\sqrt{3}} + s\left(\frac{1}{\sqrt{2}} + \frac{4}{3} + \frac{8}{\sqrt{11}} - \frac{10}{\sqrt{3}}\right) + r\left(\frac{1}{\sqrt{2}} + \frac{4}{3} + \frac{6}{\sqrt{11}} - \frac{9}{\sqrt{3}}\right) + \frac{4}{\sqrt{6}} + \frac{8}{\sqrt{7}} + \frac{4}{\sqrt{10}} - \frac{4}{\sqrt{2}} - \frac{24}{3} - \frac{40}{\sqrt{11}} + \frac{30}{\sqrt{3}},$$

the first Zagreb descriptor

$$e\chi_1(\Lambda) = 72rs - 98r - 100s + 120,$$

the hyper-Zagreb descriptor

$$e\chi_2(\Lambda) = 744rs - 1110r - 2006s + 1528,$$

the generalized Zagreb descriptor

$$eGZ(\Lambda) = 8 \times 3^\alpha(12)^\beta + 4 \times 4^\alpha\left(2 \times 3^\alpha + (r + s - 6)5^\beta + (r + s - 8)4^\beta\right) + 2 \times 5^\alpha\left(4 \times 3^\beta + (2r + 2s - 12)4^\beta + (3r + 4s - 20)6^\beta + 4 \times 5^\beta\right) + 2 \times 6^\alpha\left((6rs - 18r - 20s + 60)6^\beta + (3r + 4s - 20)5^\beta\right),$$

the harmonic descriptor

$$eH(\Lambda) = rs - \frac{1}{198}(103r + 97s) + \frac{49757}{3465},$$

the inverse sum indeg descriptor

$$eISI(\Lambda) = \frac{27rs}{2} - \frac{2227}{198}r - \frac{1019}{99}s - \frac{28598}{231},$$

the symmetric division deg descriptor

$$eSDD(\Lambda) = 12rs - \frac{1}{15}(173s + 174r) + \frac{2569}{15},$$

and the variation of the Randic´ descriptor

$$eR'(\Lambda) = rs - \frac{7}{10}(r + s) + \frac{76}{15}.$$

II. CONCLUSION

In this section, we investigated the edge version of valency-based topological indices for the Cartesian product of two path graphs $P_r \boxdot P_s$, also known as the grid graph. We derived explicit expressions for the number and types of edges, as well as their corresponding parameters ϵ_i and η_i . The several details of edge–edge interactions that arise in the grid structure. Specifically, the total number of edges in $P_r \boxdot P_s$,the strong dependence of edge-based indices on both grid dimensions.

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