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Szeged Indices of Bicyclic Graphs with Applications as Molecular Descriptor

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Abstract: Molecular descriptors are mathematical representations of molecular properties, generated through numerous algorithms. These numerical values are used to quantitatively represent the physical and chemical attributes of molecules. In the field of chemical graph theory, two indices, namely the revised Szeged index and the revised edge-Szeged index, were introduced to characterize molecular properties. The Szeged index $Sz(\Gamma)$ of a simple connected graph Γ is computed by summing the products of $n_u(e)$ and $n_v(e)$ for all edges $e = uv$ in Γ, where $n_u(e)$ denotes the number of vertices in Γ that are closer to vertex u than to vertex v, and $n_v(e)$ is defined similarly. In this paper, the role of different variants of Szeged indices in modeling different physical properties of alkanes and benzenoid hydrocarbon is investigated. Their isomer discrimination ability is also examined. In addition, we obtain lower and upper bounds on revised Szeged index, revised edge-Szeged index and the difference between vertex-edge Szeged index and edge-vertex Szeged index of bicyclic graphs.

AMS Classification: 05C07, 05C09, 05C35

Keywords: Molecular graph, Structure-property modelling, Szeged index, Edge-vertex Szeged index, Vertex-edge Szeged index, Revised Szeged index.

1. INTRODUCTION

LET Γ be a simple connected graph with vertex set $V(\Gamma)$ and edge set $E(\Gamma)$. Moreover, let $|V(\Gamma)| = n$ and $|E(\Gamma)| = m$ be the order and the size of Γ, respectively. Suppose that $z, u, v \in V(\Gamma)$ and $f = xy \in E(\Gamma)$. The length of a shortest path between u and v in Γ is denoted by $d_\Gamma(u,v)$ and called distance between them. Also, the distance between z and f is denoted by $D_\Gamma(z,f)$ is defined as $\min\{d_\Gamma(z,x), d_\Gamma(z,y)\}$.

Assuming $e = uv$ belongs to the set of edges in the graph Γ, we can define the following quantities:
$n_0(e)$ represents the count of vertices in $V(\Gamma)$ that share an equal distance from both u and v.
$n_u(e)$ signifies the number of vertices in $V(\Gamma)$ that are closer to vertex u than they are to vertex v.
$n_v(e)$ indicates the count of vertices in $V(\Gamma)$ that are closer to vertex v than they are to vertex u.

In a similar vein, we also define:
$m_0(e)$ as the count of edges in $E(\Gamma)$ that have an equal distance from both u and v,
$m_u(e)$ as the number of edges in $E(\Gamma)$ that are closer to vertex u than they are to vertex v,
$m_v(e)$ as the count of edges in $E(\Gamma)$ that are closer to vertex v than they are to vertex u.

Molecular descriptors are critical tools for bridging the gap between molecules' complicated structure and their observable features. Molecular descriptors enable scientists and researchers to examine, evaluate, and predict numerous aspects of molecules by turning complex molecular structures into numerical values.

These descriptors capture a wide range of information about molecules, including structural, electrical, and physicochemical properties. They reveal information about molecular size, shape, polarity, solubility, reactivity, and biological activity. Molecular descriptors provide a systematic way to encode and comprehend the fundamental properties that influence molecular activity by utilizing algorithms and computational tools. In drug discovery, molecular descriptors contribute in the identification of possible therapeutic candidates by examining their compatibility with biological targets, pharmacokinetics, and toxicity profiles. They also allow for the virtual screening of enormous chemical libraries in order to prioritize molecules for experimental testing. Furthermore, in environmental chemistry and materials science, molecular descriptors aid in evaluating the behavior of chemicals in complex systems and forecasting their impact on the environment and human health.

Overall, molecular descriptors provide a vocabulary for translating complicated molecular structures into usable insights, enabling informed decision-making across many scientific disciplines. Topological indices plays crucial role as molecular descriptor in mathematical chemistry.[4–8,19,20,23–26,28,31] The Wiener index, which was introduced by Wiener in 1947,[29] stands as one of the earliest topological indices. As it is the oldest index it has been studied by many different researchers, we refer the reader to papers[11,12] for more information about it. The Szeged index was presented in Ref. [13], for the first time and it is formulated as

$$Sz(\Gamma) = \sum_{e=uv} n_u(e) n_v(e).$$

In the Szeged index definition, vertices that share the same distance from both u and v are not taken into account. To incorporate these vertices, another invariant has been introduced, known as the revised Szeged index, as described in Refs. [21,22]. The revised Szeged index is defined by

$$Sz^*(\Gamma) = \sum_{e=uv} \left(n_u(e) + n_0(e)/2\right)\left(n_v(e) + n_0(e)/2\right).$$

Also, the edge Szeged index, and revised edge Szeged index,[10] are defined by

$$Sz_e(\Gamma) = \sum_{e=uv} m_u(e) m_v(e),$$

$$Sz_e^*(\Gamma) = \sum_{e=uv} \left(m_u(e) + m_0(e)/2\right)\left(m_v(e) + m_0(e)/2\right).$$

Furthermore, the edge-vertex Szeged index and the vertex-edge Szeged index, are defined by

$$Sz_{ev}(\Gamma) = \frac{1}{2} \sum_{e=uv} \left(m_u(e) n_v(e) + m_v(e) n_u(e)\right),$$

$$Sz_{ve}(\Gamma) = \frac{1}{2} \sum_{e=uv} \left(m_u(e) n_u(e) + m_v(e) n_v(e)\right).$$

The interested readers can consult Refs. [1,9,15,27,30], for mathematical properties of these indices.

Das *et al.*,[2] compared Szeged indices of trees and obtain upper and lower bounds on $Sz_{ve}(\Gamma) - Sz_{ev}(\Gamma)$ of unicyclic graphs. Study of the mathematical properties of topological indices is motivated by their applications in structure-property modeling of molecules. Mathematical properties of the aforesaid indices are discussed in several papers but their applications is not touched till now. Our goal is to investigate the importance of Sz^*, Sz_e^*, Sz_{ev} and Sz_{ve} in predicting different properties of molecules. In addition, their isomer discrimination ability is examined. Further, we obtain upper and lower bounds of Szeged indices and $Sz_{ve}(\Gamma) - Sz_{ev}(\Gamma)$ for bicyclic graphs.

2. MATERIALS AND METHODS

To facilitate the computation of present invariants, a MATLAB code is developed. To investigate the role of Sz^*, Sz_e^*, Sz_{ev} and Sz_{ve} as structural descriptors of molecule, we perform regression analysis using some in-house python code on jupyter notebook IDE. The models are built in view of alkanes and benzenoid hydrocarbon data sets. The statistical metrics are computed by utilizing the statsmodels and sklearn libraries, while the graphical depictions of the results are created through the MATLAB plotting library. The present invariants are correlated with existing well-known indices to check their uniqueness.

Besides examining their role as a molecular descriptor, the invariants are also investigated mathematically, for which following definitions and results are necessary.

Definition 2.1. Let Γ be a graph of order n. It is called bicyclic if it is connected graph and has $n+1$ edges.

Consider a bicyclic graph Γ and a subgraph denoted as *K*. In this context, *K* represents the unique bicyclic subgraph of Γ that doesn't include any pendant vertices. In simpler terms, Γ is derived from *K* by attaching trees to certain vertices of *K*. It is a recognized fact that there exist three distinct categories of bicyclic graphs having no pendant vertex (see Figure 1.).

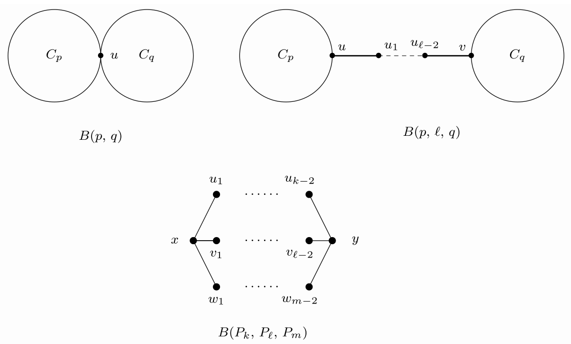

Figure 1. Three types of bicyclic structures.

Type 1. We can consider the bicyclic graph denoted as $B(p,q)$, which is formed by combining two cycles, namely C_p and C_q, with a single shared vertex.

Type 2. Another variation, denoted as $B(p,\ell,q)$, results from two cycles, C_p and C_q, connected by a unique path P_ℓ that links C_p and C_q.

Type 3. Lastly, the type represented as $B(P_k,P_\ell,P_m)$ is derived from three pairwise disjoint paths P_k,P_ℓ and P_m, all originating from one vertex *x* and leading to another vertex *y*.

Definition 2.2. Let Γ be a graph, we define

$$A(\Gamma) = \sum_{e=uv} (n_u(e) - n_v(e))^2,$$

$$L(\Gamma) = \sum_{e=uv} (m_u(e) - m_v(e))^2,$$

$$I(\Gamma) = \sum_{e=uv} (n_u(e) - n_v(e))\,(m_u(e) - m_v(e)).$$

Remark 2.3. By the above definition, we have

$$\begin{aligned} Sz_{ve}(\Gamma) - Sz_{ev}(\Gamma) &= \frac{1}{2}\sum_{e=uv} [m_u(e)(n_u(e) - n_v(e)) \\ &\quad - m_u(e)(n_u(e) - n_v(e))] \\ &= \frac{1}{2}\sum_{e=uv} (n_u(e) - n_v(e))\,(m_u(e) - m_v(e)) \\ &= \frac{1}{2} I(\Gamma). \end{aligned}$$

Lema 2.4. Let Γ be a connected graph of order n with m edges (Refs. [2,Lemma 2.2]). Then

$$Sz^*(\Gamma) = \frac{1}{4}\Big[mn^2 - \sum_{e=uv} (n_u(e) - n_v(e))^2\Big] = \frac{1}{4}[mn^2 - A(\Gamma)].$$

$$Sz_e^*(\Gamma) = \frac{1}{4}\Big[m^3 - \sum_{e=uv} (m_u(e) - m_v(e))^2\Big] = \frac{1}{4}[m^3 - L(\Gamma)].$$

Remark 2.5. Let C_p be a cycle. Then we have the following cases:

- Let p be odd. For every edge $e = xy$ of $E(C_p)$, there exists a vertex $z \in V(C_p)$ such that $d_{C_p}(x,z) = d_{C_p}(y,z)$. Moreover, exactly $(p-1)/2$ nodes of $V(C_p)$ are nearer to *x* than *y* and the other $(p-1)/2$ nodes of $V(C_p)$ are nearer to *y* than *x*. In the other word, $n_x(e) = n_y(e) = (p-1)/2$.
- Let *p* be even and $e = xy \in E(C_p)$. Exactly $p/2$ nodes of $V(C_p)$ are nearer to *x* than *y* and the other $p/2$ nodes of $V(C_p)$ are nearer to *y* than *x*. In the other word, $n_x(e) = n_y(e) = p/2$.

Remark 2.6. Let C_p be a cycle. Then we have the following cases:

- Let p be odd and $e = xy \in E(C_p)$. Exactly $(p-1)/2$ edges of $E(C_p)$ are closer to *x* than *y* and the other $(p-1)/2$ edges of $E(C_p)$ are closer to *y* than *x*. In the other word, $m_x(e) = m_y(e) = (p-1)/2$.
- Let *p* be even. For every edge $e = xy$ of $E(C_p)$, there is an edge $e' \in E(C_p) \setminus \{e\}$ such that $D_{C_p}(x,e') = D_{C_p}(y,e')$. Moreover, exactly $(p-2)/2$ edges of $E(C_p)$ are closer to *x* than *y* and the other $(p-2)/2$ edges of $E(C_p)$ are closer to *y* than *x*. In the other word, $m_x(e) = m_y(e) = (p-2)/2$.

3. RESULTS AND DISCUSSION

This section is divided into two subsections: first part is devoted to explore the role of indices under consideration as molecular descriptors and the second part aims to study their mathematical features.

3.1. Chemical Significance

The present section is directed towards examining the role of Sz^*, Sz_e^*, Sz_{ev} and Sz_{ve} as structural descriptors of molecules. The experimental values of physical properties including boiling points (*BP*), molar volumes (*MV*) at 20 °C, molar refraction (*MR*) at 20 °C, heats of vaporization (*HV*) at 25 °C, critical temperature (*CT*) and critical pressure (*CP*) of alkanes from n-butane to nonane isomers are correlated with theoretical values of Sz^*, Sz_e^*, Sz_{ev} and Sz_{ve}. The experimental values are taken from Ref. [18] and the theoretical values are generated by in-house Matlab script. We explain the outcomes by means of the following model:

$$Y = C(\pm 2E_1) + M(\pm 2E_2)X, \qquad (1)$$

where Y, C, E_i ($i = 1,2$), M and X denote property, intercept, standard error of coefficients, slope and molecular descriptor, respectively. To closely examine the model (1), we propose some additional parameters such as the correlation coefficient (*R*), standard error of model (S_e), F-test (F), and significance F (*SF*). We use *N* to signify the number of chemicals in the data set. The model parameters are generated using in-house Python code implementing statsmodels module.

The performance of Sz^* in modelling the properties under consideration is listed in Table 1. One can say from Table 1. that, Sz^* has significant predictive ability for each property where the data variance ranges from 80 % to 94 %. Particularly, it exhibits a strong correlation with *MV*, with an R^2 value of 0.941. Linear fitting of Sz^* with different properties is depicted in Figure 2.

The structure property relationship analysis for Sz_e^* is reported in Table 2. It reveals that, Sz^* sounds well except *BP* (R^2 = 0.755) and *CT* (R^2 = 0.731). In case of rest four properties the data variance ranges from 86 % to 90 %. Regression relation of Sz_e^* with different properties is plotted in Figure 3.

Table 1. Parameters of linear regression models for $Sz^{*}(\Gamma)$.

Properties	N	C	E_1	M	E_2	R^2	S_e	F	SF
BP	67	17.503	5.993	1.249	0.076	0.805	17.495	268.031	9.51×10^{-25}
CT	67	179.764	6.954	1.452	0.088	0.806	20.299	269.288	8.41×10^{-25}
CP	67	34.243	0.394	–0.103	0.005	0.867	1.149	425.296	3.19×10^{-30}
MV	65	112.579	1.658	0.658	0.021	0.941	4.37	1001.605	2.17×10^{-40}
MR	65	24.764	0.56	0.194	0.007	0.924	1.476	762.232	6.67×10^{-37}
HV	65	23.732	0.556	0.199	0.007	0.928	1.465	817.528	8.63×10^{-38}

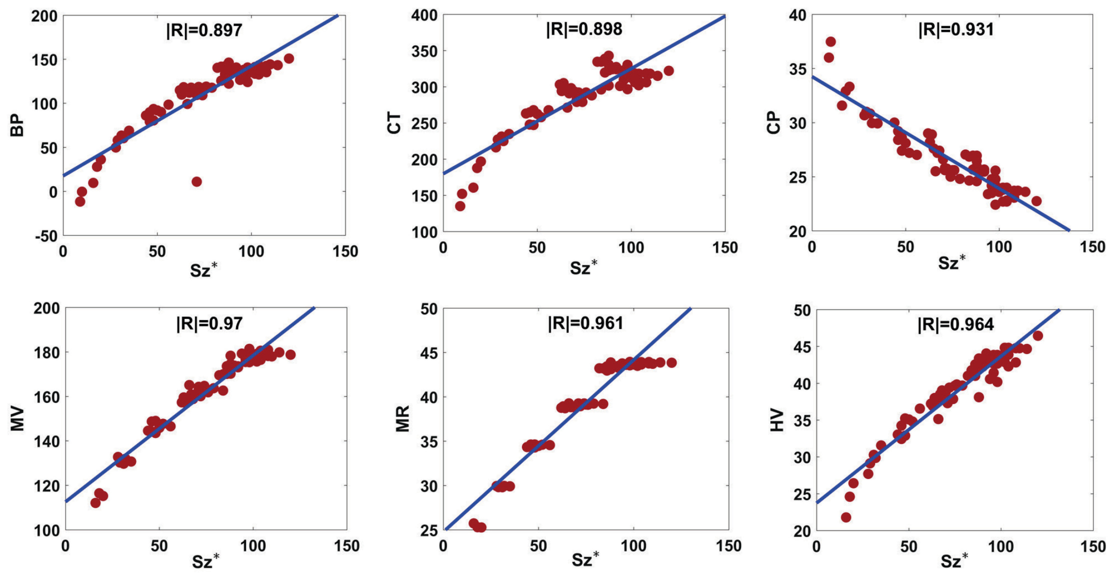

Figure 2. Linear fitting of Sz^{*} with different properties of alkanes.

Table 2. Parameters of linear regression models for $Sz_e^{*}(\Gamma)$.

Properties	C	E_1	M	E_2	R^2	S_e	F	SF
BP	29.963	6.087	1.7	0.12	0.755	19.601	200.313	1.59×10^{-21}
CT	195.75	7.409	1.945	0.146	0.731	23.859	176.968	3.21×10^{-20}
CP	33.412	0.361	–0.145	0.007	0.864	1.163	414.365	6.64×10^{-30}
MV	119.633	2.027	0.888	0.039	0.89	5.967	508.051	7.4×10^{-32}
MR	26.964	0.687	0.259	0.013	0.857	2.023	376.498	2.88×10^{-28}
HV	25.737	0.599	0.272	0.012	0.896	1.765	543.213	1.12×10^{-32}

Table 3. explores the predictive potential of Sz_{ev} . For *BP* and *CT*, its performance is not so strong, since data variances are 75 % and 73 %, respectively. On the other hand, Sz_{ev} is well correlated with *CP*, *MV*, *MR* and *HV* having data variances 86 %, 89 %, 85 % and 89 %, respectively. Linear fitting of Sz_{ev} with different properties is depicted in Figure 4.

Table 4. shows the ability of Sz_{ve} in describing different structural properties of alkanes. It is evident that Sz_{ve} is not so good in modelling *BP* (R^2 = 0.786) and *CP* (R^2 = 0.675). However it can explain *CT*, *MV*, *MR* and *HV* significantly with 86 %, 90 %, 94 % and 82 % of data variances, respectively. Linear fitting of Sz_{ve} with different properties is depicted in Figure 5. Suitable range of other parameters for a valid model is discussed in Refs. [17,18]. In view of those, we can claim that our models are statistically consistent.

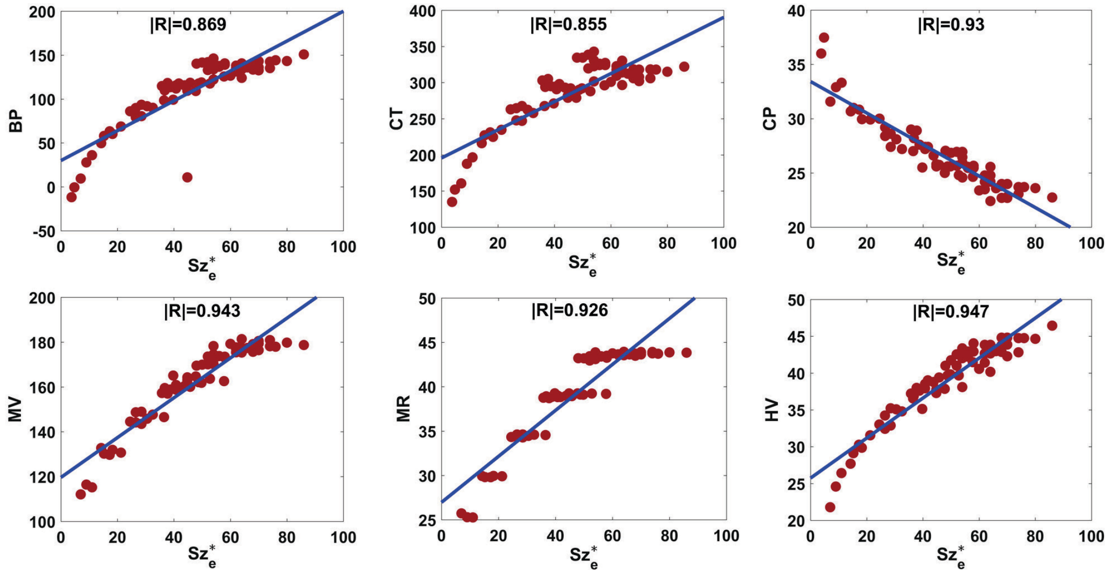

Figure 3. Linear fitting of Sz_e^* with different properties of alkanes.

Table 3. Parameters of linear regression models for $Sz_e^*(\Gamma)$.

Properties	C	E_1	M	E_2	R^2	S_e	F	SF
BP	31.935	6.02	1.722	0.123	0.751	19.759	196.093	2.68×10^{-21}
CT	198.099	7.342	1.968	0.149	0.726	24.097	172.216	6.14×10^{-20}
CP	33.255	0.357	−0.147	0.007	0.863	1.17	408.346	1×10^{-29}
MV	120.706	2.019	0.899	0.041	0.886	6.065	489.697	2.07×10^{-31}
MR	27.283	0.684	0.262	0.014	0.852	2.054	363.424	7.47×10^{-28}
HV	26.058	0.595	0.275	0.012	0.893	1.788	527.677	2.55×10^{-32}

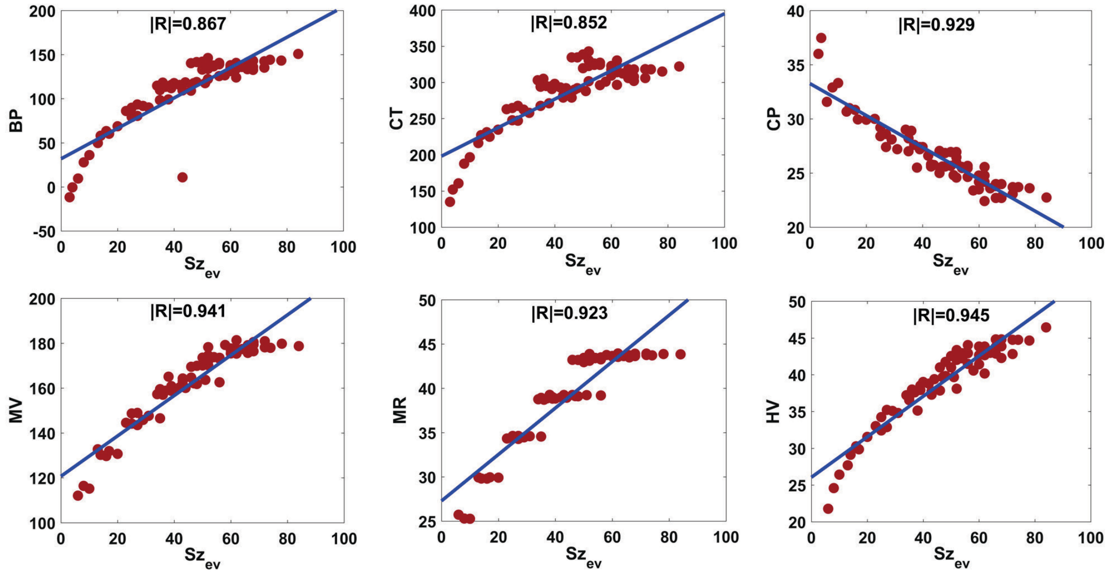

Figure 4. Linear fitting of Sz_{ev} with different properties of alkanes.

Table 4. Parameters of linear regression models for $Sz_{ve}(\Gamma)$.

Properties	C	E_1	M	E_2	R^2	S_e	F	SF
BP	30.59	5.555	0.574	0.037	0.786	18.317	238.817	1.9×10^{-23}
CT	190.806	5.217	0.698	0.035	0.86	17.201	400.562	1.72×10^{-29}
CP	32.461	0.546	−0.042	0.004	0.675	1.8	135.032	1.62×10^{-17}
MV	120.574	1.911	0.295	0.012	0.897	5.755	550.799	7.58×10^{-33}
MR	26.691	0.421	0.09	0.003	0.944	1.267	1056.703	4.42×10^{-41}
HV	26.613	0.767	0.086	0.005	0.822	2.309	291.187	2.63×10^{-25}

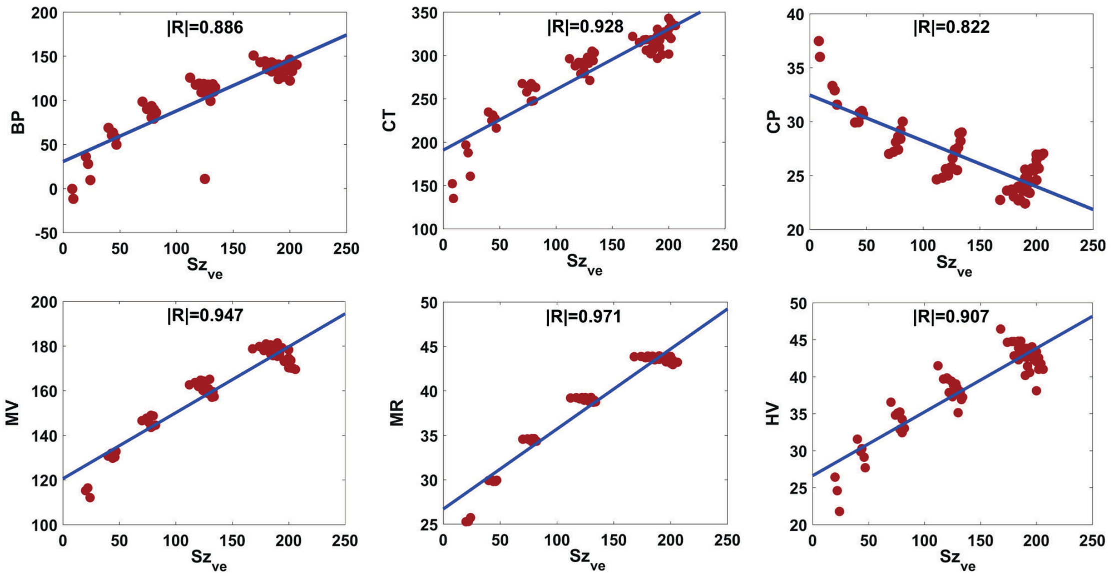

Figure 5. Linear fitting of Sz_{ve} with different properties of alkanes.

To investigate the correlation between the considered indices and some established ones, including the first Zagreb index (M_1), second Zagreb index (M_2), forgotten topological index (F), sum connectivity index (SCI), Randić index (R), inverse Randić index (RR), and symmetric division deg index (SDD), as well as additional indices such as Mostar index (Mo), Padmakar-Ivan (PI) index, and Trinajstić index (NT), a correlation matrix is computed for decane isomers (refer to Table 5.). Lučić et al.[16] established the significance of SCI and R indices in QSPR analysis. Gutman[14] highlighted the role of the aforementioned degree-based indices in the structure-property modelling of molecules. Mo, PI, and NT are indices that fall within the same category as Sz^*, Sz_e^*, Sz_{ev}, and Sz_{ve}. That is why the aforementioned indices are taken into account for comparison. The PI value for each isomer is 90. So it is not possible to get finite R for the PI index. The Mostar index is strongly correlated with Sz^*, Sz_e^*, Sz_{ev} and Sz_{ve}. On the other other hand NT has significantly low correlation with them. A correlation graph (see Figure 6.) is drawn by considering indices as nodes where two nodes are connected by an edge iff $R^2 \geq 0.8$. Three types of edge width is considered here: $R^2 \geq 0.95 \rightarrow 3.5pt$, $0.9 \leq R^2 < 0.95 \rightarrow 2.2pt$, $0.8 \leq R^2 < 0.9 \rightarrow 1pt$. From Table 5. and Figure 6., it is found that there is remarkably strong correlation among Sz^*, Sz_e^*, Sz_{ev} and Sz_{ve}. So, instead of considering four indices individually, it is possible that better performance will occur if we consider all four indices together. Now we propose a multiple regression model considering the four indices as follows:

$$Y = C(\pm 2E_1) + M_1(\pm 2E_2)Sz_e + M_2(\pm 2E_3)Sz_e^* + M_3(\pm 2E_4)Sz_{ev} + M_4(\pm 2E_5)Sz_{ve}, \quad (2)$$

where Y, C, E_i $(i = 1,2,3,4,5)$ and S_i $(i = 1,2,3,4)$ and X denote property, intercept, standard error of coefficients and slope, respectively. The parameters of model (2) for different properties are reported in Tables 6., 7.

Tables 6., 7. confirm the improvement in structure-property modelling when multiple regression model for each property is considered. In fact, remarkable data variance (99 %) is observed for MR. The F value is considerably high and SF is far smaller than 0.05. S_e is considerably low. The model (2) produces projected properties, and

Table 5. Correlation coefficient of Sz^*, Sz_e^*, Sz_{ev} and Sz_{ve} with some well-known descriptors for decanes.

	SCI	*R*	*RR*	*SDD*	M_1	M_2	*F*	*Mo*	*NT*
Sz^*	0.734	0.682	–0.929	–0.656	–0.832	–0.692	–0.811	–0.962	–0.464
Sz_e^*	0.734	0.682	–0.929	–0.656	–0.832	–0.692	–0.811	–0.962	–0.464
Sz_{ev}	0.734	0.682	–0.929	–0.656	–0.832	–0.692	–0.811	–0.962	–0.464
Sz_{ve}	–0.734	–0.682	0.929	0.656	0.832	0.692	0.811	0.962	–0.464

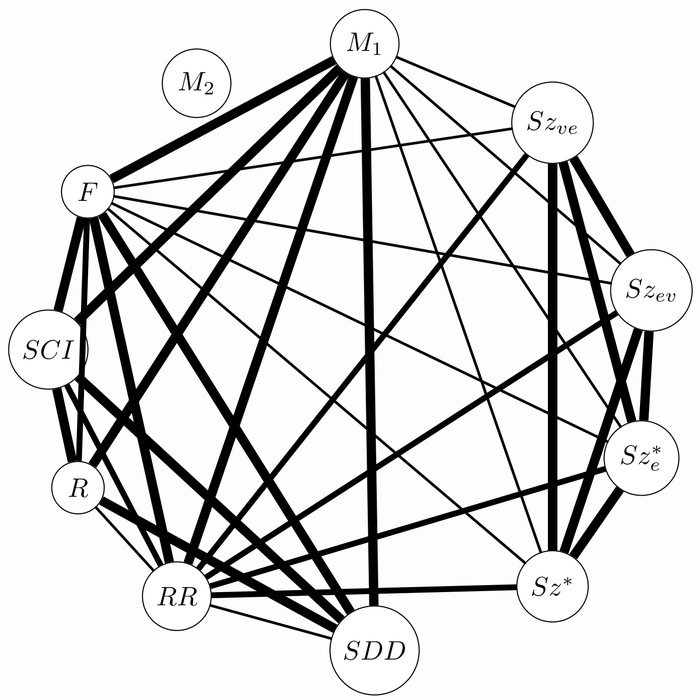

Figure 6. Correlation graph of Sz^*, Sz_e^*, Sz_{ev} and Sz_{ve} with some standard descriptors for decanes.

Table 6. Parameters of multiple linear regression model (2).

Properties	*C*	E_1	S_1	E_2	S_2	E_3	S_3	E_4	S_4	E_5
BP	–209.357	118.103	–22.809	23.830	429.919	316.787	–405.667	291.682	1.151	1.362
CT	–13.131	82.705	3.904	16.688	238.414	221.84	–234.852	204.259	0.086	0.954
CP	59.324	6.747	3.119	1.361	–52.481	18.098	49.09	16.664	–0.133	0.078
MV	26.852	42.079	–4.361	7.082	124.338	100.716	–119.549	93.266	0.164	0.379
MR	9.206	3.198	0.288	0.538	13.735	7.656	–14.021	7.089	–0.018	0.029
HV	–20.661	23.461	–4.464	3.949	82.378	56.152	–77.569	51.999	0.201	0.212

these are graphed against their corresponding experimental values in Figure 7. This graph illustrates a notable alignment between the experimental and predicted data.

Now we intend to examine the predictability of the indices considering some cyclic compounds. Experimental values of boiling point (*BP*) for benzenoid hydrocarbons are correlated with theoretical values of Sz^*, Sz_e^*, Sz_{ev} and Sz_{ve}. The findings are listed in Table 8. The data variances for the indices are 93 %, 91 %, 92 % and 92 % respectively. Linear correlation of the indices with *BP* for BHC is depicted in Figure 8.

We also study the multiple linear regression model (2) benzenoid hydrocarbons. Table 9. shows that the model is well fitted for *BP* with data variance 97 %. Figure 9. illustrates the relationship between experimental and predicted values for *BP*.

Table 7. Parameters of multiple linear regression model (2).

Properties	R^2	S_e	F	SF
BP	0.876	14.297	109.171	2.4×10^{-27}
CT	0.955	10.012	328.048	5.89×10^{-41}
CP	0.936	0.817	227.467	2.67×10^{-36}
MV	0.987	2.105	1132.098	9.56×10^{-56}
MR	0.999	0.16	17544.162	2.75×10^{-91}
HV	0.956	0.174	327.943	5×10^{-40}

Aside from structure-property modelling, an effective index should have different values for different isomers. We employ sensitivity as a metric to assess the capability of isomer discrimination. Sensitivity is defined as

$$S_T = \frac{N - N_T}{N},$$

where N represents the total number of considered isomers, and N_T is the count of isomers that cannot be differentiated using the topological index T. The S_T values of R, RR, SCI, M_1, M_2 and F for decane isomers are reported in Refs. [3,18]. Using the same dataset we obtain here that the sensitivity of PI, Mo, NT, Sz^*, Sz_e^*, Sz_{ev} and Sz_{ve} are 0.013, 0.16, 0.827, 0.533, 0.48, 0.547 and 0.533, respectively. This fact implies that the present indices have S_T values that are lower than NT, R, RR and SCI but higher than PI, Mo, M_1, M_2 and F.

3.2. Upper Bounds

In this section we obtain upper bounds on $A(\Gamma)$, $L(\Gamma)$ and $I(\Gamma)$, where Γ is a bicyclic graph. As a result, we get an upper bound on Szeged indices of bicyclic graph, by Remark 2.3. and Lemma 2.4.

3.2.1. Bicyclic graph of type 1.

Let Γ be a bicyclic graph of type 1 with order n. Hence, Γ has a subgraph $B(p,q)$, where $p,q \geq 3$. Let v_0 be the common vertex of two cycles C_p and C_q. Moreover, the vertices of C_p except common vertex are $\{v_1, v_2, \ldots, v_{p-1}\}$ and the vertices of C_q except common vertex are $\{v'_1, v'_2, \ldots, v'_{q-1}\}$ (see, Figure 10.). Since Γ is a bicyclic graph, we can consider T_i to be the tree which is hanging from vertex v_i $(i = 0,1,\ldots,p-1)$ and T_i' to be the tree which is hanging from vertex v_i' $(i = 1,2,\ldots,q-1)$. Let $|T_i| = t_i$ and $|T_i'| = t_i'$. So $t_i \geq 1$ and $t_i' \geq 1$. It is clear that $n = \sum_{i=0}^{p-1} t_i + \sum_{j=1}^{q-1} t_j'$.

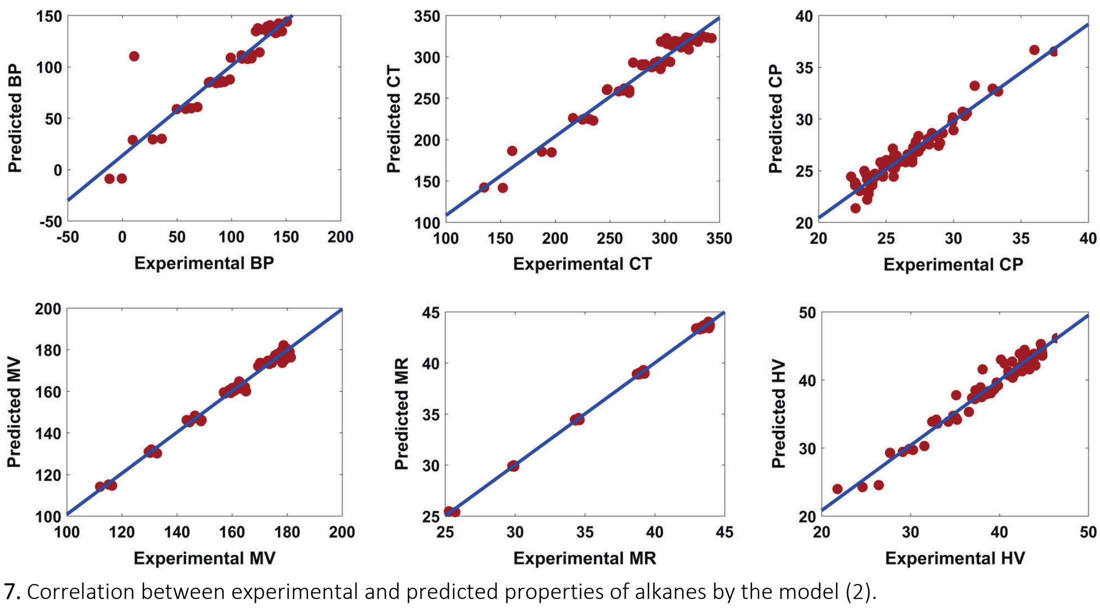

Figure 7. Correlation between experimental and predicted properties of alkanes by the model (2).

Table 8. Parameters of linear regression model for BP of benzenoid hydrocarbon.

Indices	C	E_1	M	E_2	R^2	S_e	F	SF
Sz^*	276.242	14.439	0.105	0.006	0.932	26.703	261.074	1.48×10^{-12}
Sz_e^*	290.935	15.909	0.071	0.005	0.909	30.892	190.269	2.38×10^{-11}
Sz_{ev}	287.614	14.872	0.099	0.007	0.922	28.65	224.297	5.66×10^{-12}
Sz_{ve}	291.303	14.422	0.055	0.004	0.924	28.234	231.516	4.28×10^{-12}

Table 9. Parameters of multiple linear regression model (2) for *BP* of benzenoid hydrocarbons.

Property	C	E_1	M_1	E_2	M_2	E_3	M_3	E_4	M_4	E_5	R^2	S_e	F	SF
BP	203.014	22.447	0.924	0.222	0.235	0.109	−1.204	0.36	0.056	0.021	0.968	19.979	121.082	9.56×10^{-12}

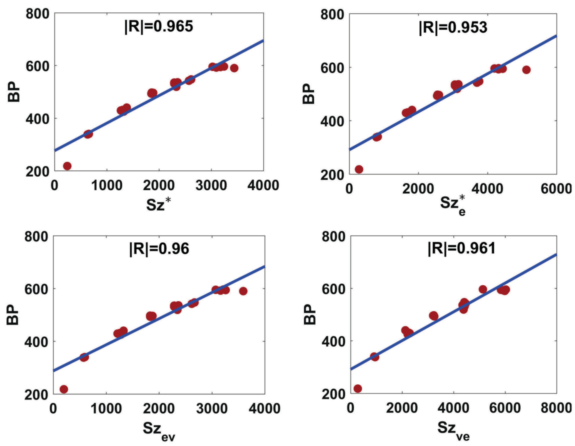

Figure 8. Linear fitting of Sz^*, Sz_e^*, Sz_{ev} and Sz_{ve} with *BP*.

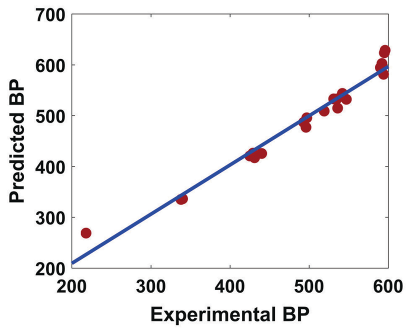

Figure 9. Correlation between exp. and pred. *BP* of BHC by the model (2).

Theorem 3.1. Let Γ be a bicyclic graph of type 1 with order *n*.

1. If p and q are even, then

$A(\Gamma) \le f_1(p,q)$,

$L(\Gamma) \le f_1(p,q) + 4n^2 - 2n(p+q) - 2p^2 + 5p - 2q^2 + 5q - 4$,

$I(\Gamma) \le f_1(p,q) + 2n^2 - n(p+q+2) - p^2 + 4p - (q-2)^2$,

where

$f_1(p,q) = p(n-p)^2 + q(n-q)^2 + (n+1-p-q)(n-2)^2$.

2. If p and q are odd, then

$A(\Gamma) \le f_2(p,q)$,

$L(\Gamma) \le f_2(p,q) + 4(n-1)(n-p-q+1)$,

$I(\Gamma) \le f_2(p,q) + 2n^2 - 3n(p+q) + p^2 + 2p + q^2 + 2q - 2$,

where

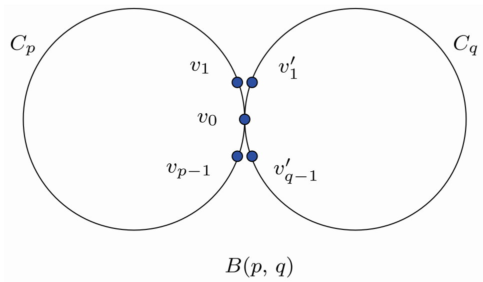

Figure 10. Bicyclic graph $B(p; q)$

$$f_2(p,q) = (n-2)^2(n-p-q+1) + 2(n-p-q+1)^2 + (p-1)(n-p+1)^2 + (q-1)(n-q+1)^2.$$

3. If p is even and q is odd, then

$A(\Gamma) \le f_3(p,q)$,

$L(\Gamma) \le f_3(p,q) + 4n^2 - 2n(2p+q-1) - 2q^2 + 3q - 5$,

$I(\Gamma) \le f_3(p,q) + 2n^2 - n(3p+q-1) + p^2 - p - q^2 + q - 4$,

where

$$f_3(p,q) = p(n-p+1)^2 + (q-1)(n-q)^2 + (n-p-q-1)^2 + (n+1-p-q)(n-2)^2.$$

Proof. The proof of the three cases are the following:

Case 1. Let p and q be even.

Let $e = xy = v_0v_{p-1}$ be the edge of C_p. In the sequel, for convenience we state the proof for $A(\Gamma)$, $L(\Gamma)$ and $I(\Gamma)$., simultaneously.

By Remark 2.5., we consider $\{v_0, v_1, \ldots, v_{p/2-1}\}$ to be the $p/2$ nodes of $V(C_p)$, that are nearer to $x = v_0$ than $y = v_{p-1}$. Consequently, all trees, which are hanging of these vertices are closer to $x = v_0$. Moreover, $\{v_{p/2}, \ldots, v_{p-1}\}$ are the $p/2$ nodes of $V(C_p)$, which are closer to $y = v_{p-1}$ than $x = v_0$, which implies that the trees hang of them are nearer to $y = v_{p-1}$. Besides, all vertices of C_q are closer to $x = v_0$ than $y = v_{p-1}$. It follows that all vertices of trees, which are hanging of $V(C_q)$ to be closer to $x = v_0$ than $y = v_{p-1}$. Therefore, we have:

$$\begin{aligned} n_x(e) - n_y(e) &= (t_0 + t_1 + \cdots + t_{p/2-1} + t_1' + \cdots + t_{q-1}') \\ &\quad -(t_{p/2} + \cdots + t_{p-1}) \\ &= n - 2(t_{p/2} + \cdots + t_{p-1}). \end{aligned}$$

Since we have $t_i \ge 1$, so we get that:

$$n_x(e) - n_y(e) \le n - 2 \times \frac{p}{2} = n - p.$$

Similarly, for arbitrary edge $e = uv \in E(C_p)$, one can obtain $n_u(e) - n_v(e) \le n - p$. By the same argument, for arbitrary edge connection $e = uv \in E(C_q)$, it is clear that $n_u(e) - n_v(e) \le n - 2 \times \frac{q}{2} = n - q$. Also, for every $e = uv$ of a tree, it is clear that $n_u(e) - n_v(e) \le n - 2$. Therefore,

$$A(\Gamma) \le f_1(p,q),$$

where

$$f_1(p,q) = p(n-p)^2 + q(n-q)^2 + (n+1-p-q)(n-2)^2.$$

By Remark 2.6, we know that the $(p-2)/2$ edges of C_p are closer to $x = v_0$ than $y = v_{p-1}$ and the other $(p-2)/2$ edges of C_p are closer to $y = v_{p-1}$ than $x = v_0$. The trees hang from the vertices in the set $\{v_0, v_1, \dots, v_{p/2-1}, v'_1, \dots, v'_{q-1}\}$ are closer to $x = v_0$ than $y = v_{p-1}$. As a result, all edges in these trees and on C_q are closer to $x = v_0$. Also, all the edges of trees those hang from the vertices in the set $\{v_{p/2}, \dots, v_{p-1}\}$ are close to $y = v_{p-1}$. It is obviously that every tree T has $|V(T)|-1$ edges. So by Remark 2.6, we have:

$$\begin{aligned} m_x(e) - m_y(e) &= [(t_0 - 1) + (t_1 - 1) + \cdots \\ &\quad + (t_{p/2-1} - 1) + (p-2)/2 + (t'_1 - 1) + \cdots \\ &\quad + (t'_{q-1} - 1) + q] - [(t_{p/2} - 1) + \cdots \\ &\quad + (t_{p-1} - 1) + (p-2)/2] \\ &= (n - t_{p/2} - \cdots - t_{p-1}) - (t_{p/2} + \cdots + t_{p-1} - 1) \\ &= n - 2(t_{p/2} + \cdots + t_{p-1}) + 1. \end{aligned}$$

Since we have $t_i \ge 1$, so we get that:

$$m_x(e) - m_y(e) \le n - 2 \times \frac{p}{2} + 1 = n - p + 1.$$

Similarly, for other edges $e = uv \in E(C_p)$, we get that $m_u(e) - m_v(e) \le n - p + 1$. By the same argument, for arbitrary edge $e = uv \in E(C_q)$, we get that $m_u(e) - m_v(e) \le n - q + 1$. Also, for every $e = uv$ of a tree, it is clear that $m_u(e) - m_v(e) \le n$. Therefore,

$$L(\Gamma) \le f_1(p,q) + 4n^2 - 2n(p+q) - 2p^2 + 5p - 2q^2 + 5q - 4.$$

By the above discussion, we get that

$$I(\Gamma) \le f_1(p,q) + 2n^2 - n(p+q+2) - p^2 + 4p - (q-2)^2.$$

Case 2. Let p and q be odd.

Since p is odd, so there is exactly one edge $e' = x'y' = v_{(p-1)/2}v_{(p+1)/2} \in E(C_p)$ such that $d_{C_p}(x', v_0) = d_{C_p}(y', v_0)$. In the sequel, for convenience we state the proof for $A(\Gamma)$, $L(\Gamma)$ and $I(\Gamma)$, simultaneously.

Consequently, for every $z \in V(C_q)$, we have $d_\Gamma(x', z) = d_\Gamma(y', z)$. Therefore,

$$\begin{aligned} n_{x'}(e') - n_{y'}(e') &= (t_1 + \ldots + t_{(p-1)/2}) \\ &\quad -(t_{(p-1)/2+1} + \ldots + t_{p-1}) \\ &= (n - t_{(p+1)/2} - \ldots - t_{p-1} - t_0 - t'_1 - \ldots - t'_{q-1}) \\ &\quad -(t_{(p+1)/2} + \ldots + t_{p-1}) \\ &= n - 2(t_{(p+1)/2} + \ldots + t_{p-1}) - t_0 - t'_1 - \ldots - t'_{q-1}. \end{aligned}$$

Since $t_i, t'_i \ge 1$, so

$$n_{x'}(e') - n_{y'}(e') \le n - 2 \times \frac{p-1}{2} - q = n - p - q + 1.$$

Now, let $e = xy \in E(C_p) \setminus \{e'\}$. Without loss of generality, let $d_{C_p}(x, v_0) \le d_{C_p}(y, v_0)$. So $V(C_q)$ is closer to x than y.

By Remark 2.5, we know that there exists a vertex in $V(C_p)$ such that its distances from x and y are equal and other nodes divide to two sets with $(p-1)/2$ nodes that one of these sets is closer to x and another is closer to y. So by the same argument as above, we have:

$$n_x(e) - n_y(e) \le n - 2 \times \frac{p-1}{2} = n - p + 1.$$

Similarly, we find $n_x(e) - n_y(e)$, for every $e = xy \in E(C_q)$. Also, for every $e = xy$ of a tree, we have $n_x(e) - n_y(e) \le n - 2$. Therefore,

$$A(\Gamma) \le f_2(p,q),$$

where

$$\begin{aligned} f_2(p,q) &= (p-1)(n-p+1)^2 + (q-1)(n-q+1)^2 \\ &\quad + 2(n-p-q+1)^2 + (n+1-p-q)(n-2)^2. \end{aligned}$$

Consequently, for every $f \in E(C_q)$, we have $D_\Gamma(x', f) = D_\Gamma(y', f)$. According to the above case we have:

$$\begin{aligned} m_{x'}(e') - m_{y'}(e') &= \left[(t_1 - 1) + \ldots + (t_{(p-1)/2} - 1) + (p-1)/2 \right] \\ &\quad - \left[(t_{(p-1)/2+1} - 1) + \ldots + (t_{p-1} - 1) + (p-1)/2 \right] \\ &= \left[n - t_{(p+1)/2} - \ldots - t_{p-1} - t_0 - t'_1 - \ldots - t'_{q-1} \right] \\ &\quad - \left[t_{(p+1)/2} + \ldots + t_{p-1} \right] \\ &= n - 2(t_{(p+1)/2} + \ldots + t_{p-1}) - t_0 - t'_1 - \ldots - t'_{q-1}. \end{aligned}$$

Then

$$m_{x'}(e') - m_{y'}(e') \le n - 2 \times \frac{p-1}{2} - q = n - p - q + 1.$$

Now, let $e = xy \in E(C_p) \setminus \{e'\}$. Without loss of generality, we can assume that $d_{C_p}(x, v_0) \le d_{C_p}(y, v_0)$. So $V(C_q)$ is closer to x than y. By Remark 2.6, the edge set of C_p divide to two sets with $(p-1)/2$ edges that one of these sets is closer to x and another is closer to y. Thus, we have:

$$m_x(e) - m_y(e) \le n - 2 \times \frac{p-1}{2} = n - p + 1.$$

Similarly, we have $m_x(e) - m_y(e) \le n - q + 1$, for every $e = xy \in E(C_q)$. Also, for every $e = xy$ of a tree, we have $n_x(e) - n_y(e) \le n$. Therefore,

$$L(\Gamma) \le f_2(p,q) + 4(n-1)(n-p-q+1).$$

By the above discussion, it is clear that

$$I(\Gamma) \le f_2(p,q) + 2n^2 - 3n(p+q) + p^2 + 2p + q^2 + 2q - 2.$$

Case 3. Let p be even and q be odd.
Similarly, from the above discussion, we obtain:

$$A(\Gamma) \le f_3(p,q), L(\Gamma) \le f_3(p,q) + 4n^2 - 2n(2p+q-1) - 2q^2 + 3q - 5, I(\Gamma) \le f_3(p,q) + 2n^2 - n(3p+q-1) + p^2 - p - q^2 + q - 4,$$

where

$$f_3(p,q) = p(n-p+1)^2 + (q-1)(n-q)^2 + (n-p-q-1)^2 + (n+1-p-q)(n-2)^2.$$

□

3.2.2. Bicyclic graph of type 2

Let Γ be a bicyclic graph of type 2 with order n. Hence, Γ has a subgraph $B(p,\ell,q)$, where $p,q \ge 3$ and $\ell \ge 2$. Let the common vertex of P_ℓ with C_p and C_q, respectively, say v_1 and $v_{p+\ell-1}$. Moreover, $V(C_p) = \{v_1, v_2, \ldots, v_p\}$, $V(C_q) = \{v_{p+\ell-1}, v_{p+\ell}, v_{p+\ell+1}, \ldots, v_{p+\ell+q-2}\}$ and also $V(P_\ell) = \{v_1, v_{p+1}, v_{p+2}, \ldots, v_{p+\ell-1}\}$ (see the Figure 11.). Since Γ is a bicyclic graph, so no cycle hangs from the vertices of $B(p,\ell,q)$. We can consider T_i to be the tree which is hanging from vertex v_i, where $i \in \{1, \ldots, p+q+\ell-2\}$. Let $|T_i| = t_i$, so $t_i \ge 1$. It is clear that $n = \sum_{i=1}^{p+q+\ell-2} t_i$.

Theorem 3.2. Let Γ be a bicyclic graph of type 2 with order n. Then

1. If p and q are even, then

$$A(\Gamma) \le g_1(p,q,\ell),$$

$$L(\Gamma) \le g_1(p,q,\ell) + \alpha,$$

$$I(\Gamma) \le g_1(p,q,\ell) + \beta,$$

where

$$g_1(p,q,\ell) = p(n-p)^2 + q(n-q)^2 + \sum_{i=-1}^{\ell-3} (n - 2(q+\ell-i-3))^2 + (n+2-p-q-\ell)(n-2)^2,$$

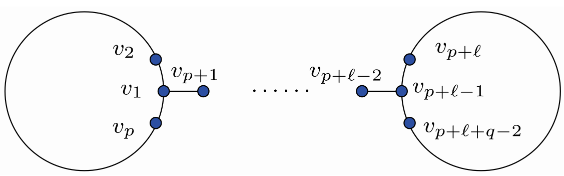

Figure 11. Bicyclic graph $B(p;\ \ell;\ q)$

$$\alpha = -4\ell(n-1) + 4n^2 - 2n(p+q-2) - 2p^2 + 5p - 2q^2 + 5q - 8$$

and

$$\beta = -2\ell(n-2) + 2n^2 - n(p+q) - p^2 + 4p - q^2 + 4q - 8.$$

2. If p and q are odd, then

$$A(\Gamma) \le g_2(p,q,\ell),$$

$$L(\Gamma) \le g_2(p,q,\ell) + \alpha + 2(-2n+p+q-1),$$

$$I(\Gamma) \le g_2(p,q,\ell) + \beta - 2n + p + q,$$

where

$$g_2(p,q,\ell) = (p-1)(n-p)^2 + (q-1)(n-q)^2 + 2(n-p-q-\ell)^2 + \sum_{i=-1}^{\ell-3} (n-2(q+\ell-i-3))^2 + (n+2-p-q-\ell)(n-2)^2.$$

3. If p is even and q is odd, then

$$A(\Gamma) \le g_3(p,q,\ell),$$

$$L(\Gamma) \le g_3(p,q,\ell) + \alpha - 2n + 2q - 1,$$

$$I(\Gamma) \le g_3(p,q,\ell) + \beta + q - n,$$

where

$$g_3(p,q,\ell) = p(n-p)^2 + (q-1)(n-q)^2 + (n-p-q-\ell)^2 + \sum_{i=-1}^{\ell-3} (n-2(q+\ell-i-3))^2 + (n+2-p-q-\ell)(n-2)^2.$$

Proof. The proof of the three cases are the following:

Case 1. Let p and q be even.

Let $e = xy = v_1 v_p \in E(C_p)$.

In this case, $\{v_1, \ldots, v_{p/2}\}$ are closer to $x = v_1$ than $y = v_p$. So the vertices of all trees hang of them to be closer to $x = v_1$. Also, $\{v_{p/2+1}, \ldots, v_p\}$ are closer to $y = v_p$ than $x = v_1$, which implies that the vertices of all trees hang of them to be closer to $y = v_p$. As a result, all vertices of C_q and P_ℓ and so the vertices of all trees hang of them are closer to $x = v_1$ than $y = v_p$. It follows that

$$\begin{aligned} n_x(e) - n_y(e) &= [t_1 + \ldots t_{p/2} + t_{p+1} + \ldots + t_{p+q+\ell-2}] \\ &\quad - [t_{p/2+1} + \ldots + t_p] \\ &= [n - t_{p/2+1} - \ldots - t_p] - [t_{p/2+1} + \ldots + t_p] \\ &= n - 2[t_{p/2+1} + \ldots + t_p]. \end{aligned}$$

Since $t_i \ge 1$, for every i, we obtain

$$n_x(e) - n_y(e) \le n - 2 \times \frac{p}{2} = n - p.$$

Similarly, for the other edges of C_p, we get the same result.

Similar to the above discussion, if $e = xy \in E(C_q)$, then $n_x(e) - n_y(e) \le n - q$.

Now, let $e = xy \in P_\ell$. If $e = v_1 v_{p+1}$, then by the same argument as the above, we have:

$$\begin{aligned} n_x(e) - n_y(e) &= [t_1 + \dots t_p] - [t_{p+1} + \dots + t_{p+q+\ell-2}] \\ &= n - 2[t_{p+1} + \dots + t_{p+q+\ell-2}] \le n - 2(q + \ell - 2). \end{aligned}$$

Otherwise, $e = v_{p+i+1} v_{p+i+2}$, where $0 \le i \le \ell - 3$. Then

$$\begin{aligned} n_x(e) - n_y(e) &= [t_1 + \dots t_{p+i+1}] - [t_{p+i+2} + \dots + t_{p+q+\ell-2}] \\ &= n - 2[t_{p+i+2} + \dots + t_{p+q+\ell-2}] \\ &\le n - 2(q + \ell - i - 3). \end{aligned}$$

Also, we know that for every $e = xy$ of a tree, $n_x(e) - n_y(e) \le n - 2$. Therefore,

$$\begin{aligned} A(\Gamma) \le{} & p(n-p)^2 + q(n-q)^2 + (n - 2(q + \ell - 2))^2 \\ & + \sum_{i=0}^{\ell-3} (n - 2(q + \ell - i - 3))^2 + (n + 2 - p - q - \ell)(n-2)^2. \end{aligned}$$

Hence,

$$A(\Gamma) \le g_1(p, q, \ell),$$

where

$$\begin{aligned} g_1(p,q,\ell) = {} & p(n-p)^2 + q(n-q)^2 \\ & + \sum_{i=-1}^{\ell-3} (n - 2(q + \ell - i - 3))^2 \\ & + (n + 2 - p - q - \ell)(n-2)^2 \end{aligned}.$$

We know that $\{v_1, \dots, v_{p/2}, v_{p+1}, \dots, v_{p+q+\ell-2}\}$ and so the trees hang of them are closer to $x = v_1$ than $y = v_p$. As a result, all edges in these trees, $E(C_q)$ and $E(P_\ell)$ are closer to $x = v_1$. Also, $\{v_{p/2+1}, \dots, v_p\}$ and so all edges of trees which hang of them are closer to $y = v_p$. So by Remark 2.6., we have:

$$\begin{aligned} m_x(e) - m_y(e) &= [(t_1 - 1) + \dots + (t_{p/2} - 1) + (p-2)/2 \\ &\quad + (t_{p+1} - 1) + \dots + (t_{p+q+\ell-2} - 1) + q + \ell - 1] \\ &\quad - [(t_{p/2+1} - 1) + \dots + (t_p - 1) + (p-2)/2] \\ &= n - 2(t_{p/2+1} + \dots + t_p) + 1. \end{aligned}$$

Since $t_i \ge 1$, we obtain

$$m_x(e) - m_y(e) \le n - 2 \times \frac{p}{2} + 1 = n - p + 1.$$

Similarly, for other edges $e = xy \in E(C_p)$, we get that $n_x(e) - n_y(e) \le n - p + 1$.

By the same argument, for any arbitrary edge $e = xy \in E(C_q)$, we get that $m_x(e) - m_y(e) \le n - q + 1$.

Let $e = xy \in E(P_\ell)$. If $e = v_1 v_{p+1}$, then similar to the above discussion, we have $m_x(e) - m_y(e) = [(t_1 - 1) + \dots + (t_p - 1) + p] - [(t_{p+1} - 1) + \dots + (t_{p+q+\ell-2} - 1) + q + \ell - 2] = n - 2(t_{p+1} + \dots + t_{p+q+\ell-2}) \le n - 2(q + \ell - 2)$.

Otherwise, $e = v_{p+i+1} v_{p+i+2}$, where $0 \le i \le \ell - 3$. In this case, we have $m_x(e) - m_y(e) = [(t_1 - 1) + \dots + (t_{p+i+1} - 1) + p + i + 1] - [(t_{p+i+2} - 1) + \dots + (t_{p+q+\ell-2} - 1) + q + \ell - i - 3] \le n - 2(q + \ell - i - 3)$.

Also, for every $e = xy$ of a tree, it is clear that $m_x(e) - m_y(e) \le n$.

Therefore,

$$L(\Gamma) \le g_1(p, q, \ell) + \alpha,$$

where

$$\begin{aligned} \alpha = {} & -4l(n-1) + 4n^2 - 2n(p+q-2) \\ & -2p^2 + 5p - 2q^2 + 5q - 8 \end{aligned}.$$

Similarly, by the above discussion, we get that

$$I(\Gamma) \le g_1(p, q, \ell) + \beta$$

where

$$\beta = -2l(n-2) + 2n^2 - n(p+q) - p^2 + 4p - q^2 + 4q - 8.$$

Case 2. Let p and q be odd.

Since p is odd, so there is exactly one edge $e' = x'y' = v_{(p+1)/2} v_{(p+3)/2} \in E(C_p)$ such that

$$d_{C_p}(x', v_1) = d_{C_p}(y', v_1).$$

Consequently, for every $z \in V(C_q)$ and $z \in V(P_\ell)$, we have $d_\Gamma(x', z) = d_\Gamma(y', z)$. Moreover, by Remark 2.5., we know that $(p-1)/2$ vertices of $V(C_p)$ are closer to $x' = v_{(p+1)/2}$ and $(p-1)/2$ other vertices of $V(C_p)$ are closer to $y' = v_{(p+3)/2}$. Therefore,

$$\begin{aligned} n_{x'}(e') - n_{y'}(e') &= (t_2 + \dots + t_{(p+1)/2}) - (t_{(p+1)/2+1} + \dots + t_p) \\ &= (n - t_{(p+3)/2} - \dots - t_p - t_1 - t_{p+1} - \dots \\ &\quad - t_{p+q+\ell-2}) - (t_{(p+3)/2} + \dots + t_p) \\ &\le n - 2 \times \frac{p-1}{2} - (q + \ell - 2) - 1 \\ &= n - p - q - \ell. \end{aligned}$$

Now, let $e = xy \in E(C_p) \setminus \{e'\}$. Without loss of generality, let $d_{C_p}(x, v_1) \le d_{C_p}(y, v_1)$. So $V(C_q)$ and $V(P_\ell)$ are closer to x than y.

By Remark 2.5., we know that there exists a vertex in $V(C_p)$ such that its distances from x and y are equal and other vertices divide to two sets with $(p-1)/2$ vertices such that one of these sets is closer to x and another is closer to y. So by the same argument as above, we have

$$n_x(e) - n_y(e) \le n - 2 \times \frac{p-1}{2} - 1 = n - p.$$

Similarly, we find $n_x(e) - n_y(e)$, for every $e = xy \in E(C_q)$.

If $e = xy \in E(P_\ell)$, then similar to the above case, we have $n_x(e) - n_y(e) \le (n - 2(q + \ell - i - 3))$, where $-1 \le i \le \ell - 3$.

Also, for every $e = xy$ of a tree, we have $n_x(e) - n_y(e) \le n - 2$. Therefore,

$$A(\Gamma) \le g_2(p,q,\ell),$$

where

$$g_2(p,q,\ell) = (p-1)(n-p)^2 + (q-1)(n-q)^2 + 2(n-p-q-\ell)^2 + \sum_{i=-1}^{\ell-3}(n-2(q+\ell-i-3))^2 + (n+2-p-q-\ell)(n-2)^2.$$

For every $f \in E(C_q)$ and $f \in E(P_\ell)$, we have $D_\Gamma(x',f) = D_\Gamma(y',f)$. By Remark 2.6., we know that $(p-1)/2$ edges of $E(C_p)$ are closer to x' and $(p-1)/2$ other edges of $E(C_p)$ are closer to y'. According to the above case, we have

$$\begin{aligned} m_{x'}(e') - m_{y'}(e') &= [(t_2-1)+\ldots+(t_{(p+1)/2}-1)+(p-1)/2] \\ &\quad -[(t_{(p+1)/2+1}-1)+\ldots+(t_p-1)+(p-1)/2] \\ &= [n-t_{(p+3)/2}-\ldots-t_p-t_1-t_{p+1}-\ldots \\ &\quad -t_{p+q+\ell-2}]-[t_{(p+3)/2}+\ldots+t_p] \\ &\le n-2\times\frac{p-1}{2}-1-(q+\ell-2)=n-p-q-\ell. \end{aligned}$$

Now, let $e = xy \in E(C_p) \setminus \{e'\}$. Without loss of generality, let $d_{C_p}(x,v_1) \le d_{C_p}(y,v_1)$. So $V(C_q)$ and $V(P_\ell)$ are closer to x than y. We know that $(p-1)/2$ edges of $E(C_p)$ are closer to x and the other $(p-1)/2$ edges of $E(C_p)$ are closer to y, by Remark 2.6. Therefore,

$$m_x(e) - m_y(e) \le n - p + 1.$$

Similarly, we find $m_x(e) - m_y(e)$, for every $e = xy \in E(C_q)$.

Moreover, for $e = xy \in E(P_\ell)$, similar to the above case, we have $m_x(e) - m_y(e) \le n - 2(q+\ell-i-3)$, where $-1 \le i \le \ell - 3$.

Also, for every $e = xy$ of a tree, we have $m_x(e) - m_y(e) \le n$.

Consequently,

$$L(\Gamma) \le g_2(p,q,\ell) + \alpha + 2(-2n+p+q-1).$$

By the above discussion, it is clear that

$$I(\Gamma) \le g_2(p,q,\ell) + \beta - 2n + p + q.$$

Case 3. Let p be even and q be odd.

Similarly to the above discussion, we obtain

$$A(\Gamma) \le g_3(p,q,\ell),$$

$$L(\Gamma) \le g_3(p,q,\ell) + \alpha - 2n + 2q - 1,$$

$$I(\Gamma) \le g_3(p,q,\ell) + \beta + q - n,$$

where

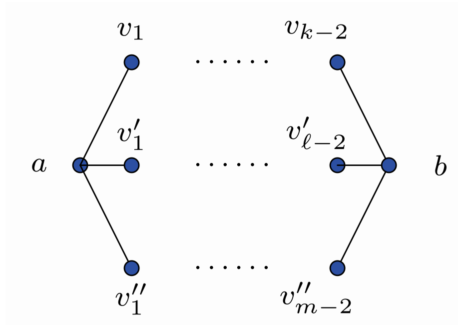

Figure 12. Bicyclic graph $B(P_k; P_\ell; P_m)$.

$$g_3(p,q,\ell) = p(n-p)^2 + (q-1)(n-q)^2 + (n-p-q-\ell)^2 + \sum_{i=-1}^{\ell-3}(n-2(q+\ell-i-3))^2 + (n+2-p-q-\ell)(n-2)^2.$$

3.2.3. Bicyclic Graph of Type 3

Let Γ be a bicyclic graph of type 3 with order n. Hence, Γ has a subgraph $B(P_k,P_\ell,P_m)$, where $k \le \ell \le m$. Let the common vertices of three paths P_k, P_ℓ and P_m, say a and b. Moreover, let $V(P_k) = \{a,v_1,v_2,\ldots,v_{k-2},b\}$, $V(P_\ell) = \{a,v'_1,v'_2,\ldots,v'_{\ell-2},b\}$ and $V(P_m) = \{a,v''_1,v''_2,\ldots,v''_{m-2},b\}$ (see, Figure 12.). In the following of this section, we use v_0, v'_0 or v''_0 instead of a and we use v_{k-1}, $v'_{\ell-1}$ or v''_{m-1} instead of b. Since Γ is a bicyclic graph, so no cycle hangs from the vertices of $B(P_k,P_\ell,P_m)$. As a result, we can consider T_i, T'_j and T''_s to be the trees which are hanging from vertices v_i, v'_i and v''_i respectively, where $i \in \{0,1,\ldots,k-1\}, j \in \{0,1,\ldots,\ell-1\}$ and $s \in \{1,2,\ldots,m-1\}$. Let $|T_i| = t_i$, $|T'_i| = t'_i$ and $|T''_i| = t''_i$, so $t_i, t'_i, t''_i \ge 1$. It is clear that $n = \sum_{i=0}^{k-1} t_i + \sum_{j=0}^{\ell-2} t'_j + \sum_{s=1}^{m-2} t''_j$. We can consider the following cycles in $B(P_k,P_\ell,P_m)$:

$$l_1 = \{a\ v_1 \ldots v_{k-2} b\ v''_{m-2} v''_{m-3} \ldots v''_1 a\},$$

$$l_2 = \{a\ v'_1 \ldots v'_{\ell-2} b\ v''_{m-2} v''_{m-3} \ldots v''_1 a\},$$

$$l_3 = \{a\ v_1 \ldots v_{k-2} b\ v'_{\ell-2} v'_{\ell-3} \ldots v'_1 a\}.$$

Consider $F^k_{m,\ell} = \sum_{i=0}^{k-2}(n-m-\ell-2i)^2$.

Theorem 3.3. Let Γ be a bicyclic graph of type 3 with order n.

1. If k, ℓ and m are even or if k, ℓ and m are odd, then

$$A(\Gamma) \le \mathcal{F}_1(k,\ell,m),$$

$$L(\Gamma) \le F^k_{m,\ell-1} + F^\ell_{m,k-1} + F_{k,\ell-1}^{\frac{m+\ell-2}{2}} - F_{k,\ell-1}^{\frac{m-\ell-2}{2}} + \alpha_2,$$

$$I(\Gamma) \le \mathcal{F}_1(k,\ell,m) + \beta_2,$$

where

$$\mathcal{F}_1(k,\ell,m) = F^k_{m,\ell} + F^\ell_{m,k} + F_{k,\ell}^{\frac{m+\ell-2}{2}} - F_{k,\ell}^{\frac{m-\ell-2}{2}} +(m-\ell+1)(n-k-m+2)^2 +(n-m-k-\ell-3)(n-2)^2,$$

$$\alpha_2 = (m-\ell+1)(n-k-m+3)^2 + (n-m-k-\ell-3)n^2,$$

$$\beta_2 = -k^2 + k(-\ell-3m+n+9) - \ell^2 - \ell(m-8) -2m^2+2mn+12m+12n^2-43n+4.$$

2. If k and ℓ are even and m is odd or if k and ℓ are odd and m is even, then

$$A(\Gamma) \le \mathcal{F}_2(k,\ell,m),$$

$$L(\Gamma) \le F^k_{m,\ell-3} + F^\ell_{m,k-3} + F_{k,\ell-4}^{\frac{m+\ell-1}{2}} - F_{k,\ell-4}^{\frac{m-\ell+3}{2}} + \alpha_2,$$

$$I(\Gamma) \le \mathcal{F}_2(k,\ell,m) + \beta_2 + k(m-\ell-2n+2) -\ell^2 - l(n-7) + m^2 - 3mn -3m - 10n^2 + 30n - 8,$$

where

$$\mathcal{F}_2(k,\ell,m) = F^k_{m,\ell-2} + F^\ell_{m,k-2} + F_{k,\ell-3}^{\frac{m+\ell-1}{2}} - F_{k,\ell-3}^{\frac{m-\ell+3}{2}} +(m-\ell+1)(n-m-k+2)^2 +(n-m-k-\ell-3)(n-2)^2.$$

3. If k and m are even and ℓ is odd or if k and m are odd and ℓ is even, then

$$A(\Gamma) \le \mathcal{F}_3(k,\ell,m),$$

$$L(\Gamma) \le F^k_{m,\ell-3} + F^m_{m,k-4} + F_{k,\ell-3}^{\frac{m+\ell-1}{2}} - F_{k,\ell-3}^{\frac{m-\ell+3}{2}} + \alpha_2 +(\ell-m)(k+m-n-3)^2,$$

$$I(\Gamma) \le \mathcal{F}_3(k,\ell,m) + \beta_2 + k(m-\ell-2n+2) -\ell(n-3) - 3mn + m - 10n^2 + 30n - 7,$$

where

$$\mathcal{F}_3(k,\ell,m) = F^k_{m,\ell-2} + F^m_{m,k-3} + F_{k,\ell-2}^{\frac{m+\ell-1}{2}} - F_{k,\ell-2}^{\frac{m-\ell+3}{2}} +(n-m-k+2)^2 +(n-m-k-\ell-3)(n-2)^2.$$

4. If ℓ and m are even and k is odd or if ℓ and m are odd and k is even, then

$$A(\Gamma) \le \mathcal{F}_4(k,\ell,m),$$

$$L(\Gamma) \le F^k_{m,\ell-4} + F_{m,k-3}^{\frac{k+\ell-1}{2}} - F_{m,k-3}^{\frac{\ell-k+3}{2}} + F_{\ell,k-3}^{\frac{k+m-1}{2}} - F_{\ell,k-3}^{\frac{m-k+3}{2}} +\alpha_2 + (\ell-m-1)(k+m-n-3)^2 +(-2k+\ell+m+2)(\ell+m-n-3)^2,$$

$$I(\Gamma) \le \mathcal{F}_4(k,\ell,m) + \beta_2 - 2k^2 + k(2m-2n+9) -\ell(m+n-1) + m^2 - 3mn -3m - 10n^2 + 30n - 9,$$

where

$$\mathcal{F}_4(k,\ell,m) = F^k_{m,\ell-3} + F_{m,k-2}^{\frac{k+\ell-1}{2}} - F_{m,k-2}^{\frac{\ell-k+3}{2}} + F_{\ell,k-2}^{\frac{k+m-1}{2}} - F_{\ell,k-2}^{\frac{m-k+3}{2}} -(2k-\ell-m-2)(\ell+m-n-2)^2 +(n-m-k-\ell-3)(n-2)^2.$$

Proof. The proof of the four cases are the following:

Case 1. Let k, ℓ and m be even.

Step 1. Let $e = xy \in E(P_k)$.

Hence, $e = xy = v_i v_{i+1}$, where $0 \le i \le k-2$. Clearly, this edge is on l_1. The length of l_1 is equal to $k+m-2$, so it is an even cycle. As a result, $(k+m-2)/2$ vertices on l_1 are closer to $x = v_i$ than $y = v_{i+1}$, by Remark 2.5. It follows that all vertices of trees, which are hanging from them are closer to $x = v_i$. Besides, the other $(k+m-2)/2$ vertices on l_1 and so all vertices of trees, which hang of them are closer to $y = v_{i+1}$ than $x = v_i$, by Remark 2.5. Therefore, it is enough to discuss about $A = \{v'_1, \ldots, v'_{\ell-2}\}$. We know that $e \in l_3$. Notice, l_3 is an even cycle, thus there is no vertex on l_3 such that has the same distances from $x = v_i$ and $y = v_{i+1}$, by Remark 2.5. Since $\ell \ge k$, so for every $0 \le i \le k-2$, there is $0 \le j \le \ell-1$ such that $d_\Gamma(v'_j, v_{i+1}) < d_\Gamma(v'_j, v_i)$, it follows that

$$i+j > \ell-1-j+k-1-(i+1) \Rightarrow j \ge (\ell+k-2)/2-i-1.$$

Also, if $v'_z \in A$ such that $z \ge j$, then $d_\Gamma(v'_z, v_{i+1}) < d_\Gamma(v'_z, v_i)$. In addition, all vertices of trees which are hanging from such v'_z are closer to v_{i+1} than v_i.

Therefore,

$$n_x(e) - n_y(e) \le n - 2[(k+m-2)/2 + \sum_{\frac{\ell+k-2}{2}-i-1}^{\ell-2} 1] = n-m-\ell-2i.$$

Step 2. Let $e = xy \in E(P_\ell)$.

It is clear that $B(P_k, P_\ell, P_m)$ is isomorphic to $B(P_\ell, P_m, P_k)$, hence in sequel of this step we can consider it.

Completely similar to the above step, we get that

$$n_x(e) - n_y(e) \le n - 2[(k+\ell-2)/2 + \sum_{\frac{\ell+m-2}{2}-i-1}^{\ell-2} 1] = n-m-k-2i.$$

Step 3. Let $e = xy \in E(P_m)$.

Hence, $e = xy = v''_i v''_{i+1}$, where $0 \le i \le m-2$. Clearly, this edge is on l_1. Similar to the above, $(k+m-2)/2$ vertices on l_1 and all vertices of trees hang of them are closer to $x = v''_i$ than $y = v''_{i+1}$, by Remark 2.5. Moreover, the other $(k+m-2)/2$ vertices on l_1 and so all vertices of trees, which hang of them are closer to $y = v''_{i+1}$ than $x = v''_i$, by Remark 2.5. Consequently, we discuss about vertices in $A=\{v'_1,\dots,v'_{\ell-2}\}$. On the other hand, $e\in I_2$. By Remark 2.5., there is no vertex on I_2 such that has the same distances from $x=v''_i$ and $y=v''_{i+1}$. If $v'_j\in A$ such that $d_\Gamma(v'_j,v''_{i+1})<d_\Gamma(v'_j,v''_i)$, then similar to the above, we have $j\geq(\ell+m-2)/2-i-1$. Notice, $m\geq\ell$. Since $1\leq j\leq\ell-2$, so $(m-\ell)/2\leq i\leq((m+\ell)/2-3$. It is clear that, if $v'_z\in A$ such that $j\leq z$, then all vertices of trees which are hanging from such v'_z are closer to $y=v''_{i+1}$ than $x=v''_i$. Therefore,

$$n_x(e)-n_y(e)\leq n-2\Big[(k+m-2)/2+\sum_{\frac{\ell+m-2}{2}-i-1}^{\ell-2}1\Big]$$
$$=n-k-\ell-2i.$$

Otherwise, suppose that $d_\Gamma(v'_j,v''_{i+1})>d_\Gamma(v'_j,v''_i)$ for every $v'_j\in A$. Thus we have

$$n_x(e)-n_y(e)\leq n-2(\frac{k+m-2}{2})=n-k-m+2.$$

Consequently, we have

$$n_x(e)-n_y(e)\leq\begin{cases} n-k-\ell-2i & \text{if } \dfrac{m-\ell}{2}\leq i\leq\dfrac{m+\ell}{2}-3,\\ n-k-m+2 & \text{otherwise.}\end{cases}$$

Step 4. Let $e=xy$ be an edge of a tree hangs of a vertex in $B(P_k,P_\ell,P_m)$.

We know that $n_x(e)-n_y(e)\leq n-2$.

Consequently, by the above four steps, we have:

$$A(\Gamma)\leq\mathcal{F}_1(k,\ell,m),$$

where

$$\mathcal{F}_1(k,\ell,m)=F^k_{m,\ell}+F^\ell_{m,k}+F_{k,\ell}^{\frac{m+\ell-2}{2}}-F_{k,\ell}^{\frac{m-\ell-2}{2}}$$
$$+(m-\ell+1)(n-k-m+2)^2$$
$$+(n-m-k-\ell-3)(n-2)^2.$$

If $e=xy\in I_1$, then by Remark 2.6., we know that the number of edges on I_1, which are closer to x than y is equal to the number of edges on I_1, which are closer to y than x. Therefore, edges on I_1 are not effective in calculating $m_x(e)-m_y(e)$.

We know that the number of edges on a tree T is equal to $|V(T)|-1$. On the other hand, by Remark 2.5., the number of trees that are hanging from the vertices on I_1, which are closer to x than y is equal to the number of trees that are hanging from the vertices on I_1, which are closer to y than x. Consequently, the number of (-1) caused by these trees in $m_x(e)$ is equal to the number of (-1) caused by those trees in $m_y(e)$. Thus, they are not effective in calculating $m_x(e)-m_y(e)$.

Now, we discuss about the edges on P_ℓ and on trees which are hanging from the vertices $A=\{v'_1,\dots,v'_{\ell-2}\}$. We know that there are $\ell-1$ edges on P_ℓ and $\ell-2$ trees on middle vertices of path. Hence, for every $v'_j\in A$ such that v'_j is closer to x than y, there is an edge on P_ℓ, which is closer to x than y, and converse. It follows that in calculating $m^*=m_x(e)-m_y(e)$ we have to calculate $n^*=n_x(e)-n_y(e)$ and the maximum difference between value of m^* and n^* is equal to 1.

Let $e\in E(P_\ell)$. Since $B(P_k,P_\ell,P_m)$ is isomorphic to $B(P_\ell,P_m,P_k)$, so we can consider it and again similar to the above argument, we get that the maximum difference between the values of m^* and n^* is equal to 1.

Let $e=xy$ be an edge of a tree. It is clear that $m_x(e)-m_y(e)\leq n$.

Therefore,

$$L(\Gamma)\leq F^k_{m,\ell-1}+F^\ell_{m,k-1}+F_{k,\ell-1}^{\frac{m+\ell-2}{2}}-F_{k,\ell-1}^{\frac{m-\ell-2}{2}}+\alpha_2,$$

where

$$\alpha_2=(m-\ell+1)(n-k-m+3)^2+(n-m-k-\ell-3)n^2.$$

By the above discussion, we get that

$$I(\Gamma)\leq\mathcal{F}_1(k,\ell,m)+\beta_2,$$

where

$$\beta_2=-k^2+k(-\ell-3m+n+9)-\ell^2-\ell(m-8)$$
$$-2m^2+2mn+12m+12n^2-43n+4.$$

Moreover, if k, ℓ and m are odd, then we get the same result.

Case 2. Let k and ℓ be even and m be odd.

Step 1. Let $e=xy\in E(P_k)$.

It is clear that $B(P_k,P_\ell,P_m)$ is isomorphic to $B(P_k,P_m,P_\ell)$, hence in sequel of this step we can consider it.

Let $e=xy=v_iv_{i+1}$, where $0\leq i\leq k-2$. Obviously, $e\in I_3$ and I_3 is an even cycle, so by Remark 2.5., there are $(k+\ell-2)/2$ vertices on I_3 such that they are closer to $x=v_i$ than $y=v_{i+1}$, as a result all vertices of trees which are hanging from them are closer to $x=v_i$ than $y=v_{i+1}$. Also by Remark 2.5., the other $(k+\ell-2)/2$ vertices on I_3 and so all vertices of trees which are hanging from them are closer to $y=v_{i+1}$ than $x=v_i$. Therefore, it is enough that we discuss about the vertices in $A=\{v''_1,\dots,v''_{m-2}\}$. On the other hand, $e\in I_1$ and I_1 is an odd cycle. By Remark 2.5., there is a vertex v on I_1 such that $d_{\Gamma'}(v,v_i)=d_{\Gamma'}(v,v_{i+1})$. Since $m>k$, so $v\in A$. Let $v=v''_j$, it follows that

$$i+j=m-1-j+k-1-(i+1)\ \Rightarrow\ j=(m+k-3)/2-i.$$

It is clear that if $v''_z\in A$ such that $z>j$, then $d_{\Gamma'}(v''_z,v_i)>d_{\Gamma'}(v''_z,v_{i+1})$. In addition, all vertices of trees which are hanging from such v''_z are closer to $y=v_{i+1}$ than

$x = v_i$.

Therefore,

$$n_x(e) - n_y(e) \le n - 2\Big[(k+\ell-2)/2 + \sum_{j+1}^{m-2} 1\Big] - 1$$
$$= n - m - \ell - 2i + 2.$$

Step 2. Let $e = xy \in E(P_\ell)$.

Again, since $B(P_k, P_\ell, P_m)$ is isomorphic to $B(P_k, P_m, P_\ell)$, so in sequel of this step we can consider it.

Let $e = xy = v'_i v'_{i+1}$, where $0 \le i \le \ell - 2$. Similar to the above step $(k+\ell-2)/2$ vertices on l_3 and all vertices of trees which are hanging from them are closer to $x = v'_i$ than $y = v'_{i+1}$. Moreover, the other $(k+\ell-2)/2$ vertices on l_3 and so all vertices of trees which are hanging from them are closer to $y = v'_{i+1}$ than $x = v'_i$. Furthermore, we discuss about the vertices in $A = \{v''_1, \ldots, v''_{m-2}\}$. Also, since $m > \ell$, so there is a vertex $v''_j \in A$ such that $d_{\Gamma'}(v''_j, v'_i) = d_{\Gamma'}(v''_j, v'_{i+1})$. Consequently, $j = (m+\ell-3)/2 - i$ and if $v''_z \in A$ such that $z > j$, then $d_{\Gamma'}(v''_z, v'_i) > d_{\Gamma'}(v''_z, v'_{i+1})$. As a result,

$$n_x(e) - n_y(e) \le n - 2[(k+\ell-2)/2 + \sum_{j+1}^{m-2} 1] - 1$$
$$= n - m - k - 2i + 2.$$

Step 3. Let $e = xy \in E(P_m)$.

Let $e = xy = v''_i v''_{i+1}$, where $0 \le i \le m-2$. In this case $e \in l_1$. Since l_1 is an odd cycle, so there is a vertex on l_1, which has the same distances from $x = v''_i$ and $y = v''_{i+1}$ on Γ, by Remark 2.5. Hence the vertices on tree hangs of it have the same distances from v''_i and v''_{i+1} on Γ, too. In addition, $(k+m-3)/2$ vertices on l_1 are closer to v''_i than v''_{i+1}, as a result all vertices of trees which are hanging from them are closer to v''_i than v''_{i+1}. Also by Remark 2.5., the other $(k+m-3)/2$ vertices on l_1 and so all vertices of trees which are hanging from them are closer to v''_{i+1} than v''_i. Therefore, it is enough that we discuss about the vertices in $A' = \{v'_1, \ldots, v'_{\ell-2}\}$. On the other hand, $e \in l_2$ and l_2 is an odd cycle, which implies that there is a vertex v on l_2 such that $d_\Gamma(v, v''_i) = d_\Gamma(v, v''_{i+1})$. If $v \in l_1 \cap l_2$, then all vertices in *A*' are closer to either v''_i or v''_{i+1}. Since in formula of $A(\Gamma)$ we need the square of $n_x(e) - n_y(e)$ for every edge *xy* in Γ, so it makes no difference to suppose that they are closer to v''_i or v''_{i+1}. Let all vertices in *A*' be closer to v''_i. Therefore,

$$n_x(e) - n_y(e) \le n - 2[(k+m-3)/2] - 1 = n - m - k + 2.$$

Otherwise, $v \in l_1 \cap A'$. Let $v = v'_j$. Therefore $j = (m+\ell-3)/2 - i$. On the other hand, $1 \le j \le \ell - 2$, it follows that $(m-\ell+1)/2 \le i \le (m+\ell-5)/2$. Similar to the above steps $v'_z \in A'$ such that $z > j$, then $d_\Gamma(v'_z, v''_i) > d_\Gamma(v'_z, v''_{i+1})$. As a result,

$$n_x(e) - n_y(e) \le n - 2[(k+m-3)/2 + \sum_{j+1}^{\ell-2} 1] - 1$$
$$= n - \ell - k - 2i + 3.$$

Therefore, in this case we have

$$n_x(e) - n_y(e) \le \begin{cases} n-\ell-k-2i+3 & \text{if } \dfrac{m-\ell+1}{2} \le i \le \dfrac{m+\ell-5}{2}, \\ n-m-k+2 & \text{otherwise.} \end{cases}$$

Step 4. Let $e = xy$ be an edge of a tree hangs from a vertex in $B(P_k, P_\ell, P_m)$.

We know that $n_x(e) - n_y(e) \le n - 2$. Consequently, by the above four steps, we have:

$$A(\Gamma) \le \mathcal{F}_2(k, \ell, m),$$

where

$$\mathcal{F}_2(k,\ell,m) = F^k_{m,\ell-2} + F^\ell_{m,k-2} + F^{\frac{m+\ell-1}{2}}_{k,\ell-3} - F^{\frac{m-\ell+3}{2}}_{k,\ell-3}$$
$$+(m-\ell+1)(n-m-k+2)^2$$
$$+(n-m-k-\ell-3)(n-2)^2.$$

Similar to the above discussion, we have

$$L(\Gamma) \le F^k_{m,\ell-3} + F^\ell_{m,k-3} + F^{\frac{m+\ell-1}{2}}_{k,\ell-4} - F^{\frac{m-\ell+3}{2}}_{k,\ell-4} + \alpha_2.$$

By the above argument, we get that

$$I(\Gamma) \le \mathcal{F}_2(k,\ell,m) + \beta_2 + k(-\ell+m-2n+2) - \ell^2$$
$$-\ell(n-7) + m^2 - 3mn - 3m - 10n^2 + 30n - 8.$$

Moreover, if *k* and ℓ are odd and *m* is even, then we get the same result.

Case 3. Let *k* and *m* be even and ℓ be odd.
Similar to the above case we get that

$$A(\Gamma) \le \mathcal{F}_3(k,\ell,m), L(\Gamma) \le F^k_{m,\ell-3} + F^m_{m,k-4} + F^{\frac{m+\ell-1}{2}}_{k,\ell-3} - F^{\frac{m-\ell+3}{2}}_{k,\ell-3}$$
$$+\alpha_2 + (\ell-m)(k+m-n-3)^2, I(\Gamma)$$
$$\le \mathcal{F}_3(k,\ell,m) + \beta_2 + k(-\ell+m-2n+2)$$
$$-\ell(n-3) - 3mn + m - 10n^2 + 30n - 7.$$

Moreover, if *k* and *m* are odd and ℓ is even, then we get the same result.

Case 4. Let ℓ and *m* be even and *k* be odd.
Similar to the above case we get that

$$A(\Gamma) \le \mathcal{F}_4(k,\ell,m),$$

$$L(\Gamma) \le F^k_{m,\ell-4} + F^{\frac{k+\ell-1}{2}}_{m,k-3} - F^{\frac{\ell-k+3}{2}}_{m,k-3} + F^{\frac{k+m-1}{2}}_{\ell,k-3} - F^{\frac{m-k+3}{2}}_{\ell,k-3}$$
$$+\alpha_2 + (\ell-m-1)(k+m-n-3)^2$$
$$+(-2k+\ell+m+2)(\ell+m-n-3)^2,$$

$$I(\Gamma) \le \mathcal{F}_4(k,\ell,m) + \beta_2 + -2k^2 + k(2m-2n+9) - \ell(m+n-1) + m^2 - 3mn - 3m - 10n^2 + 30n - 9.$$

Moreover, if ℓ and m are odd and k is even, then we get the same result. □

4. LOWER BOUND

In this section, we obtain lower bound on $I(\Gamma)$, where Γ is a bicyclic graph. As a result, we are comparing Szeged indices of bicyclic graph, by Remark 2.3.

Theorem 4.1. Let Γ be a bicyclic graph of order *n*. Then $I(\Gamma) \ge 0$. □

Proof. Since Γ is a bicyclic graph, so it has a subgraph *K*, where *K* is $B(p,q)$, $B(p,\ell,q)$ or $B(P_k,P_\ell,P_m)$. For any $e = uv \in E(\Gamma)$, we consider $I = (n_u(e) - n_v(e))\,(m_u(e) - m_v(e))$.

We consider the following two cases:

Case 1. Let $e = uv \in E(K)$. In this case, similar to the above calculating, we can consider $n_u(e) = m_u(e) - 1$, $n_u(e) = m_u(e)$ or $n_u(e) = m_u(e) + 1$.

If $n_u(e) = m_u(e)$ and $n_v(e) = m_v(e)$, then obviously $I \ge 0$. If $n_u(e) = m_u(e)$ and $n_v(e) = m_v(e) - 1$, then $I = (n_u(e) - n_v(e))^2 - (n_u(e) - n_v(e))$, which implies that $I \ge 0$. If $n_u(e) = m_u(e)$ and $n_v(e) = m_v(e) + 1$, then similarly we get that $I \ge 0$. Patently, it is impossible that $I = 0$ for all edges $e = uv$ on $E(K)$. So there is at least one edge on *K* such that $(n_u(e) - n_v(e))\,(m_u(e) - m_v(e)) \ge 1$.

Case 2. Let $e = uv$ be an edge of a tree in Γ. We are discussing T_1 and will be the same for all other trees. Without loss of generality, let $d_\Gamma(u,v_1) \le d_\Gamma(v,v_1)$. Consider $T_1 = \check{T}_1 \cup \{uv\} \cup \hat{T}_1$ and so $t_1 = |T_1| = |\check{T}_1| + |\hat{T}_1|$. Let Γ be a bicycle graph of type 1 (for other types we have the same discussion).

So we have

$$n_u(e) - n_v(e) = (t'_1 + \ldots + t'_{q-1} + t_0 + t_2 \ldots + t_{p-1} + |\check{T}_1|) - (|\hat{T}_1|) = n - 2|\hat{T}_1|.$$

Also, we know that

$$m_u(e) - m_v(e) = \left[(t'_1 - 1) + \ldots + (t'_{q-1} - 1) + (t_0 - 1) + (t_2 - 1) \ldots + (t_{p-1} - 1) + (|\check{T}_1| - 1) + p + q\right] - \left[|\hat{T}_1| - 1\right] = n - 2(|\hat{T}_1| - 1).$$

Let $|\hat{T}_1| = x$. Therefore,

$$(n_u(e) - n_v(e))(m_u(e) - m_v(e)) = (n-2x)^2 + 2(n-2x).$$

We consider $f(n) = (n-2x)^2 + 2(n-2x)$. Since *n* is a natural number, so $f(n)$ is negative merely for $n = 2x - 1$, also we have $f(2x-1) = -1$. Therefore, either $(n_u(e) - n_v(e))$ $(m_u(e) - m_v(e)) \ge 0$ or $(n_u(e) - n_v(e))(m_u(e) - m_v(e)) = -1$. We claim that in Γ there is at most one tree which has an edge $e = uv$ such that $(n_u(e) - n_v(e))(m_u(e) - m_v(e)) = -1$. On the contrary, let T_1 and T_2 be two trees in Γ that have such edge. Hence, $t_1 = |T_1| = |\check{T}_1| + |\hat{T}_1|$ and $t_2 = |T_2| = |\check{T}_2| + |\hat{T}_2|$ and by the above argument we have $n = 2|\hat{T}_1| - 1 = 2|\hat{T}_2| - 1 = 2x - 1$. On the other hand, we know that $n > |\widehat{T_1}| + |\widehat{T_2}| = 2x$, which is a contradiction.

Consequently, sum of the value $(n_u(e) - n_v(e))$ $(m_u(e) - m_v(e))$ for all edges $e = uv \in E(\Gamma)$, which is $I(\Gamma)$, to be positive. □

5. CONCLUDING REMARKS

In this report, usefulness of Sz^*, Sz_e^*, Sz_{ev} and Sz_{ve} as structural descriptors of molecules is demonstrated using alkanes and benzenoid hydrocarbons. In case of simple model of alkanes based on (1), the indices Sz^*, Sz_e^*, Sz_{ev} and Sz_{ve} are found to yield best prediction for *MV*, *HV*, and *MR* respectively. When we look into the multiple linear regression model (2) of alkanes, significant improvement on data variances is observed for all properties, specially *MR* is modelled with powerful accuracy. When *BP* of benzenoid hydrocarbon is modelled individually by means of (1), Sz^* sounds the best. In view of the model (2), this performance enhances remarkably. When the considered four indices are correlated with some well-known degree based indices for decane isomers, a strong correlation with *RR* is found which suggests to find mathematical connection between them. The isomer discrimination ability of current indices is sometimes stronger than that of well-known indices and sometimes weaker. In addition, upper and lower bounds on Szeged indices and $Sz_{ve} - Sz_{ev}$ of bicyclic graphs are computed.

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Supplementary Information. Numerical values of all properties that are considered in this investigation are reported in tabular form as supplementary material. Theoretical indices are also listed in the supplementary file for alkanes and decane isomers. Supporting information to the paper is attached to the electronic version of the article at: https://doi.org/10.5562/cca4051.

PDF files with attached documents are best viewed with Adobe Acrobat Reader which is free and can be downloaded from Adobe's web site.

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