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ON THE TRANSMISSION-BASED GRAPH TOPOLOGICAL INDICES

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Abstract. The distance $d(u, v)$ between vertices u and v of a connected graph G is equal to the number of edges in a minimal path connecting them. The transmission of a vertex v is defined by $\sigma(v) = \sum_{u \in V(G)} d(v, u)$. A topological index is said to be a transmission-based topological index (TT index) if it includes the transmissions $\sigma(u)$ of vertices of G. Because $\sigma(u)$ can be derived from the distance matrix of G, it follows that transmission-based topological indices form a subset of distance-based topological indices. So far, relatively limited attention has been paid to TT indices, and very little systematic studies have been done. In this paper our aim was i) to define various types of transmission-based topological indices ii) establish lower and upper bounds for them, and iii) determine a family of graphs for which these bounds are best possible. Additionally, it has been shown in examples that using a group theoretical approach the transmission-based topological indices can be easily computed for a particular set of regular, vertex-transitive, and edge-transitive graphs. Finally, it is demonstrated that there exist TT indices which can be successfully applied to predict various physicochemical properties of different organic compounds. Some of them give better results and have a better discriminatory power than the most popular degree-based and distance-based indices (Randić, Wiener, Balaban indices).

1. Introduction and Preliminaries

Let G be a simple connected graph with the finite vertex set $V(G)$ and the edge set $E(G)$, and denote by $n = |V(G)|$ and $m = |E(G)|$ the number of vertices and edges, respectively. Using the standard terminology in graph theory, we refer the reader to [44]. The degree $d(u)$ of the vertex $u \in V(G)$ is the number of the edges incident to u. The edge of the graph G connecting the vertices u and v is denoted by uv.

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The role of molecular descriptors (especially topological descriptors) is remarkable in mathematical chemistry especially in QSPR/QSAR investigations. In mathematical chemistry, the *first Zagreb* index $M_1(G)$ and the *second Zagreb* index $M_2(G)$ belong to the family of the most important degree-based molecular descriptors. They are defined as [22, 23, 25, 31, 36]

$$M_1(G) = \sum_{uv\in E(G)} d(u) + d(v) = \sum_{u\in V(G)} d^2(u), \quad M_2(G) = \sum_{uv\in E(G)} d(u)d(v).$$

Similarly, the *first variable Zagreb* index and the *second variable Zagreb* index are defined as [33, 36, 46]

$$M_1^\lambda(G) = \sum_{u\in V(G)} d(u)^{2\lambda}, \quad M_2^\lambda(G) = \sum_{uv\in E(G)} d(u)^\lambda d(v)^\lambda,$$

where λ is a real number.

The *Randić* index $R(G)$, the *ordinary sum-connectivity* index $X(G)$, the *harmonic* index $H(G)$ and *geometric-arithmetic* index $GA(G)$ are also widely used degree-based topological indices [17, 40, 45, 48–50]. By definition,

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d(u)d(v)}}, \quad X(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d(u)+d(v)}},$$

$$H(G) = \sum_{uv\in E(G)} \frac{2}{d(u)+d(v)}, \quad GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}.$$

Let $\Delta = \Delta(G)$ and $\delta = \delta(G)$ be the maximum and the minimum degrees, respectively, of vertices of G. The average degree of G is $\frac{2m}{n}$. A connected graph G is said to be *bidegreed* with degrees Δ and δ, $\Delta > \delta \geq 1$, if at least one vertex of G has degree Δ and at least one vertex has degree δ, and if no vertex of G has degree different from Δ or δ. A connected bidegreed bipartite graph is called *semi-regular* if each vertex in the same part of a bipartition has the same degree. A graph G is called *regular* if all its vertices have the same degree, otherwise it is said to be *irregular*. In many applications and problems in theoretical chemistry, it is important to know how a given graph is irregular. The (vertex) regularity of a graph is defined in several approaches. Two most frequently used graph topological indices that measure how irregular a graph is, are the *irregularity* and *variance of degrees*. Let $\mathrm{imb}(e) = |d(u) - d(v)|$ be the *imbalance* of an edge $e = uv \in E(G)$. In [1], the *irregularity* of G, which is a measure of irregularity of graph G, defined as

$$\mathrm{irr}(G) = \sum_{e\in E(G)} \mathrm{imb}(e) = \sum_{uv\in E(G)} |d_G(u) - d_G(v)|. \tag{1.1}$$

The *variance of degrees* of graph G is defined as [7]

$$\mathrm{Var}(G) = \frac{1}{n}\sum_{u\in V(G)} \left(d(u) - \frac{2m}{n}\right)^2 = \frac{M_1(G)}{n} - \frac{4m^2}{n^2}. \tag{1.2}$$

Another measure of irregularity, which is called *degree deviation*, defined as [37]

$$s(G) = \sum_{u \in V(G)} \left| d(u) - \frac{2m}{n} \right|.$$

It is worth mentioning that $\frac{s(G)}{n}$ is nothing but the *mean deviation* of the data set $(d(u) \mid u \in V(G))$.

The *distance* between the vertices u and v in graph G is denoted by $d(u, v)$ and it is defined as the number of edges in a minimal path connecting them. The *eccentricity* $\varepsilon(v)$ of a vertex v is the maximum distance from v to any other vertex. The *diameter* $\mathrm{diam}(G)$ of G is the maximum eccentricity among the vertices of G. The *transmission* (or *status*) of a vertex v of G is defined as $\sigma(v) = \sigma_G(v) = \sum_{u \in V(G)} d(v, u)$. A graph G is said to be *transmission regular* [3] if $\sigma(u) = \sigma(v)$ for any vertex u and v of G. A transmission regular graph G is called *k-transmission regular* if there exists a positive integer k, for which $\sigma(v) = k$ for any vertex v of G. In K_n, the complete graph of order n, each vertex has transmission $n - 1$. So it is $(n - 1)$-transmission regular. The the cycle C_n and the complete bipartite graph $K_{a,a}$ are transmission regular. It has been verified that there exist regular and non-regular transmission regular graphs [3]. Consider the polyhedron depicted in Figure 1. It is the rhombic dodecahedron that contains 14 vertices, (8 vertices of degree 3 and 6 vertices of degree 4), 24 edges and 12 faces, all of them are congruent rhombi. The graph G_{RD} of the rhombic

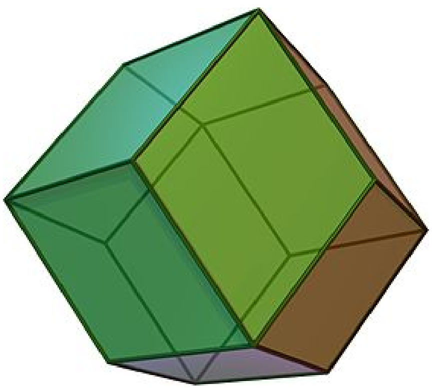

FIGURE 1. The rhombic dodecahedron

dodecahedron is a bidegreed, semi-regular 28-transmission regular graph (see Figure 2). An interesting observation is that the 14-vertex polyhedral graph G_{RD} depicted in Figure 2 is identical to the semi-regular graph published earlier in an alternative form in [3]. It is conjectured that G_{RD} is the smallest non-regular, bipartite, polyhedral (3-connected) and transmission regular graph.

If ω is a vertex weight of graph G, then one can see that

$$\sum_{\{u,v\} \subseteq V(G)} (\omega(u) + \omega(v))\, d(u, v) = \sum_{v \in V(G)} \omega(v)\sigma(v). \tag{1.3}$$

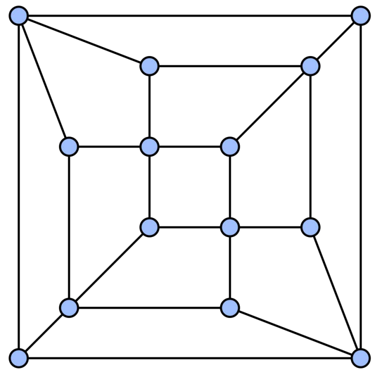

FIGURE 2. The edge-graph of the rhombic dodecahedron which is a 28-transmission regular graph but not regular

It is easy to construct various transmission-based indices having the same structure as the known degree-based topological indices. Based on this analogy-concept, the corresponding transmission-based indices are defined.

Let us define the *transmission Randić* index $RS(G)$, the *transmission ordinary sum-connectivity* index $XS(G)$, the *transmission harmonic* index $HS(G)$ and the *transmission geometric-arithmetic* index $GAS(G)$ as follows:

$$RS(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{\sigma(u)\sigma(v)}}, \quad XS(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{\sigma(u)+\sigma(v)}},$$

$$HS(G) = \sum_{uv\in E(G)} \frac{2}{\sigma(u)+\sigma(v)}, \quad GAS(G) = \frac{n}{2m} \sum_{uv\in E(G)} \frac{2\sqrt{\sigma(u)\sigma(v)}}{\sigma(u)+\sigma(v)}.$$

It follows that $GAS(G) \leq \frac{n}{2}$, with equality if and only if G is a transmission regular graph.

The *Wiener* index $W(G)$, the *Balaban* index $J(G)$ and the *sum-Balaban* index $SJ(G)$ represent a particular class of transmission-based topological indices. They are defined as [4–6, 9, 10, 16, 21, 51]

$$\begin{aligned} W(G) =& \frac{1}{2} \sum_{u\in VG)} \sum_{v\in V(G)} d(u,v) = \frac{1}{2} \sum_{u\in VG)} \sigma(u), \\ J(G) =& \frac{m}{m-n+2} \sum_{uv\in E(G)} \frac{1}{\sqrt{\sigma(u)\sigma(v)}} = \frac{m}{m-n+2} RS(G), \\ SJ(G) =& \frac{m}{m-n+2} \sum_{uv\in E(G)} \frac{1}{\sqrt{\sigma(u)+\sigma(v)}} = \frac{m}{m-n+2} XS(G). \end{aligned}$$

In [39] the *first transmission Zagreb* index $MS_1(G)$ and the *second transmission Zagreb* index $MS_2(G)$ are defined as

$$MS_1(G) = \sum_{uv\in E(G)} \sigma(u)+\sigma(v) = \sum_{u\in V(G)} d(u)\sigma(u), \quad MS_2(G) = \sum_{uv\in E(G)} \sigma(u)\sigma(v).$$

It is important to note that $MS_1(G)$ coincides with the *degree distance* $DD(G)$ that was introduced in [11, 24] and [43].

In fact by (1.3),

$$DD(G) = \sum_{\{u,v\}\subseteq V(G)} (d(u)+d(v))d(u,v) = \sum_{v\in V(G)} d(v)\sigma(v) = MS_1(G). \tag{1.4}$$

Consequently, if G is a k-transmission regular graph with m vertices, then $DD(G) = MS_1(G) = 2mk$.

Let us propose the *variable degree transmission Zagreb* index $MSD^\lambda(G)$ and the *variable transmission Zagreb* index $MS^\lambda(G)$ as follows

$$MSD^\lambda(G) = \sum_{u\in V(G)} d(u)\sigma(u)^{2\lambda-1}, \quad MS^\lambda(G) = \sum_{u\in V(G)} \sigma(u)^{2\lambda},$$

where λ is a real number.

The *eccentric distance sum* of a graph G, denoted by $\xi^d(G)$, defined as [20]

$$\xi^d(G) = \sum_{u\in V(G)} \varepsilon(u)\sigma(u).$$

It follows from (1.3) that

$$\xi^d(G) = \sum_{\{u,v\}\subseteq V(G)} (\varepsilon(u)+\varepsilon(v))d(u,v) = \sum_{v\in V(G)} \varepsilon(v)\sigma(v). \tag{1.5}$$

Starting with (1.6) and (1.7) we introduce two transmission-based irregularity indices defined as follows. Let G be a connected graph with n vertices and m edges. The *transmission imbalance* of an edge $e = uv \in E(G)$ is defined as $\mathrm{imb}_{\mathrm{Tr}}(e) = |\sigma_G(u) - \sigma_G(v)|$. Let us define the *transmission irregularity* $\mathrm{irr}_{\mathrm{Tr}}(G)$ and the *transmission variance* $\mathrm{Var}_{\mathrm{Tr}}(G)$ of G as follows:

$$\mathrm{irr}_{\mathrm{Tr}}(G) = \sum_{e\in E(G)} \mathrm{imb}_{\mathrm{Tr}}(e) = \sum_{uv\in E(G)} |\sigma_G(u) - \sigma_G(v)|, \tag{1.6}$$

$$\begin{aligned}\mathrm{Var}_{\mathrm{Tr}}(G) &= \frac{1}{n}\sum_{u\in V(G)} \left(\sigma_G(u) - \frac{2W(G)}{n}\right)^2 = \frac{1}{n}\sum_{u\in V(G)} \sigma_G(u)^2 - \frac{4W(G)^2}{n^2} \\ &= \frac{MS^1(G)}{n} - \frac{4W(G)^2}{n^2} \geq 0,\end{aligned} \tag{1.7}$$

where $\frac{2W(G)}{n}$ is the average vertex transmission of G. It is obvious that $\mathrm{Var}_{\mathrm{Tr}}(G)$ is equal to zero if and only if G is transmission regular.

Let us also define the transmission-based topological indices $QS_e(G)$ and $QS_{v,e}(G)$ as follows

$$QS_e(G) = \frac{1}{m}\mathrm{irr}_{\mathrm{Tr}}(G), \quad QS_{v,e}(G) = \frac{n}{2}\left(1 + \frac{1}{m}\mathrm{irr}_{\mathrm{Tr}}(G)\right) = \frac{n}{2}\left(1 + QS_e(G)\right).$$

Remark 1.1. Let G be an n-vertex graph. Comparing topological indices $GAS(G)$ and $QS_{v,e}(G)$, we get

$$GAS(G) \leq \frac{n}{2} \leq QS_{v,e}(G).$$

Equalities hold in both sides simultaneously if and only if G is transmission regular.

2. Establishing Lower and Upper Bounds

Lemma 2.1. *Let G be a connected graph with $n \geq 2$ vertices and m edges. Then*

$$\begin{aligned} 0 \leq &\mathrm{irr}_{\mathrm{Tr}}(G) \leq m(n-2), \\ 0 \leq &\sum_{uv \in E(G)} (\sigma(u) - \sigma(v))^2 \leq m(n-2)^2. \end{aligned}$$

The equality on the right-hand sides holds if and only if G is isomorphic to S_n. The equality on the left-hand sides holds if and only if G is transmission regular.

Proof. For an arbitrary edge uv of G, we have $|\sigma(u) - \sigma(v)| \leq n-2$. Therefore,

$$\mathrm{irr}_{\mathrm{Tr}}(G) = \sum_{uv \in E(G)} |\sigma(u) - \sigma(v)| \leq \sum_{uv \in E(G)} (n-2) = m(n-2).$$

It is trivial that in both formulas the equality on the right-hand side holds if and only if G isomorphic to S_n, since the star is the only graph where equality holds for each edge. □

Corollary 2.1. *Let T be a tree with $n \geq 2$ vertices. Then*

$$\begin{aligned} 0 \leq &\mathrm{irr}_{\mathrm{Tr}}(T) \leq (n-1)(n-2), \\ 0 \leq &\sum_{uv \in E(T)} (\sigma(u) - \sigma(v))^2 \leq (n-1)(n-2)^2. \end{aligned}$$

The equality on the right-hand sides holds if and only if G is isomorphic to S_n. The equality on the left-hand sides holds if and only if G is transmission regular.

Proof. It is a consequence of Lemma 2.1 and the fact that a tree with n vertices has exactly $n-1$ edges. □

Corollary 2.2. *Let G be a connected graph with $n \geq 2$ vertices. Then*

$$(n-2) \geq QS_e(G) \geq 0$$

and

$$\frac{n(n-1)}{2} \geq QS_{v,e}(G) \geq \frac{n}{2}.$$

The upper bounds are achieved if and only if G is isomorphic to S_n and the lower bounds are achieved if and only if G is transmission regular.

Proof. It is a direct consequence of Lemma 2.1. □

Lemma 2.2. *Let G be a connected graph with $n \geq 3$ vertices and with maximum vertex degree Δ. Then for each arbitrary vertex u of G*

$$\sigma(u) \geqslant 2(n-1) - d(u) \geqslant 2(n-1) - \Delta \geqslant n-1.$$

Proof. Because $n-1 \geq \Delta \geq d(u)$ one obtains that

$$\begin{aligned}\sigma(u) = \sum_{(w\in V|d(u,w)=1)} d(u,w) + \sum_{(w\in V|d(u,w)>1)} d(u,w) = d(u) + \sum_{(w\in V|d(u,w)>1)} d(u,w) \\ \geqslant d(u) + 2(n-1-d(u)) = 2n-2-d(u) \geqslant 2(n-1) - \Delta \geqslant n-1.\end{aligned}$$ □

Remark 2.1. There are several graphs containing a vertex u for which $\sigma(u) = n-1$. For example, $\sigma(u) = d(u) = n-1$ for any vertex u of a complete graph K_n.

Remark 2.2. Let G be a connected graph. It is easy to see that for any $u \in V(G)$, $\sigma(u) \geqslant 2(n-1) - d(u)$, with equality if and only if $\varepsilon(u) \leq 2$. This implies that

(i) $\sigma(u) = 2(n-1) - d(u)$ for any vertex u of a connected graph G if and only if $\mathrm{diam}(G) \leq 2$;
(ii) if G is a connected graph with $\mathrm{diam}(G) \leq 2$, then G is transmission regular if and only if G is regular.

Proposition 2.1. *Let G be a connected graph with n vertices. Then*

$$MSD^{\frac{3}{2}}(G) \geq 2(n-1)MS^1(G) - MS^{\frac{3}{2}}(G),$$

with equality if and only if $\mathrm{diam}(G) \leq 2$.

Proof. It follows from Lemma 2.2 that

$$\sum_{u\in V(G)} d(u)\sigma^2(u) \geq \sum_{u\in V(G)} (2n-2-\sigma(u))\,\sigma^2(u) = 2(n-1) \sum_{u\in V(G)} \sigma^2(u) - \sum_{u\in V(G)} \sigma^3(u),$$

and by Remark 2.2, the equality holds if and only if $\mathrm{diam}(G) \leq 2$. □

Proposition 2.2. *Let G be a connected graph with n vertices. Then*

$$MS_1(G) \geq 4(n-1)W(G) - MS^1(G),$$

with equality if and only if $\mathrm{diam}(G) \leq 2$.

Proof. It follows from Lemma 2.2 that

$$\sum_{u\in V(G)} d(u)\sigma(u) \geq \sum_{u\in V(G)} (2n-2-\sigma(u))\,\sigma(u) = 2(n-1) \sum_{u\in V(G)} \sigma(u) - \sum_{u\in V(G)} \sigma^2(u).$$

It follows from Remark 2.2 that the equality holds if and only if $\mathrm{diam}(G) \leq 2$. □

Lemma 2.3. *Let G be a connected graph with n vertices and m edges. If* $\mathrm{diam}(G) \leq 2$*, then*

(i) $\mathrm{irr}_{\mathrm{Tr}}(G) = \mathrm{irr}(G) \geq 0$;
(ii) $QS_{v,e}(G) = \frac{n}{2}\left(1 + \frac{1}{m}\mathrm{irr}(G)\right) \geq \frac{n}{2}$.

In particular, in both cases equality holds if and only if G is regular.

Proof. (i) It is a direct consequence of Lemma 2.1 and Remark 2.2.
(ii) It follows directly from part (i). ☐

Corollary 2.3. *Let $K_{p,q}$ be the complete bipartite graph with $p+q$ vertices and with parts of size p and q. Then*
(i) $\mathrm{irr}_{\mathrm{Tr}}(K_{p,q}) = pq\,|p-q| \geq 0$;
(ii) $QS_{v,e}(K_{p,q}) = \frac{p+q}{2}\,(1+|p-q|) \geq \frac{p+q}{2}$, *specially* $QS_{v,e}(S_n) = \frac{n(n-1)}{2}$.
In particular, the equalities in (i) *and* (ii) *hold if and only if $p=q$.*

Proof. (i) Since $\mathrm{diam}(K_{p,q}) = 2$ and $|E(K_{p,q})| = pq$, it follows from Lemma 2.3 (i) that $\mathrm{irr}_{\mathrm{Tr}}(K_{p,q}) = \mathrm{irr}(K_{p,q}) = \sum_{uv\in E(K_{p,q})} |p-q| = pq\,|p-q|$.
(ii) Since $\mathrm{diam}(K_{p,q}) = 2$ and $|V(K_{p,q})| = p+q$, it follows from Lemma 2.3 (ii) that
$$QS_{v,e}(K_{p,q}) = \frac{p+q}{2}\,(1+|p-q|) \geq \frac{p+q}{2}.$$
Specially, let $n \geq 2$ and $p=1$ and $q=n-1$. Then $K_{p,q}$ is isomorphic to the star S_n, $(n=p+q)$. Consequently, we obtain that
$$QS_{v,e}(S_n) = \frac{n}{2}(1+|2-n|) = \frac{n(n-1)}{2}.$$
It follows from Lemma 2.3 that the equalities in (i) and (ii) hold if and only if $K_{p,q}$ is regular if and only if $p=q$. ☐

An edge uv of a connected graph G is said to be a *strong edge* of G, if $|d(u)-d(v)| > 0$. Denote by $es(G)$ the number of strong edges of G. It is obvious that if G is a connected graphs, then $es(G) = 0$ if and only if G is regular. From this observation it follows that the topological invariant $es(G)$ can be considered as a graph irregularity index. There are several graphs in which each edge is strong, that is $es(G) = |E(G)|$. For example, $es(K_{p,q}) = |E(K_{p,q})| = pq$ if p is not equal to q. It can be easily constructed a tree graph T with an arbitrary large edge number $m(T)$, for which $es(T) = m(T)$. Consider the $(n \geq 5)$-vertex windmill graph denoted by $Wd(n)$. It is a graph with diameter 2, with the vertex number $n = 2k+1$ and with the edge number $m = 3k$, where $k \geq 2$ is an arbitrary positive integer. Note that $es(Wd(n)) = 2k = \frac{2}{3}m = n-1$.

Proposition 2.3. *For the windmill graph $Wd(n)$ we have*
(i) $\mathrm{irr}_{\mathrm{Tr}}(Wd(n)) = es(Wd(n))(n-3) = \frac{2}{3}m(n-3) = (n-1)(n-3)$;
(ii) $QS_{v,e}(Wd(n)) = \frac{n}{2}\left(1+\frac{2}{3}(n-3)\right)$.

Proof. (i) Let E_0 be the set of strong edges of $Wd(n)$. It is easy to see that
$$E_0 = \Big\{uv \in E(Wd(n)) \mid d(u)=2, d(v)=n-1\Big\}, \quad es(Wd(n)) = |E_0|.$$

Since $\operatorname{diam}(Wd(n)) = 2$, it follows from Lemma 2.3 (i) that

$$\begin{aligned}\operatorname{irr}_{\mathrm{Tr}}(Wd(n)) = \operatorname{irr}(Wd(n)) &= \sum_{uv\in E_0} |d(u) - d(v)| = \sum_{uv\in E_0} |2-(n-1)| \\ &= es(Wd(n))\,|2-(n-1)| \\ &= \frac{2}{3}m(n-3) = (n-1)(n-3).\end{aligned}$$

(ii) It follows from part (i) that

$$\begin{aligned}QS_{v,e}(Wd(n)) &= \frac{n}{2}\left(1 + \frac{1}{m}\operatorname{irr}_{\mathrm{Tr}}(Wd(n))\right) = \frac{n}{2}\left(1+\frac{2}{3}(n-3)\right) \\ &= \frac{n}{2}\left(1+\frac{1}{m}(n-1)(n-3)\right).\end{aligned}$$

□

Lemma 2.4. [32] *Let P_n be a path of order n such that $V(P_n) = \{v_0, v_1, \dots, v_{n-1}\}$ and $E(P_n) = \{v_i v_{i+1} \mid i = 0, \dots, n-2\}$. Then for each $0 \le i \le n-1$*

$$\sigma_{P_n}(v_i) = \frac{1}{2}\Big(2i^2 - 2(n-1)i + (n-1)^2 + (n-1)\Big).$$

The following is a direct consequence of Lemma 2.4.

Proposition 2.4. *The transmission irregularity index of P_n is given by*

$$\operatorname{irr}_{\mathrm{Tr}}(P_n) = \begin{cases} \frac{n(n-2)}{2}, & \text{if } n \text{ is even,} \\ \frac{(n-1)^2}{2}, & \text{if } n \text{ is odd.}\end{cases}$$

For an edge uv of a connected graph G, define the positive integers N_u and N_v where N_u is the number of vertices of G whose distance to vertex u is smaller than distance to vertex v, and analogously, N_v is the number of vertices of G whose distance to the vertex v is smaller than to u. The number of vertices equidistant from u and v is denoted by N_{uv}. An edge uv of G is called a distance-balanced edge if $N_u = N_v$. A graph G is said to be *distance-balanced* [26] if its each edge is distance-balanced. It is known that a connected graph G is transmission regular if and only if G is distance balanced [3, 26].

The *Szeged* index $Sz(G)$ and the *revised Szeged* index $Sz^*(G)$ of a connected graph G are defined as [29, 35, 38]

$$Sz(G) = \sum_{uv\in E(G)} N_u N_v, \qquad Sz^*(G) = \sum_{uv\in E(G)} \left(N_u + \frac{N_{uv}}{2}\right)\left(N_v + \frac{N_{uv}}{2}\right).$$

Remark 2.3. For any connected graph G with n vertices, the following known relations are fulfilled [3, 12, 13, 16, 28, 29, 35, 38, 47].

(i) For any edge uv of G, $n = N_u + N_v + N_{uv}$. This implies that a graph G is bipartite if and only if $n = N_u + N_v$ holds for any edge uv of G.
(ii) The inequality $Sz(G) \ge W(G)$ is fulfilled.
(iii) $Sz(G) \le Sz^*(G)$ with equality if and only if G is bipartite.

(iv) For an n-vertex tree T, $W(S_n) \leq W(T) \leq W(P_n)$.
(v) For a tree graph T, $Sz^*(T) = Sz(T) = W(T)$.

The fundamental properties of Wiener index and their extremal graphs are summarized in [9, 12, 13, 16, 21]. Transmission regular graphs are characterized by the following property.

Lemma 2.5. [3,26,29] *Let G be a connected graph with n vertices and m edges. Then*

$$Sz^*(G) \leq \frac{n^2 m}{4},$$

with equality if and only if G is transmission regular.

Lemma 2.6 ([3, 12])**.** *Let G be a connected graph and let uv be an edge of G. Then*

$$\sigma(u) - \sigma(v) = N_v - N_u.$$

Lemma 2.7. *Let G be a connected graph. Then the following hold:*
(i) $\mathrm{irr}_{\mathrm{Tr}}(G) = \sum_{uv \in E(G)} |N_u - N_v| \geq 0$;
(ii) $\sum_{uv \in E(G)} (N_u - N_v)^2 = MSD^{\frac{3}{2}}(G) - 2MS_2(G) \geq 0$;
(iii) $\sum_{uv \in E(G)} (\sigma(u) - \sigma(v))^2 = \sum_{uv \in E(G)} \left(N_u^2 + N_v^2\right) - 2Sz(G) \geq 0$;
(iv) $\sum_{uv \in E(G)} \left(N_u^2 + N_v^2\right) = MSD^{\frac{3}{2}}(G) + 2Sz(G) - 2MS_2(G)$.

In (i)*,* (ii)*, and* (iii) *the equality holds if and only if G is transmission regular.*

Proof. (i) This is a direct consequence of Lemma 2.6.
(ii)

$$\begin{aligned} 0 \leq \sum_{uv \in E(G)} (N_u - N_v)^2 &= \sum_{uv \in E(G)} (\sigma(u) - \sigma(v))^2 \\ &= \sum_{uv \in E(G)} \left(\sigma^2(u) + \sigma^2(v)\right) - 2 \sum_{uv \in E(G)} \sigma(u)\sigma(v) \\ &= \sum_{u \in V(G)} d(u)\sigma^2(u) - 2MS_2(G) \\ &= MSD^{\frac{3}{2}}(G) - 2MS_2(G). \end{aligned}$$

(iii)

$$\begin{aligned} 0 \leq \sum_{uv \in E(G)} (\sigma(u) - \sigma(v))^2 &= \sum_{uv \in E(G)} (N_u - N_v)^2 \\ &= \sum_{uv \in E(G)} \left(N_u^2 + N_v^2\right) - 2Sz(G). \end{aligned}$$

(iv) It follows from the proof of the part (ii) and (iii) that

$$\begin{aligned}\sum_{uv\in E(G)}\left(N_u^2+N_v^2\right) &= \sum_{uv\in E(G)}(\sigma(u)-\sigma(v))^2+2Sz(G)\\ &= MSD^{\frac{3}{2}}(G)-2MS_2(G)+2Sz(G).\end{aligned}$$ □

Remark 2.4. Based on Lemma 2.7, the transmission-based topological index $QS_{v,e}(G)$ can be represented in the following alternative form:

$$QS_{v,e}(G)=\frac{n}{2}\left(1+\frac{1}{m}\sum_{uv\in E(G)}|\sigma(u)-\sigma(v)|\right)=\frac{n}{2}\left(1+\frac{1}{m}\sum_{uv\in E(G)}|N_u-N_v|\right).$$

Proposition 2.5. *Let G be a connected graph with n vertices and m edges. Then*

$$n^2m\geq MSD^{\frac{3}{2}}(G)+4Sz(G)-2MS_2(G),$$

with equality if and only if G is a bipartite graph.

Proof. Let G be a connected graph with n vertices. It follows from Remark 2.3 (i) that for any edge uv of G, $N_u+N_v\leq n$, with equality if and only if G is bipartite. This implies that

$$n^2\geq(N_u+N_v)^2=\left(N_u^2+N_v^2\right)+2N_uN_v,$$

with equality if and only if G is bipartite. Consequently, by Lemma 2.7 (iv) we have

$$\begin{aligned}n^2m=\sum_{uv\in E(G)}n^2 &\geq \sum_{uv\in E(G)}\left(N_u^2+N_v^2\right)+2\sum_{uv\in E(G)}N_uN_v\\ &= \sum_{uv\in E(G)}\left(N_u^2+N_v^2\right)+2Sz(G)\\ &= MSD^{\frac{3}{2}}(G)+4Sz(G)-2MS_2(G),\end{aligned}$$

with equality if and only if G is bipartite. □

Proposition 2.6. *Let G be a connected graph with n vertices. Then*

$$\operatorname{irr}_{\mathrm{Tr}}(G)=\sum_{uv\in E(G)}|N_u-N_v|\geq\frac{1}{n}\sum_{uv\in E(G)}\left|N_u^2-N_v^2\right|, \tag{2.1}$$

with equality if and only if G is a bipartite graph.

Proof. Let G be a connected graph with n vertices. It follows from Remark 2.3 (i) that for any edge uv of G, $N_u+N_v\leq n$, with equality if and only if G is bipartite. Therefore, it follows from Lemma 2.6 and

$$\left|N_u^2-N_v^2\right|=(N_u+N_v)\,|N_u-N_v|\leq n\,|N_u-N_v|=n\,|\sigma(u)-\sigma(v)|,$$

with equality if and only if G is bipartite. This implies that (2.1) holds with equality if and only if G is bipartite. □

Corollary 2.4. *Let T_n be an n vertex tree. Then*

$$\begin{aligned} MS_2(T_n) =& 2W(T_n) + \frac{1}{2} MSD^{\frac{3}{2}}(T_n) - \frac{n^2(n-1)}{2}, \\ \mathrm{irr}_{\mathrm{Tr}}(T_n) =& \frac{1}{n} \sum_{uv \in E(T_n)} \left| N_u^2 - N_v^2 \right|. \end{aligned}$$

Proof. It is a consequence of Proposition 2.5, Proposition 2.6 and Remark 2.3, since a tree with n vertices is bipartite and has exactly $n-1$ edges. ☐

Proposition 2.7. [12] *Let G_B be a connected bipartite graph with n vertices and m edges. Then*

$$Sz^*(G_B) = Sz(G_B) = \frac{n^2 m}{4} - \frac{1}{4} \sum_{uv \in E(G_B)} (\sigma(u) - \sigma(v))^2 \leq \frac{n^2 m}{4},$$

with equality if and only if G is transmission regular.

Corollary 2.5. *Let G_B be a connected bipartite graph with n vertices and m edges. Then*

$$QS_{v,e}(G_B) \leq \sqrt{n^2 - \frac{4}{m} Sz(G_B)},$$

with equality if and only if $|\sigma(u) - \sigma(v)|$ is constant for any edge $uv \in G_B$.

Proof. Using Cauchy-Schwartz inequality and Proposition 2.7 one obtains for G_B that

$$\left(\frac{1}{m} \sum_{uv \in E(G_B)} |\sigma(u) - \sigma(v)| \right)^2 \leq \frac{1}{m} \sum_{uv \in E(G_B)} (\sigma(u) - \sigma(v))^2 = n^2 - \frac{4}{m} Sz(G_B),$$

with equality if and only if $|\sigma(u) - \sigma(v)|$ is constant for any edge $uv \in G_B$. Consequently,

$$\frac{1}{m} \sum_{uv \in E(G_B)} |\sigma(u) - \sigma(v)| \leq \sqrt{n^2 - \frac{4}{m} Sz(G_B)},$$

with equality if and only if $|\sigma(u) - \sigma(v)|$ is constant for any edge $uv \in G_B$. Because

$$QS_{v,e}(G_B) - \frac{n}{2} = \frac{n}{2m} \sum_{uv \in E(G_B)} |\sigma(u) - \sigma(v)|,$$

we have

$$QS_{v,e}(G_B) - \frac{n}{2} \leq \frac{n}{2} \sqrt{n^2 - \frac{4}{m} Sz(G_B)},$$

with equality if and only if $|\sigma(u) - \sigma(v)|$ is constant for any edge $uv \in G_B$. ☐

Lemma 2.8. [12] *Let T_n be an n-vertex tree. Then*

$$Sz(T_n) = W(T_n) = \frac{1}{4} \left(n(n-1) + MS_1(T_n) \right).$$

The following proposition demonstrates that the Wiener index and the first transmission Zagreb index are closely related.

Proposition 2.8. *Let T_n be an n-vertex tree. Then*

$$MS_1(T_n) = 4W(T_n) - n(n-1) = 4Sz(T_n) - n(n-1). \tag{2.2}$$

Proof. For any connected graph G we have

$$MS_1(G) = \sum_{uv \in E(G)} (\sigma(u) + \sigma(v)) = \sum_{u \in V(G)} d(u)\sigma(u).$$

Therefore, by Lemma 2.8 the result follows. □

Remark 2.5. As a consequence of (2.2), we conclude that in the family of n-vertex trees there is a linear correspondence (a perfect linear correlation) between the topological indices $W(T_n)$ and $MS_1(T_n)$.

In [39] it is reported that for a connected graph G, $W(G) < MS_1(G)$. This relation can be strengthened as follows.

Proposition 2.9. *Let G be a connected graph with minimum degree δ and maximum degree Δ. Then*

$$2\delta W(G) \leq MS_1(G) \leq 2\Delta W(G),$$

and equalities hold in both sides if and only if G is a regular graph.

Proof. Because for any connected graph G, $MS_1(G) = \sum_{uv \in E(G)} (\sigma(u) + \sigma(v)) = \sum_{u \in V(G)} d(u)\sigma(u)$, and for any vertex u of G, $\delta \leq d(u) \leq \Delta$, we have that

$$2\delta WG) \leq \sum_{uv \in E(G)} (\sigma(u) + \sigma(v)) = \sum_{u \in V(G)} d(u)\sigma(u) \leq 2\Delta WG).$$

Consequently, if G is an r-regular graph, we have $MS_1(G) = 2rW(G)$. □

Corollary 2.6. *Let T_n be an n-vertex tree. Then*

$$(n-1)(3n-4) \leq MS_1(T_n) \leq \frac{1}{3}n(n-1)(2n-1),$$

where

(i) *the right-hand side equality holds if and only if T_n is the path P_n;*
(ii) *the left-hand side equality holds if and only if T_n is the star S_n.*

Proof. For an n-vertex tree T_n we have $W(S_n) \leq W(T_n) \leq W(P_n)$, where $W(S_n) = (n-1)^2$ and $W(P_n) = \frac{(n^3-n)}{6}$. Therefore, from Proposition 2.8, we have the following inequalities:

$$MS_1(T_n) \leq \frac{4n(n-1)(n+1)}{6} - n(n-1) = \frac{1}{3}n(n-1)(2n-1),$$

with equality if and only if T_n is the path P_n, and

$$MS_1(T_n) \geq 4(n-1)^2 - n(n-1) = (n-1)(3n-4),$$

with equality if and only if T_n is the star S_n. □

The following is a direct consequence of Proposition 2.9.

Corollary 2.7. *If G_{be} is a benzenoid graph with $\Delta = 3$ and $\delta = 2$, then*

$$4W(G_{be}) \leq MS_1(G_{be}) \leq 6W(G_{be}).$$

It is easy to show that the inequality represented by

$$MS_2(G) = \sum_{uv\in E(G)} \sigma(u)\sigma(v) \leq \frac{1}{2} MSD^{\frac{3}{2}}(G),$$

can be sharpened in the following form.

Proposition 2.10. *Let G be a connected graph with m edges. Then*

$$MS_2(G) \leq \frac{1}{2} MSD^{\frac{3}{2}}(G) - \frac{1}{2m} \mathrm{irr}_{\mathrm{Tr}}(G)^2,$$

with equality if and only if $|\sigma(u) - \sigma(v)|$ is constant for any $uv \in E(G)$.

Proof. Using Cauchy-Schwartz inequality we have

$$\begin{aligned}\left(\frac{1}{m}\sum_{uv\in E(G)} |\sigma(u)-\sigma(v)|\right)^2 &\leq \frac{1}{m}\sum_{uv\in E(G)} (\sigma(u)-\sigma(v))^2, \\ &= \frac{1}{m}\sum_{uv\in E(G)} (\sigma^2(u)+\sigma^2(v)) - \frac{2}{m}\sum_{uv\in E(G)} \sigma(u)\sigma(v),\end{aligned}$$

with equality if and only if $|\sigma(u) - \sigma(v)|$ is constant for any $uv \in E(G)$. It follows that

$$MS_2(G) \leq \frac{1}{2} MSD^{\frac{3}{2}}(G) - \frac{1}{2m} \mathrm{irr}_{\mathrm{Tr}}(G)^2,$$

with equality if and only if $|\sigma(u) - \sigma(v)|$ is constant for any $uv \in E(G)$. □

Corollary 2.8. *Let G be a connected graph with m edges. If* $\mathrm{diam}(G) \leq 2$, *then*

$$MS_2(G) \leq \frac{1}{2} MSD^{\frac{3}{2}}(G) - \frac{1}{2m} \mathrm{irr}(G)^2,$$

with equality if and only if $|d(u) - d(v)|$ is constant for any $uv \in E(G)$.

Proof. Let G be a connected graph with m edges. It follows from Remark 2.2 that for any $uv \in E(G)$, $|d(u) - d(v)|$ is constant if $\mathrm{diam}(G) \leq 2$. Now the result follows from Lemma 2.3 and Proposition 2.10. □

Lemma 2.9. [14, 43] *Let G be a connected graph with n vertices and m edges. Then*

$$W(G) \geq n(n-1) - m,$$

with equality if and only if $\mathrm{diam}(G) \leq 2$. (*For example, the equality holds for complete graphs, complete bipartite and complete multipartite graphs, moreover wheel graphs and windmill graphs composed of triangles.*)

Proposition 2.11. *Let G be a connected k-transmission regular with n vertices and m edges. Then*

$$k = \frac{2W(G)}{n} \geq 2(n-1) - \frac{2m}{n},$$

with equality if and only if $\mathrm{diam}(G) \leq 2$.

Proof. Since G is k-transmission regular, $W(G) = \frac{nk}{2}$ holds. Now the result follows from Lemma 2.9. □

Proposition 2.12. *Let G be a connected graph with n vertices and m edges. Then*

$$MS^1(G) \geq 4(n-1)W(G) - MS_1(G) \geq 4(n-1)\left(n^2 - n - m\right) - MS_1(G),$$

and equalities hold in both sides simultaneously if $\mathrm{diam}(G) \leq 2$.

Proof. The result follows directly, using Lemma 2.9 and Proposition 2.2. □

Proposition 2.13. *Let G be a connected graph with n vertices and m edges. Then*

$$MS_1(G) \leq \sqrt{m\left(MSD^{\frac{3}{2}}(G) + 2MS_2(G)\right)}, \tag{2.3}$$

with equality if and only if $\sigma(u) + \sigma(v)$ is constant for each edge $uv \in E(G)$.

Proof. Using the Cauchy-Schwartz inequality, we obtain

$$\begin{aligned}\left(\frac{1}{m}\sum_{uv\in E(G)}(\sigma(u)+\sigma(v))\right)^2 &\leq \frac{1}{m}\sum_{uv\in E(G)}(\sigma(u)+\sigma(v))^2\\ &= \frac{1}{m}\left(\sum_{uv\in E(G)}\left(\sigma^2(u)+\sigma^2(v)\right) + 2\sum_{uv\in E(G)}\sigma(u)\sigma(v)\right),\end{aligned}$$

with equality if and only if $\sigma(u) + \sigma(v)$ is constant for each edge $uv \in E(G)$. This implies that

$$\left(\frac{1}{m}MS_1(G)\right)^2 \leq \frac{1}{m}\left(MSD^{\frac{3}{2}}(G) + 2MS_2(G)\right),$$

with equality if and only if $\sigma(u) + \sigma(v)$ is constant for each edge $uv \in E(G)$. Consequently, we have

$$MS_1(G) \leq \sqrt{m\left(MSD^{\frac{3}{2}}(G) + 2MS_2(G)\right)}.$$ □

Let G be a connected graph with n vertices. Let us define the topological invariant $\Phi(G)$ as follows

$$\Phi(G) = \frac{\left(\sum\limits_{u\in V(G)}\sigma(u)\right)^2}{n\sum\limits_{u\in V(G)}\sigma^2(u)} = \frac{4W(G)^2}{nMS^1(G)}.$$

The following theorem shows that $\Phi(G)$ quantifies the degree of transmission regularity of a connected graph G.

Theorem 2.1. *Let G be a connected graph with n vertices. Then $\Phi(G) \leq 1$, with equality if and only if G is transmission regular.*

Proof. Using Cauchy-Schwartz inequality, we obtain

$$\left(\sum_{u\in V(G)} \sigma(u)\right)^2 \leq n \sum_{u\in V(G)} \sigma(u)^2,$$

with equality if and only if $\sigma(u) = \sigma(v)$ for each $u, v \in V(G)$. This completes the proof. □

Proposition 2.14. *Let G be a connected graph with n vertices and m-edges. If $\rho_D(G)$ denotes the distance spectral radius of G, then*

$$2(n-1) - \frac{2m}{n} \leq \frac{2W(G)}{n} \leq \rho_D(G).$$

The left-hand side equality holds if and only if $\operatorname{diam}(G) \leq 2$. *The right-hand side equality holds if and only if G is transmission regular.*

Proof. The left-hand side inequality is nothing but Lemma 2.9. From Theorem 2.1 and [2, Theorem 5.5] one obtains that $\frac{2W(G)}{n} \leqslant \sqrt{\frac{1}{n}MS^1(G)} \leqslant \rho_D(G)$, with equality if and only if G is transmission regular. □

Let us finish this section with following result showing how $W(G)$, $MS_1(G)$, and $\xi^d(G)$ relates to each other.

Theorem 2.2. [27] *Let G be a connected graph on $n \geqslant 3$ vertices. Then*

$$MS_1(G) \leqslant 2nW(G) - \xi^d(G),$$

with equality if and only if $G \cong P_4$, or $G \cong K_n - ke$, for $k = 0, 1, \ldots, \lfloor \frac{n}{2} \rfloor$, where ke denotes a matching of size k.

3. Vertex and Edge Transitive Graphs

In this section, following Darafsheh [8, 34], we aim to use a method which applies group theory to graph theory. For more details regarding the theory of groups and graph theory one can see [15] and [19], respectively.

Let Γ be a group acting on a set X. We shall denote the action of $\alpha \in \Gamma$ on $x \in X$ by x^α. Then $U \subseteq X$ is call an *orbit* of Γ on X if for every $x, y \in U$ there exists $\alpha \in \Gamma$ such that $x^\alpha = y$. The action of group Γ on X is called *transitive* if X is itself an orbit of Γ on X.

Let G be a graph. A bijection α on $V(G)$ is called an *automorphism* of G if it preserves $E(G)$. In other words, α is an automorphism if for each $u, v \in V(G)$, $e = uv \in E(G)$ if and only if $u^\alpha v^\alpha \in E(G)$. Let us denote by $\operatorname{Aut}(G)$ the set of all automorphisms of G.

It is known that $\operatorname{Aut}(G)$ forms a group under the composition of mappings. This is a subgroup of the symmetric group on $V(G)$. Note that $\operatorname{Aut}(G)$ acts on $V(G)$

naturally, i.e., for each $\alpha \in \mathrm{Aut}(G)$ and $v \in V(G)$ the action of α on v, v^α, is defined as $\alpha(v)$. The action of $\mathrm{Aut}(G)$ on $V(G)$ induces an action on $E(G)$. In fact, for $\alpha \in \mathrm{Aut}(G)$ and $e = uv \in E(G)$, the action of α on $e = uv$, e^α, is defined as $u^\alpha v^\alpha$.

A graph G is called *vertex-transitive* (*edge-transitive*) if the action of $\mathrm{Aut}(G)$ on $V(G)$ ($E(G)$) is transitive.

Let G be a graph, $V_1, V_2, \ldots, V_t$ be the orbits of $\mathrm{Aut}(G)$ under its natural action on $V(G)$. Then for each $1 \leq i \leq t$ and for $u, v \in V_i$, $\sigma(u) = \sigma(v)$. In particular, if G is vertex transitive ($t = 1$), then for each $u, v \in V(G)$, $\sigma(u) = \sigma(v)$. Therefore vertex-transitive graphs are transmission regular. It is known that any vertex-transitive graph is (vertex degree) regular [19] and transmission regular [8], but note vice versa.

Lemma 3.1. *Let G be a connected k-transmission regular graph with n vertices and m edges. Then*

$$\begin{aligned} SJ(G) =& \frac{m^2}{(m-n+2)\sqrt{2k}}, \quad GAS(G) = \frac{n}{2}, \quad HS(G) = \frac{m}{k}, \\ J(G) =& \frac{m^2}{(m-n+2)k}. \end{aligned}$$

Lemma 3.2. *Let G be a connected vertex-transitive graph with n vertices and m edges and the valency r. Then*

$$\begin{aligned} SJ(G) =& \frac{m^2\sqrt{n}}{2(m-n+2)\sqrt{W(G)}}, \quad GAS(G) = \frac{2W(G)}{n}, \\ HS(G) =& \frac{nm}{2W(G)} = \frac{n^2 r}{4W(G)}, \\ J(G) =& \frac{m^2 n}{2(m-n+2)W(G)} = \frac{mn^2 r}{4(m-n+2)W(G)}. \end{aligned}$$

Proof. If G is a connected vertex-transitive graph with n vertices and m edges, then G is of valency r (r-regular) and k-transmission regular, for some natural numbers r and k. It follows that $2m = nr$ and $2W(G) = nk$. □

Lemma 3.3. *Let G be a connected k-transmission regular with n vertices and m edges. Then*

$$HS(G) \leq \frac{m}{2(n-1) - \frac{2m}{n}},$$

with equality if and only if $\mathrm{diam}(G) \leq 2$.

Proof. Follows from Proposition 2.11 and the fact that for a k-transmission regular graph G with n vertices and m edges, $HS(G) = \frac{m}{k}$. □

Theorem 3.1. *Let G be a connected graph with n vertices and m edges. Let us denote the orbits of the action* $\mathrm{Aut}(G)$ *on* $E(G)$ *by* $E_1, E_2, \ldots, E_l$*. Suppose that for* *each* $1 \leq i \leq t$, $e_i = u_i v_i$ *is a fixed edge in the orbit* E_i. *Then*

$$\begin{aligned} HS(G) =& \sum_{i=1}^{l} \frac{2|E_i|}{\sigma(u_i) + \sigma(v_i)}, \quad SJ(G) = \frac{m}{m-n+2} \sum_{i=1}^{l} \frac{|E_i|}{\sqrt{\sigma(u_i) + \sigma(v_i)}}, \\ GAS(G) =& \frac{n}{2m} \sum_{i=1}^{l} \frac{|E_i|\sqrt{\sigma(u_i)\sigma(v_i)}}{\sigma(u_i) + \sigma(v_i)}, \quad \mathrm{irr}_{\mathrm{Tr}}(G) = \sum_{i=1}^{l} |E_i| \left|\sigma(u_i) - \sigma(v_i)\right|, \\ MS_1(G) =& \sum_{i=1}^{l} |E_i|(\sigma(u_i) + \sigma(v_i)), \quad MS_2(G) = \sum_{i=1}^{l} |E_i|\sigma(u_i)\sigma(v_i). \end{aligned}$$

Corollary 3.1. *Let* G *be a connected graph with* n *vertices and* m *edges. If* G *is edge-transitive and* uv *is a fixed edge of* G, *then*

$$\begin{aligned} HS(G) =& \frac{2m}{\sigma(u) + \sigma(v)}, \quad SJ(G) = \frac{m^2}{(m-n+2)\sqrt{\sigma(u) + \sigma(v)}}, \\ GAS(G) =& \frac{n}{2} \frac{\sqrt{\sigma(v)\sigma(v)}}{\sigma(u) + \sigma(v)}, \quad MS_2(G) = m\sigma(u)\sigma(v), \\ \mathrm{irr}_{\mathrm{Tr}}(G) =& m\left|\sigma(u) - \sigma(v)\right|, \quad QS_e(G) = \left|\sigma(u) - \sigma(v)\right|, \\ QS_{v,e}(G) =& \frac{n}{2}\left(1 + \left|\sigma(u) - \sigma(v)\right|\right), \quad MS_1(G) = m(\sigma(u) + \sigma(v)). \end{aligned}$$

Fullerenes are zero-dimensional nanostructures, discovered experimentally in 1985 [30]. Fullerenes C_n can be drawn for $n = 20$ and for all even $n \geq 24$. They have n carbon atoms, $\frac{3n}{2}$ bonds, 12 pentagonal and $\frac{n}{2} - 10$ hexagonal faces. The most important member of the family of fullerenes is C_{60} [30]. The smallest fullerene is C_{20}. It is a well-known fact that among all fullerene graphs only C_{20} and C_{60} (see Figure 3) are vertex-transitive [18]. Since for every vertex of $v \in V(C_{20})$, $\sigma(v) = 50$ and for every $v \in V(C_{60})$, $\sigma(v) = 278$, then

$$\begin{aligned} SJ(C_{20}) =& 7.5, \quad GAS(C_{20}) = 50, \quad HS(C_{20}) = 0.6, \\ J(C_{20}) =& 1.5, \quad SJ(C_{60}) = 10.73, \quad GAS(C_{60}) = 278, \\ HS(C_{60}) =& 0.32, \quad J(C_{60}) = 0.9. \end{aligned}$$

A nanostructure called *achiral polyhex nanotorus* (or *toroidal fullerenes* of parameter p and length q, denoted by $T = T[p, q]$ is depicted in Figure 4 and its 2-dimensional molecular graph is in Figure 5. It is regular of valency 3 and has pq vertices and $\frac{3pq}{2}$ edges. It follows the following proposition.

Proposition 3.1.

$$\begin{aligned} SJ(T) =& \frac{9(pq)^2\sqrt{pq}}{8(pq+2)\sqrt{W(T)}}, \quad GAS(T) = \frac{2W(T)}{pq}, \\ HS(T) =& \frac{3(pq)^2}{4W(T)}, \quad J(T) = \frac{9(pq)^3}{8(pq+2)W(T)}. \end{aligned}$$

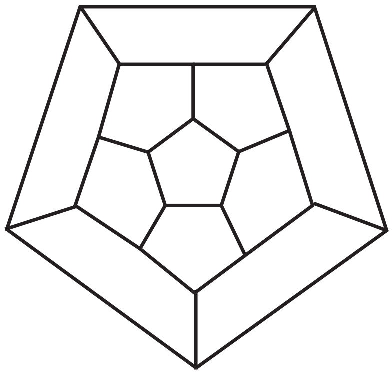

FIGURE 3. 2-dimensional graph of fullerene C_{20}

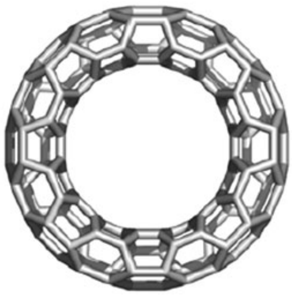

FIGURE 4. A achiral polyhex nanotorus (or toroidal fullerene) $T[p, q]$

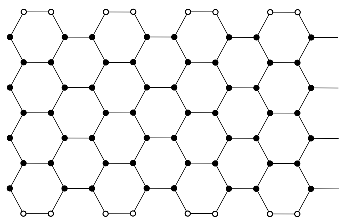

FIGURE 5. A 2-dimensional lattice for an achiral polyhex nanotorus $T[p, q]$

The vertex set of the hypercube H_n consists of all n-tuples $(b_1, b_2, \ldots, b_n)$ with $b_i \in \{0, 1\}$. Two vertices are adjacent if the corresponding tuples differ in precisely one place. Moreover, H_n has exactly $2n$ vertices and $n2^{n-1}$ edges.

Lemma 3.4. [8] *The hypercube H_n is $(n2^{n-1})$-transmission regular which is vertex- and edge-transitive.*

Therefore from Lemma 3.1 and Lemma 3.4 we have the following result.

Corollary 3.2.

$$SJ(H_n) = \frac{n^2 2^{2(n-1)}}{(n2^{n-1} - 2n + 2)\sqrt{n2^n}}, \quad GAS(H_n) = n, \quad HS(H_n) = 2n^2 2^{2(n-1)},$$
$$J(H_n) = \frac{n^2 2^{2(n-1)}}{(n2^{n-1} - 2n + 2)n2^{n-1}}.$$

4. On the Application Possibilities of Transmission-Based Topological Indices in QSPR Studies

As we have already mentioned, the transmission-based topological indices represent a particular family of distance-based topological invariants. In what follows we demonstrate in examples the promising applications of TT indices in QSPR studies. In the literature we found some TT indices used successfully for predicting physico-chemical properties of unbranched alkanes. Ren [41] introduced a topological index denoted by Xu, it is defined for an n-vertex connected graph G as follows:

$$Xu(G) = \sqrt{n} \log \left(\frac{\sum_{u \in V(G)} d(u)\sigma^2(u)}{\sum_{u \in V(G)} d(u)\sigma(u)} \right).$$

Analyzing the mono-parametric correlations with different degree-based and distance-based indices (Randić connectivity index, Balaban's J index), the linear prediction model based on $Xu(G)$ index gives the best results.

Shamsipur et al. [42] proposed a family of bond-additive TT topological indices, called as shamsipur indices (Sh_1–Sh_{10} indices) and used them for prediction of different physico-chemical properties of a large number of alkanes and alkane isomers. In [42] for 379 organic compounds ten different versions of Sh indices were calculated and their ability were evaluated in QSPR studies. The resulting regression data were compared with the results based on several known topological indices, and in most cases, betters results were obtained by the Sh_1–Sh_{10} indices. For example, using the Sh_1 index defined as

$$Sh_1(G) = \log \left(\sum_{uv \in E(G)} \frac{\sigma(u)\sigma(v)}{d(u)d(v)} \right),$$

a correlation coefficient of 0,983 between the boiling point (BP) and Sh_1 was obtained.

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