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Connectivity-, Wiener- and Harary-Type Indices of Dendrimers

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Formulas for calculating connectivity-based indices (Randić-type index calculated on vertices, χ, and on edges, ε, Zagreb index, M_2, and Bertz index, B) and distance-based indices (Wiener , W, hyper-Wiener, WW, and Harary-type indices, H_{We} and H_{Wp}) in regular homogeneous dendrimers are derived. Values of the above topological indices for families of dendrimers, with up to 10 orbits, are calculated. Mutual intercorrelation of these indices, in the considered dendrimers, is evaluated.

Key words: connectivity indicies, dendrimers, distance indicies

INTRODUCTION

Dendrimers are hyperbranched molecules, synthesized mainly by two procedures: (i) by »divergent growth«,[1–3] when branched blocks are added around a central *core*, thus obtaining a new, larger orbit or generation, and (ii) by »convergent growth«,[4–7] when large branched blocks , previously built up starting from the periphery, are attached to the core. These rigorously tailored structures show a spherical shape, which can be functionalized,[8–11]

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thus modifying their physico-chemical or biological properties. Excellent reviews in the field are available.[12–14]

Topology of dendrimers is basically that of a tree (dendros in Greek means tree). Some particular definitions in dendrimers are needed :

Vertices in a dendrimer, except for the external endpoints, are considered as branching points. The number of edges that enlarge the number of points of a newly added generation is called the progressive degree, p.[15–17] It equals the classical degree (*i.e.*, the number of all edges emerging from a point), k, minus one: $p = k - 1$.

A regular dendrimer has all branching points with the same degree, otherwise it is irregular.

A dendrimer is called *homogeneous* if all its radial chains (*i.e.,* the chains starting from the core and ending in an external point) have the same length.[12] In graph theory, they correspond to the Bethe lattices.[18]

A tree has either a monocenter or a dicenter[19] (*i.e.,* two points joined by an edge). Accordingly, a dendrimer is called *monocentric* or *dicentric*. Examples are given in Figure 1. The numbering of orbits (generations)[12] starts with zero for the core and ends with r**,** which is the radius of the dendrimer

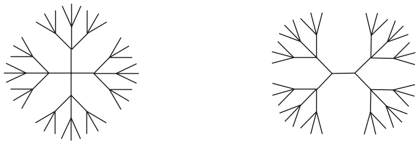

Figure 1. Monocentric and dicentric regular dendrimers.

(*i.e.*, the number of edges along a radial chain, starting from the core and ending at an external node).

CONNECTIVITY INDICES

The vertex (atom) connectivity index was introduced by Randić[20] as a measurement of the molecular branching in alkanes. It was subsequently extended by Kier and Hall to account for heteroatoms and it was renamed as the molecular connectivity index.[21] The original Randić index is calculated by

$$\chi = \chi(\mathrm{G}) = \sum_{(ij) \in E(\mathrm{G})} (k_i k_j)^{-1/2} \tag{1}$$

where the summation is carried out over all pairs of adjacent vertices, in a molecular graph, G, which is always a connected graph.

In order to calculate the vertex connectivity index for regular dendrimers, we need to introduce some mathematical results that will be given below.

In a regular monocentric dendrimer graph, of degree k, the number of vertices in the s^{th} orbit or generation, n_s, is given by:

$$n_s = k(k-1)^{s-1} \; ; \; s > 0 \; . \tag{2}$$

In the case of a dicentric dendrimer, n_s is obtained as follows:

$$n_s = 2(k-1)^{s} \; ; \; s > 0 \; . \tag{3}$$

A general expression to calculate the number of vertices in the s^{th} orbit of a regular dendrimer can be obtained from a combination of expressions (2) and (3):

$$n_s = (2-z)(k+z-1)(k-1)^{s-1} \; ; \; s > 0 \tag{4}$$

or using the progressive degree, p, one obtains:

$$n_s = (2-z)(p+z)p^{s-1} \; ; \; s > 0 \tag{5}$$

where z = 1 for a monocentric dendrimer and z = 0 for a dicentric one.

The number of external vertices (*i.e.*, endpoints) is given by:

$$n_r = (2-z)(p+z)p^{r-1} \tag{6}$$

where r is the radius of the dendrimer and equals the number of its orbits.

The total number of vertices, N, in a dendrimer will be:

$$N = (2-z) + \sum_{s=1}^{r} (2-z)(p+z)p^{s-1} \tag{7}$$

which is equivalent to

$$N = 2\sum_{s=0}^{r} p^{s} - zp^{r} \; . \tag{8}$$

By developing the sum in Eq.(8), one obtains

$$N = \frac{2(p^{(r+1)}-1)}{(p-1)} - zp^{r} . \tag{9}$$

In order to calculate the χ index, we can consider it as a combination of two χ indices, one of them χ_{ii} calculated from contributions coming from internal vertices in the dendrimer, *i.e.*, those different from the end points, and the other χ_{ie} calculated from the end point contributions:

$$\chi = \chi_{ii} + \chi_{ie} \, . \tag{10}$$

The χ_{ii} index is calculated as:

$$\chi_{ii} = (N_{r-1} - 1)\left[(p+1)^2\right]^g \tag{11}$$

where N_{r-1} is the number of internal vertices, *i.e.* those inside the r–1 orbit. This number is obtained from the total number of vertices by subtracting the number of endpoints, n_r:

$$N_{r-1} = (N - n_r) = \frac{2(p^r - 1)}{p-1} - zp^{(r-1)} \; ; \; \mathrm{r} \geq 1 \, . \tag{12}$$

By substituting the expressions for N and n_r in Eq. (12) and then that of N_{r-1} in Eq. (11), one obtains

$$\chi_{ii} = (N - n_r - 1)\left[(p+1)^2\right]^g \tag{13}$$

and subsequently

$$\chi_{ii} = \left[\frac{2(p^{(r+1)} - 1)}{p-1} - zp^r - (2-z)(p+z)p^{(r-1)}\right](p+1)^{2g} \, . \tag{14}$$

Following a similar procedure for χ_{ie}, one obtains:

$$\chi_{ie} = n_r (p+1)^g = (2-z)(p+z)p^{r-1}(p+1)^g \tag{15}$$

and the global index (see Eq. (10))

$$\chi = (N - n_r - 1)(p+1)^{2g} + n_r (p+1)^g \tag{16}$$

or by expanding N and n_r

$$\chi = \left[\frac{2(p^{(r+1)} - 1)}{p-1} - zp^r - (2-z)(p+z)p^{(r-1)} - 1\right](p+1)^{2g} +$$

$$+ (2-z)(p+z)p^{(r-1)}(p+1)^g . \tag{17}$$

By making in Eq. (16) $g = -1/2$, the classical Randić index, $\chi_{-1/2}$, is obtained

$$\chi_{-1/2} = (N - n_r - 1)(p+1)^{-1} + n_r (p+1)^{-1/2} \tag{18}$$

$$\chi_{-1/2} = \frac{2(p^{(r+1)} - 1)}{(p^2 - 1)} - \frac{(2-z)(p+z)p^{(r-1)} - 1}{(p+1)} + (2-z)(p+z)p^{(r-1)}(p+1)^{-1/2} \; . \quad (19)$$

When g = 1, the Zagreb Group index, M_2,[22] can be obtained

$$M_2 = (N - n_r - 1)(p+1)^2 + n_r(p+1) \quad (20)$$

$$M_2 = \frac{(p+1)}{(p-1)}\left[4p^{(r+1)} - (p+1)^2 + z(z-3)p^r(p-1)\right] . \quad (21)$$

From Eq. (13), it is easy to calculate the Bertz index[23] (see also the Platt and Gordon-Scantlebury indices)[23a] of a dendrimer as

$$B = (N - n_r)\binom{p+1}{2} = \left[\frac{2(p^{(r+1)} - 1)}{(p-1)} - p^r z - (2-z)(p+z)p^{(r-1)}\right]\frac{(p+1)p}{2} \quad (22)$$

which equals the number of connected pairs of edges in a regular dendrimer.

BOND (EDGE) CONNECTIVITY INDEX

The bond (edge) connectivity index,[24] ε, was introduced by Estrada as a measurement of molecular volume in alkanes. It was subsequently extended to molecules containing heteroatoms[25] and to account for spatial[26] (3D) features of organic molecules. The ε index is calculated by using the Randić graph theoretical invariant in which the vertex degree is substituted by edge degree. Mathematically, the index is obtained as follows:

$$\varepsilon = \varepsilon(\mathrm{G}) = \sum_{(ij)\in E(L(\mathrm{G}))} (\delta_i \delta_j)^g \quad (23)$$

where the summation runs over all edges in the line graph, L(G), which is derived from G by substituting edges by points and then connecting those points whenever the edges which they represent are adjacent in G. In Eq. (23), δ_i is the degree of vertex $i \in V(L(\mathrm{G}))$ (*i.e.*, the degree of the corresponding edge in G):

$$\delta_i = p_u + p_v \; ; \; (u,v) \in E(\mathrm{G}) \; . \quad (24)$$

Thus, an edge $(i, j) \in E(L(\mathrm{G}))$ corresponds to a subgraph of two adjacent edges in G. The exponent g is taken to be –1/2, like for the Randić index.

In regular dendrimers, ε can be calculated as a sum of three indices accounting for contributions associated to pairs of internal-internal adjacent edges, ε_{ii}, pairs of internal-external adjacent edges ε_{ie}, and pairs of external-external adjacent edges ε_{ee}. One edge will be called internal if it is inside the $(r–2)^{th}$ orbit and external if it is outside this orbit (*i.e.*, if it is incident to an external vertex). It is straightforward that the internal edges of the regular dendrimer have the same degree, $\delta_i = 2p$, and the external ones have the degree $\delta_e = p$, where p is the progressive degree of internal vertices in the dendrimer. Now, the expression for the edge connectivity index can be written as:

$$\varepsilon = \varepsilon_{\text{ii}} + \varepsilon_{\text{ie}} + \varepsilon_{\text{ee}} \quad . \tag{25}$$

The ε_{ii} index can be obtained as

$$\varepsilon_{\text{ii}} = N_{r-2} \binom{p+1}{2} (\delta_i)^{2g} \tag{26}$$

where $N_{r–2}$ is the number of internal vertices inside the $r–2$ orbit (itself included). It can be calculated by Eq. (8), when the summation runs till $r–2$.

$$N_{r-2} = (N - n_r - n_{r-1}) = \frac{2(p^{(r-1)} - 1)}{p-1} - zp^{(r-2)} \; ; \; r \geq 2 \; . \tag{27}$$

The internal edge connectivity index, ε_{ii}, is then calculated as

$$\varepsilon_{-1/2,\text{ii}} = N_{r-2} \binom{p+1}{2} (2p)^{-1} = \left(\frac{2(p^{(r-1)})}{p-1} - zp^{(r-2)} \right) \left(\frac{p+1}{4} \right) \; ; \quad r \geq 2 \; . \tag{28}$$

The internal-external edge connectivity index, ε_{ie}, can be calculated by

$$\varepsilon_{\text{ie}} = n_r (\delta_i \delta_e)^g \tag{29}$$

which can be given as

$$\varepsilon_{-1/2,\text{ie}} = n_r (2p^2)^{-1/2} = (2-z)(p+z)p^{(r-1)} \left(\frac{1}{p\sqrt{2}} \right) . \tag{30}$$

The ε_{ee} index is calculated by

$$\varepsilon_{\text{ee}} = n_{r-1} \binom{p}{2} (\delta_e)^{2g} \tag{31}$$

where n_{r-1} is

$$n_{r-1} = (2-z)(p+z)p^{(r-2)} \tag{32}$$

and next

$$\varepsilon_{-1/2,\mathrm{ee}} = n_{r-1}\binom{p}{2}(p)^{-1} = (2-z)(p+z)p^{(r-2)}\left(\frac{p-1}{2}\right) \; ; \; r \geq 2 \; . \tag{33}$$

The edge connectivity index of regular dendrimers can be obtained by combining Eqs. (28), (30) and (33) in expression (25). Tables I and II list values of the above presented connectivity indices, up to generation ten, in regular dendrimers.

TABLE I

Vertex and edge connectivity indices for regular dendrimers having p = 2 and 3, and generations up to 10 orbits

	N	$\chi_{-1/2}$	$\varepsilon_{-1/2}$	N	$\chi_{-1/2}$	$\varepsilon_{-1/2}$
r		z = 1			z = 0	
			p = 2			
1	4	1.732	1.500	6	2.643	2.414
2	10	4.464	4.371	14	6.285	6.328
3	22	9.928	10.243	30	13.571	14.157
4	46	20.856	21.985	62	28.142	29.814
5	94	42.713	45.471	126	57.284	61.127
6	190	86.426	92.441	254	115.568	123.755
7	382	173.851	186.382	510	232.135	249.010
8	766	348.703	374.265	1022	465.270	499.519
9	1534	698.405	750.029	2046	931.540	1000.539
10	3070	1397.810	1501.558	4094	1864.080	2002.577
			p = 3			
1	5	2	2.000	8	3.25	3.414
2	17	7	7.828	26	10.75	12.243
3	53	22	25.485	80	33.25	38.728
4	161	67	78.456	242	100.75	118.184
5	485	202	235.368	728	303.25	356.551
6	1457	607	714.103	2186	910.75	1071.654
7	4373	1822	2144.308	6560	2733.25	3216.962
8	13120	5467	6434.923	19680	8200.75	9652.885
9	39370	16400	19306.770	59050	24603.25	28960.655
10	118100	49210	57922.310	177100	73810.75	86883.966

TABLE II

Bertz and Zagreb group indices for regular dendrimers having $p = 2$ and 3, and generations up to 10 orbits

	N	B	M_2	N	B	M_2
r		$z = 1$			$z = 0$	
			$p = 2$			
1	4	3	9	6	6	21
2	10	12	45	14	18	69
3	22	30	117	30	42	165
4	46	66	261	62	90	357
5	94	138	549	126	186	741
6	190	282	1125	254	378	1509
7	382	570	2277	510	762	3045
8	766	1146	4581	1022	1530	6117
9	1534	2298	9189	2046	3066	12261
10	3070	4602	18405	4094	6138	24549
			$p = 3$			
1	5	6	16	8	12	40
2	17	30	112	26	48	184
3	53	102	400	80	156	616
4	161	318	1264	242	480	1912
5	485	966	3856	728	1452	5800
6	1457	2910	11632	2186	4368	17464
7	4373	8742	34960	6560	13116	52456
8	13120	26238	104944	19680	39360	157432
9	39370	78726	314896	59050	118092	472360
10	118100	236190	944752	177100	354288	1417144

WIENER-TYPE INDICES

The Wiener index,[27] W, or the »path number« , in acyclic structures, can be defined by

$$W = W(\mathrm{G}) = \sum_{(i,j)\in E(\mathrm{G})} N_{i,(i,j)} N_{j,(i,j)} \tag{34}$$

where $N_{i,(i,j)}$ and $N_{j,(i,j)}$ denote the number of vertices lying on the two sides of edge $(i,j) \in E(\mathrm{G})$, with $E(\mathrm{G})$ being the set of edges in a connected graph, G. The summation runs over all edges in G. The product $N_{i,(i,j)}\, N_{j,(i,j)}$ is the number of external paths (*i.e.*, the paths which contain edge (i,j) as a sub-path) and represents the contribution of edge (i,j) to the global index, W. It is just the (i,j)-entry $((i,j) \in E(\mathrm{G}))$ in the edge-defined Wiener matrix[28,29]

$$[\boldsymbol{W}_\mathrm{e}]_{i,j} = N_{i,(i,j)}\, N_{j,(i,j)} \ ; \ (i,j) \in E(\mathrm{G}) \ . \tag{35}$$

For non-adjacent vertices, $(i,j) \notin E(\mathrm{G})$, the entries in $\boldsymbol{W}_\mathrm{e}$ are zero. From this, W can be calculated as the half sum of its entries

$$W_{\;W\mathrm{e}} = (1/2)\sum_i \sum_j \; [\boldsymbol{W}_\mathrm{e}]_{i,j} \; . \tag{36}$$

In the following, a subscript matrix symbol associated with the index symbol will specify the matrix on which the index is calculated.

When (i,j) represents a path, $(i,j) \in P(\mathrm{G})$, with $P(\mathrm{G})$ being the set of paths in graph, then a relation similar to Eq. (34) will define the *hyper-Wiener* index,[30] WW

$$WW = WW(\mathrm{G}) = \sum_{(i,\,j) \in P(\mathrm{G})} N_{i,(i,\,j)} N_{j,(i,\,j)} \; . \tag{37}$$

The summation goes over all paths in G. $N_{i,(i,j)}$ and $N_{j,(i,j)}$ represent now the number of vertices lying on the two sides of the path $(i,j) \in P(\mathrm{G})$. The product $N_{i,(i,j)} N_{j,(i,j)}$ equals the number of external paths that contain the path (i,j) as a sub-path and is the contribution of the path (i,j) to the global index, WW. It is the (i,j)-entry in the path-defined Wiener matrix[28,29]

$$[\boldsymbol{W}_\mathrm{p}]_{i,j} = N_{i,(i,j)}\, N_{j,(i,j)} \; ; \; (i,j) \in P(\mathrm{G}) \; . \tag{38}$$

From $\boldsymbol{W}_\mathrm{p,}$ the index WW is calculated as the half sum of its entries

$$WW_{\;\boldsymbol{W}\mathrm{p}} = (1/2)\sum_i \sum_j \; [\boldsymbol{W}_\mathrm{p}]_{i,j} \; . \tag{39}$$

In both $\boldsymbol{W}_\mathrm{e}$ and $\boldsymbol{W}_\mathrm{p}$ matrices, the diagonal entries are zero.

In cycle-containing graphs, Wiener matrices are not defined. Wiener indices are here calculated by means of the distance-type matrices.

The distance matrix,[19] $\boldsymbol{D}_\mathrm{e}$, collects the topological distances in the graph, *i.e.*, the number of edges, $N_{e,(i,j)\, \in P(\mathrm{G})}$, which separate two vertices, i and j, on the shortest path, $(i,j) \in P(\mathrm{G})$

$$[\boldsymbol{D}_\mathrm{e}]_{i,j} = \begin{cases} N_{e,(i,j) \in P(\mathrm{G})}; \left|(i,j)\right| = \min, \text{if } i \neq j \\ 0 \text{ if } i = j \end{cases} \; . \tag{40}$$

The subscript e in the symbol of the distance matrix means that it is edge-defined (*i.e.*, its entries count edges on the path (i,j)). In Eq. (40), $\left|(i,j)\right|$ is the cardinality of the path (i,j) taken as a set of subsequently connected edges; it is just the length of the path (i,j). In case $\left|(i,j)\right| = \min$, it equals the topological distance between i and j. The Wiener index is calculated as the half sum of entries in $\boldsymbol{D}_\mathrm{e}$, meaning the number of all distances in G (*i.e.*, the number of internal edges contained in all shortest paths in the graph)

$$W_{De} = (1/2)\sum_i \sum_j [\boldsymbol{D}_e]_{i,j} \ . \qquad (41)$$

A similar matrix[31] can be constructed when paths, p, of length $1 \le |p| \le |(i,j)|$ are counted in the path (i,j)

$$[\boldsymbol{D}_\mathbf{p}]_{i,j} = \begin{cases} N_{p,(i,j)\in P(G)}; |(i,j)| = \min, \text{if } i \neq j \\ 0 \text{ if } i = j \end{cases} . \qquad (42)$$

It is a path-defined matrix and the number of paths, $N_{p,(i,j)\in P(G)}$, can be calculated from the entries $[\boldsymbol{D}_e]_{i,j}$ by

$$N_{p,(i,j)\in P(G)} = \binom{[\boldsymbol{D}_e]_{ij} + 1}{2} = \{([D_e]_{i,j})^2 + [D_e]_{i,j}\}/2 \ . \qquad (43)$$

The half sum of entries in $\boldsymbol{D}_p$ yields the hyper-Wiener index[31]

$$WW_{Dp} = (1/2)\sum_i \sum_j [\boldsymbol{D}_p]_{i,j} \qquad (44)$$

whose meaning is the number of all internal paths (*i.e.*, the paths *internal* with respect to endpoints i and j) contained in all shortest paths in the graph. In a connected graph, the number of internal paths equals the number of external paths, (*i.e.*, the paths containing the path (i,j) as a sub-path), as stated by Klein, Lukovits and Gutman.[32]

By virtue of the equality of the sum of »external« and »internal« paths in a tree graph, it is straightforward that: $W_{De} = W_{We}$ and $WW_{Dp} = WW_{Wp}$ (*i.e.*, Wiener-type indices calculated on the distance-type and Wiener-type matrix, respectively).

HARARY-TYPE INDICES

In chemical graph theory, the distance matrix accounts for the »through bond« interactions of atoms in molecules. However, these interactions decrease as the distance between atoms increases. This is the reason why the »reciprocal distance« matrix, $\boldsymbol{RD}_e(G)$ was recently introduced. Entries in this matrix are defined by

$$[\boldsymbol{RD}_e]_{i,j} = 1 \ / \ [\boldsymbol{D}_e]_{i,j} \ . \qquad (45)$$

$\boldsymbol{RD}_e$ matrix allows the calculation of a Wiener index[7] analogue, as the half sum of its entries

$$H_{De} = H_{De}(G) = (1/2)\sum_i \sum_j [\boldsymbol{RD}_e]_{i,j} \ . \qquad (46)$$

The resulting number was named,[33–35] the »Harary index«, in the honor of Frank Harary. Since topological matrices are considered »natural« sources in deriving graph descriptors, Diudea[36] has extended the use of »reciprocal (topological) property« matrices in defining novel Harary-type indices, H_M.

$$H_{M_{e/p}} = (1/2)\sum_i \sum_j 1/[\boldsymbol{M}]_{i,j} = (1/2)\sum_i \sum_j [\boldsymbol{RM}]_{i,j} \tag{47}$$

the subscript M being the identifier for a square matrix $\boldsymbol{M}$, which collects some topological property. Note that the subscript e/p refers to the length of the path (i,j) on which the matrix is defined: e means a path equal to one edge (*i.e.*, $(i,j) \in E(\mathrm{G})$) while p denotes a path of length $1 \leq |p| \leq |(i,j)| \in P(\mathrm{G})$. When the symbol of a topological index is associated with the subscript e, it is an *index* but it becomes a *hyper-index* when associated with a subscript p.

Despite the equalities $W_{D\mathrm{e}} = W_{W\mathrm{e}}$ and $WW_{D\mathrm{p}} = WW_{W\mathrm{p}}$, the Harary numbers calculated on distance-type and Wiener-type matrices, respectively, do not obey such a relation (*i.e.*, $H_{W\mathrm{e}} \neq H_{D\mathrm{e}}$ and $H_{W\mathrm{p}} \neq H_{D\mathrm{p}}$).

WIENER- AND HARARY-TYPE INDICES IN DENDRIMERS

The Wiener and hyper-Wiener indices have been calculated[16,17] by formulas derived *via* the layer matrix of cardinality,[37] $\boldsymbol{LC}$, which is related to the distance matrix, $\boldsymbol{D}_{\mathrm{e}}$. In fact, formulas for calculating $W_{D\mathrm{e}}$ and $WW_{D\mathrm{p}}$ have been derived.

In this paper, general formulas for evaluating $W_{W\mathrm{e}}$ and $WW_{W\mathrm{p}}$ and their corresponding Harary indices, $H_{W\mathrm{e}}$ and $H_{W\mathrm{p}}$, will be derived.

The procedure for evaluating the $N_{i,(i,j)}$ and $N_{j,(i,j)}$ numbers (*cf.* Eqs. (34) and (37)) is based on the wedgeal enumeration of vertices in a dendrimer.[16,38] A *wedge* is a fragment of the dendrimer (*i.e.*, a subdendrimer)[38] that results from deleting any edge, except those incident in an external, nonbranching point, in a dendrimer. If the cut edge ends at the core, the wedge is called *maximal*. The vertices of a wedge have the same degree as the corresponding ones in the whole dendrimer, except the cut point, whose degree is smaller by one. The number of vertices, F_i, in the wedge starting at orbit i can be calculated by[16]

$$F_i = \sum_{s=i}^{r} p^{(r-s)} = \frac{p^{(r-i+1)} - 1}{p - 1} \; . \tag{48}$$

Hyper-Wiener and hyper-Harary-type indices, TI_p, in dendrimers can be expressed as a sum of 'interactions' between the core and any vertex i, $TI_{0,i}$, between vertices lying on the same orbit, $TI_{i,i}$, and between vertices i and j located on different orbits, $TI_{i,j}$

$$TI_p = TI_{0,i} + TI_{i,i} + TI_{i,j} \quad (49)$$

$$TI_{0,i} = (2-z)(p+1)^z \sum_{i=1}^{r} p^{(i-z)} \Big[\big[(N - F_1)F_i\big]^g + (1-z)\big[(N/2)F_i\big]^g \Big] \quad (50)$$

$$TI_{i,i} = (1-z)\big[(N/2)^2\big]^g + \sum_{i=1}^{r} \left(\frac{(2-z)(p+1)^z p^{(i-z)}}{2} \right) \big[(F_i)^2\big]^g \quad (51)$$

$$TI_{i,j} = (2-z)(p+1)^z \sum_{i=1}^{r-1} p^{(i-z)} \sum_{j=i+1}^{r} \left\{ \begin{matrix} \big[(2-z)(p+1)^z p^{(j-z)} - p^{(j-i)}\big](F_i F_j)^g + \\ + p^{(j-i)}\big[(N - F_{i+1})F_j\big]^g \end{matrix} \right\}; r > 1 \quad (52)$$

where N is the total number of vertices in the dendrimer (see Eq.(9)) and F_i is the number of vertices in a wedgeal fragment starting at orbit i (see Eq.(48)). When g = 1 the TI is WW_{Wp} while in case g = –1, the index is H_{Wp}.

A similar procedure leads to the edge-defined indices, TI_{e} : W_{We} (g = 1) and H_{We} (g = –1)

$$TI_{\mathrm{e}} = (1-z)\left(\left(\frac{N}{2} \right)^2 \right)^g + (p+1)^z (2p)^{(1-z)} \sum_{i=1}^{r} p^{(i-1)} \big((N - F_i)F_i \big)^g \; . \quad (53)$$

Values of the Wiener-type and Harary-type indices are collected in Tables III and IV.

TABLE III

Wiener-Type indices for regular dendrimers having p = 2 and 3, and generations up to 10 orbits

p	*r*	*W*		*WW*	
		z = 0	z = 1	z = 0	z = 1
2	1	29	9	47	12
	2	285	117	667	237
	3	1981	909	6195	2535
	4	11645	5661	46179	20427
	5	62205	31293	301251	139923
	6	312829	160893	1798531	863523
	7	1510397	788733	10085123	4958787
	8	7084029	3740157	53986819	27022467
	9	32518141	17310717	278891523	141535491
	10	146825213	78661629	1400838147	718754307

TABLE III (continued)

p	*r*	*W*		*WW*	
		$z = 0$	$z = 1$	$z = 0$	$z = 1$
3	1	58	16	97	22
	2	1147	400	2842	862
	3	16564	6304	55546	18988
	4	207157	82336	885067	322684
	5	2392942	975280	12486859	4737346
	6	26310703	10897456	162614932	63370330
	7	279816808	117191488	2001654484	795156568
	8	2905693033	1226857792	23632595701	9524050936
	9	29637785506	12591244624	270225628693	110124165742
	10	298120420579	127267866832	3012581235310	1238679833686

TABLE IV

Harary-Type indices for regular dendrimers having $p = 2$ and 3, and generations up to 10 orbits

p	*r*	H_{We}		H_{Wp}	
		$z = 0$	$z = 1$	$z = 0$	$z = 1$
2	1	0.91111	1.00000	8.24444	4.00000
	2	0.75700	0.80952	39.48428	21.00000
	3	0.67978	0.70526	171.93340	93.99806
	4	0.64248	0.65479	718.89205	398.36215
	5	0.62434	0.63034	2942.94684	1642.52530
	6	0.61544	0.61840	11913.41433	6674.41687
	7	0.61105	0.61251	47945.57042	26914.25133
	8	0.60886	0.60959	192376.55943	108099.91432
	9	0.60778	0.60814	770707.04503	433297.01294
	10	0.60724	0.60742	3085243.85345	1734996.10484
3	1	0.91964	1.00000	17.41964	7.00000
	2	0.79410	0.82692	179.54978	77.12500
	3	0.75027	0.76122	1696.45922	744.63142
	4	0.73578	0.73939	15533.98437	6873.80590
	5	0.73099	0.73219	140639.34503	62412.87700
	6	0.72941	0.72980	1268302.06937	563405.57044
	7	0.72888	0.72901	11422421.63083	5075774.57299
	8	0.72870	0.72875	102824974.44435	45697411.49634
	9	0.72864	0.72866	925494391.69444	411323103.15047
	10	0.72862	0.72863	832965848.383902	3702047217.72089

From Table IV one can see that the H_{We} values decrease as the radius (*i.e.*, generation) of the dendrimer increases. For the family of dendrimers having the progressive degree 2, the limit of convergence is 0.6067 while for the family with the progressive degree 3, the limit is 0.7286, irrespective of whether they are mono- or dicentric-dendrimers. The convergence is a feature of H_{We} that differentiates this index from all the discussed indices.

Connectivity-type indices are highly intercorrelated (correlating coefficient, $r > 0.9999$) in the set of homogeneous dendrimers with the degree 3 and 4 and generation up to ten. When the distance-based indices are considered, the correlation of the connectivity-type indices lowers to about 0.97 and drops to about 0.05 *vs*. H_{We}. This behavior suggests that the distance-based indices are more »structure-related« in comparison to the connectivity-based ones. This is supported by the correlation *vs*. the number of vertices (*i.e.*, carbon atoms), which is about 0.97 for the distance-based indices, except H_{We} and over 0.9999 for the connectivity-based indices. Index H_{We} is practically orthogonal *vs*. all the other indices discussed herein. The above results might be used in structure-property studies. Unfortunately, well defined families of dendrimers are still difficult to obtain and characterize.

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SAŽETAK

Indeksi povezanosti i indeksi nalik na Wienerov i Hararyjev za dendrimere

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Izvedene su formule za izračunavanje različitih indeksa povezanosti za pravilne homogene dendrimere (Randićevi indeksi za čvorove (χ) i bridove (ε), Zagrebački indeks (M_2) i Bertzov indeks (B)) i različitih indeksa udaljenosti (Wienerov indeks, W, hiper-Wienerov indeks, WW, Hararyjevi indeksi H_{We} i H_{Wp}). Razmotrene su međusobne korelacije tih indeksa.