Molecular Topology. 25.[1] Hyper-Wiener Index of Dendrimers

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General formulas for the calculation of the hyper-Wiener index, **R**, in regular dendrimers are proposed. They are derived on the basis of Randić algorithm[2] by using progressive vertex degrees and orbit numbers[3] as parameters. A second evaluation of **R** is made on the ground of Klein−Lukovits−Gutman formula.[4]

1. INTRODUCTION

Wiener[5] has introduced the first structurally related number, **W**, for correlating with the thermodynamic properties of saturated hydrocarbons.[5,6] He calculated **W** as the sum of contributions $\mathbf{W}_e$, of all edges in an acyclic molecular graph, **G**

$$\mathbf{W} = \mathbf{W}(\mathbf{G}) = \sum_{e\in G} \mathbf{W}_e = \sum_{e\in G} \mathbf{N}_{L,e}\mathbf{N}_{R,e} \qquad (1)$$

where $\mathbf{N}_{L,e}$ and $\mathbf{N}_{R,e}$ denote the number of vertices lying to the left and to the right of edge e, and summation runs over all edges in **G**.

Hosoya,[7] expressed **W**, to hold for any connected graph, as the half sum of all entries in the distance matrix **D**

$$\mathbf{W} = \frac{1}{2}\sum_i\sum_j [\mathbf{D}]_{ij} \qquad (2)$$

Other formulas relate **W** with the distance sums, **DS**,[8−11] or with the distance walk degrees, $\mathbf{DW}_i^{(1)}$,[12]

$$\mathbf{W} = \frac{1}{2}\sum_i \mathbf{DS}_i = \frac{1}{2}\sum_i \mathbf{DW}_i^{(1)} \qquad (3)$$

or also with the Laplacian eigenvalues, $\mathbf{x}_i$,[13−15]

$$\mathbf{W} = \mathbf{N}\sum_{i=2}^{N} \frac{1}{\mathbf{x}_i} \qquad (4)$$

Among the various modifications of **W**, the Schultz index[12,16,17] and the hyper-Wiener index[1,2,18−21] are the most important.

Randić[2] extended eq 1 for all the paths in a tree-graph, thus resulting the so-called hyper-Wiener index, **R**

$$\mathbf{R} = \mathbf{R}(\mathbf{G}) = \sum_{p\in G} \mathbf{R}_p = \sum_{p\in G} \mathbf{N}_{L,p}\mathbf{N}_{R,p} \qquad (5)$$

where $\mathbf{R}_p$ represents the contribution of the path ***p*** to the global value **R**, and $\mathbf{N}_{L,p}$ and $\mathbf{N}_{R,p}$ have the same meaning as for eq 1 but referring to a path ***p***, instead of an edge **e**. The product equals the number of all paths which include the selected path. The index **R** can be also expressed as the half sum of the Wiener matrix entries, $[\mathbf{W}]_{ij}$,[18,19]

$$\mathbf{R} = \frac{1}{2}\sum_i\sum_j [\mathbf{W}]_{ij} \qquad (6)$$

For *N*-alkanes (paths $\mathbf{P}_N$), Lukovits[20] found the formula

$$\mathbf{R}_N = \mathbf{W}_N + \mathbf{W}_{N-1} + \mathbf{W}_{N-2} + \ldots\ \mathbf{W}_2 + \mathbf{W}_1 = \mathbf{N}(\mathbf{N}+1)[\mathbf{N}(\mathbf{N}+1) - 2]/24 \qquad (7)$$

where $\mathbf{R}_N$ denotes the **R** number of a **N** path and $\mathbf{W}_N$, $\mathbf{W}_{N-1}$, etc. are the Wiener indices of a **N** path and **N** − **1** path, etc.

Very recently, Klein, Lukovits, and Gutman[4] extended the definition of **R** to account for cycle-containing structures

$$\mathbf{R} = \frac{1}{4}\sum_i\sum_j (([\mathbf{D}]_{ij})^2 + [\mathbf{D}]_{ij}) = (\mathbf{MOM}[\mathbf{D}^2] + \mathbf{W})/2 \qquad (8)$$

The above formula relates the **R** index with the **W** index and the second moment of distance, $\mathbf{MOM}[\mathbf{D}^2]$

$$\mathbf{MOM}[\mathbf{D}^2] = \frac{1}{2}\sum_i [\mathbf{D}^2]_{ii} \qquad (9)$$

The Wiener and hyper-Wiener numbers are "seen" as an approximate measure of the expansiveness of graphs, in **R** dominating, however, the large distances. They show good correlation with various physico-chemical[12,15,19,21] and biological[22−24] properties of organic compounds.

In this paper general formulas for evaluating the hyper-Wiener index in dendrimers are presented. They are derived according to both eqs 5 and 8 and exemplified on several types of regular dendrimers.

2. HYPER-WIENER INDEX IN REGULAR DENDRIMERS

Dendrimers are hyperbranched molecules, synthesized by repeatable steps, either by adding branching blocks around a central *core* (thus obtaining a new, larger orbit or generation—the "divergent growth" approach) or by building large branched blocks starting from the periphery and then attaching them to the core (the "convergent growth" approach—see refs in ref 25). These rigorously tailored structures are mainly organic compounds, but inorganic components were also used.[26,27] They show spherical shape, which can be functionalized,[28−32] thus resulting in new and interesting properties. Reviews in the field are available.[33−35]

Some definitions in dendrimer topology are needed.

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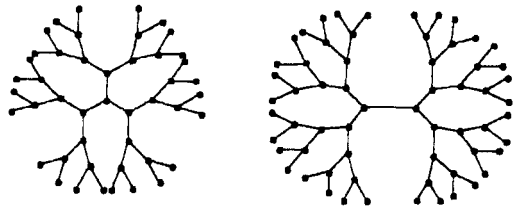


Figure 1. Regular monocentric ($D_{2,4}$) and dicentric ($DD_{2,4}$) dendrimers.

The vertices of a dendrimer, except the external end points, are considered as branching points. The number of edges emerging from each branching point is called progressive degree, **p**,[3] (*i.e.*, the edges which enlarge the number of points of a newly added orbit). It equals the classical degree, **k**, minus one: $\mathbf{p} = \mathbf{k} - \mathbf{1}$. If all the branching points have the same degree, the dendrimer is called regular. 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.[35] In graph theory, they correspond to the Bethe lattices.[36]

It is well-known[37] that any tree has either a monocenter or a dicenter (*i.e.*, two points joined by an edge). Accordingly, the dendrimers are called *monocentric* and *dicentric*, respectively. Examples are given in the Figure 1. The numbering of orbits (generations[3,35]) starts with zero for the core and ends with **r**, which equals the radius of the dendrimer (*i.e.*, the number of edges from the core to the external nodes).

A regular monocentric dendrimer, of progressive degree **p** and generation **r** is herein denoted by $\mathbf{D}_{p,r}$, whereas the corresponding dicentric dendrimer, by $\mathbf{DD}_{p,r}$.

Two procedures were developed for evaluating the **R** and **W** numbers: (a) enumerating procedure, based on eq 5 and (b) layer matrix procedure, which applies eq 8.

(a) Enumerating Procedure. The enumeration of points within the subgraphs lying to the left and to the right of a selected path (see eq 5) may be accomplished by

$$\mathbf{N}_i = \sum_{s=1}^{r} p^{(r-s)} \tag{10}$$

where **r** denotes the maximal orbit number in the dendrimer and **i** is the orbit number of one of the endpoints of the path *p*. The number of all vertices in dendrimer is given by

$$\mathbf{N}(\mathbf{D}_{p,r}) = (2 - \mathbf{z})p^{r} + 2\sum_{i=0}^{r-1} p^{i} = 2\sum_{i=0}^{r} p^{i} - \mathbf{z}p^{r} \tag{11}$$

where $\mathbf{z} = 1$ for a monocentric and $\mathbf{z} = 0$ for a dicentric dendrimer, respectively.

Now, we can calculate $\mathbf{R}_p$ (*p* labeled by its endpoints) as well as their sum over all paths, cf. eq 5, which is just the hyper-Wiener index, **R**.

$$\mathbf{R}_{0i} = (p + 1)^{z}(2 - \mathbf{z})\sum_{p=1}^{r} p^{(i-z)}[(\mathbf{N} - \mathbf{N}_1)\mathbf{N}_i + (1 - \mathbf{z})(\mathbf{N}/2)\mathbf{N}_i] \tag{12}$$

$$\mathbf{R}_{ii} = (1 - \mathbf{z})(\mathbf{N}/2)^2 + \sum_{i=1}^{r}\binom{(p + 1)^{z}(2 - \mathbf{z})p^{(iz)}}{2}\mathbf{N}_i^2 \tag{13}$$

$$\mathbf{R}_{ij} = (p + 1)^{z}(2 - \mathbf{z})\sum_{i=1}^{r-1} p^{(i-z)} \sum_{j=i+1}^{r} \{\mathbf{N}_i\mathbf{N}_j[(p + 1)^{z}(2 - \mathbf{z})p^{(j-z)} - p^{(j-i)}] + (\mathbf{N} - \mathbf{N}_{i+1})\mathbf{N}_j p^{(j-i)}\} \tag{14}$$

$$\mathbf{R}(\mathbf{D}_{p,r}) = \mathbf{R}_{0i} + \mathbf{R}_{ii} + \mathbf{R}_{ij} \tag{15}$$

The parameter **z** enables the use of eqs 11−15 both for monocentric and dicentric regular dendrimers. By evaluating the sums in these equations, the results are two analytical relations: one for monocentric ($\mathbf{z} = 1$) and another for dicentric ($\mathbf{z} = 0$) dendrimers. For $\mathbf{z} = 1$

$$\mathbf{R}(\mathbf{D}_{p,r}) = \{2p^{2r}(p^2 - 1)^2\,\mathbf{r}^2 + p^{2r}(p^2 - 1)(p^2 - 8p - 5)\mathbf{r} + (p + 1)(p^{r} - 1)[p^{r}(p^2 + 10p + 3) - 2]\}/2(p - 1)^4 \tag{16}$$

For $\mathbf{z} = 0$

$$\mathbf{R}(\mathbf{DD}_{p,r}) = \{4p^{2r+2}(p - 1)^2\,\mathbf{r}^2 + 4p^{2r+2}(p - 4)(p - 1)\mathbf{r} + p^{2r+2}(p^2 - 3p + 16) - p^{r+1}(p^2 + 10p + 5) + (p + 1)\}/(p-1)^4 \tag{17}$$

Note that *n*-alkanes ($\mathbf{P}_N$) can be viewed as regular dendrimers, with $\mathbf{p} = \mathbf{1}$. Taking into account that $\mathbf{N}_i = \mathbf{r} - \mathbf{i} + \mathbf{1}$ and $\mathbf{r} = (\mathbf{N} - (\mathbf{2} - \mathbf{z}))/\mathbf{2}$, the evaluation of the sums in eqs 10−15 leads to

$$\mathbf{R}(\mathbf{P}_N) = \mathbf{N}(\mathbf{N} - 1)(\mathbf{N} + 1)(\mathbf{N} + 2)/24 \tag{18}$$

which is independent of **z** and is equivalent with the Lukovits relation[20] (see eq 7).

(b) Layer matrix procedure. A layer matrix, **LM**, collects the properties of vertices **u** located in concentric shells (layers) at distance **j** around each vertex $\mathbf{i} \in \mathbf{G}$. The **j**-*th* layer of vertex **i**, $\mathbf{G}(\mathbf{u})_j$, and the matrix entries can be written as

$$\mathbf{G}(\mathbf{u})_j = \{\mathbf{u}: \mathbf{D}_{iu} = \mathbf{j}\} \tag{19}$$

$$[\mathbf{LM}]_{ij} = \sum_{u \in G(u)_j} \mathbf{M}_u \tag{20}$$

where **M** is a given property.

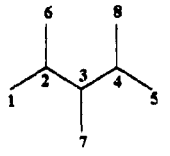
Thus the **LM** can be expressed as

$$\mathbf{LM} = \{[\mathbf{LM}]_{ij};\ \mathbf{i} \in \mathbf{V}(\mathbf{G});\ \mathbf{j} \in [0,1,...,\mathbf{d}]\} \tag{21}$$

d being the diameter of **G**, *i.e.*, the largest distance in **G**. The dimensions of such a matrix are $\mathbf{N}^*(\mathbf{d}+\mathbf{1})$. For more details about **LM**, see ref 38.

When **M** equals unity, the layer matrix just counts the vertices lying in each layer around **i**, until the distance $\mathbf{j} = \mathbf{ecc}_i$ (eccentricity of vertex **i**, *i.e.*, the largest distance from **i** to all other vertices in **G**). We denoted this matrix by **LC** (layer matrix of cardinality). By the layer counter, $\mathbf{j} = \mathbf{D}_{iu}$, the matrix **LC** is related to the distance matrix, **D**, their

j	0	1	2	3	4
	1	1	2	2	2
	1	3	2	1	0
	1	3	4	0	0
	1	3	2	2	0
	1	1	2	2	2
	1	1	2	2	2
	1	1	2	4	0
	1	1	2	2	2



234M3C5

Figure 2. The LC matrix for 2,3,4-trimethylpentane (234M3C5).

entries being the distance degrees and itself a collection of distance degree sequences. Figure 2 illustrates the **LC** matrix for the graph 2,3,4-trimethylpentane. In the followings, the column $\mathbf{j} = \mathbf{0}$ (whose elements equal unity) will be neglected. The **LC** matrix of a regular dendrimer, in the line form,[39] is as follows

$$\mathbf{A} = (2 - \mathbf{z})\{(p + 1)p^{(\mathbf{j}-1)}; (1 - \mathbf{z})p^{\mathbf{r}}\} \quad \mathbf{j} = 1,2,...,\mathbf{r} \tag{22}$$

$$\mathbf{B} = (2 - \mathbf{z})p^{(\mathbf{s}-\mathbf{z})}(p + 1)^{\mathbf{z}}\{(p + 1)p^{(\mathbf{j}-1)}; \mathbf{E}\} \quad \mathbf{j} = 1,2,...,\mathbf{r} - \mathbf{s}; \quad \mathbf{s} = 1,2,...,\mathbf{r} - 2 \tag{23}$$

$$\mathbf{C} = (2 - \mathbf{z})p^{(\mathbf{s}-\mathbf{z})}(p + 1)^{\mathbf{z}}\{(\mathbf{r} - \mathbf{s})(p + 1); \mathbf{E}\} \quad \mathbf{s} = \mathbf{r} - 1, \mathbf{r} \tag{24}$$

$$\mathbf{E} = \{(p^{(\mathbf{r}-\mathbf{s})})_{\mathbf{j}}; \ (p^{(\mathbf{r}-\mathbf{s}+\mathbf{k})})_{\mathbf{j}}; \ (p^{(\mathbf{r}-\mathbf{s}+\mathbf{k})})_{\mathbf{j}}; \ (\mathbf{z}p^{\mathbf{r}})_{\mathbf{j}}\} \quad \mathbf{j} = \mathbf{r} - \mathbf{s} + 1; \ \mathbf{j} = \mathbf{r} - \mathbf{s} + 2\mathbf{k}; \ \mathbf{j} = \mathbf{r} - \mathbf{s} + 2\mathbf{k} + 1; \ \mathbf{j} = \mathbf{r} + \mathbf{s}; \ \mathbf{k} = 1,2,...,\mathbf{s} - \mathbf{z} \tag{25}$$

where **A**, **B**, and **C** denote the type of rows (starting from the core) within the **LC** matrix of a dendrimer, and **E** is a common part within several rows of **LC** (see also ref 40).

Thus **LC** can serve as a basis for evaluating the Wiener-related numbers, **W** and **R** (see eqs 2 and 8).

By taking into account the layer counter **j**, the expansion of the **LC** matrix of a dendrimer (eqs 22−25) offers the parameters in eq 8, **MOM(D²)**, and **W**

$$\mathbf{MOM}[\mathbf{D}^2] = (\mathbf{A} + \mathbf{B} + \mathbf{C})/2 \tag{26}$$

$$\mathbf{A} = (2 - \mathbf{z})[\sum_{\mathbf{j}=1}^{\mathbf{r}}(\mathbf{p} + 1)\mathbf{p}^{(\mathbf{j}-1)}\mathbf{j}^2 + (1 - \mathbf{z})\mathbf{p}^{\mathbf{r}}(\mathbf{r} + 1)^2] \tag{27}$$

$$\mathbf{B} = (2 - \mathbf{z})(p + 1)^{\mathbf{z}}\sum_{\mathbf{s}=1}^{\mathbf{r}-2}[p^{(\mathbf{s}-\mathbf{z})}(\sum_{\mathbf{j}=1}^{\mathbf{r}-\mathbf{s}}(p + 1)p^{(\mathbf{j}-1)}\mathbf{j}^2 + \mathbf{E})] \tag{28}$$

$$\mathbf{C} = (2 - \mathbf{z})(p + 1)^{\mathbf{z}} \sum_{\mathbf{s}=\mathbf{r}-1}^{\mathbf{r}} p^{(\mathbf{s}-\mathbf{z})}[(\mathbf{r} - \mathbf{s})(p + 1) + \mathbf{E}] \tag{29}$$

$$\mathbf{E} = \mathbf{p}^{(\mathbf{r}-\mathbf{s})}(\mathbf{r} - \mathbf{s} + 1)^2 + \mathbf{z}p^{\mathbf{r}}(\mathbf{r} + \mathbf{s})^2 + \sum_{\mathbf{k}=1}^{\mathbf{s}-\mathbf{z}}\mathbf{p}^{(\mathbf{r}-\mathbf{s}+\mathbf{k})}[(\mathbf{r} - \mathbf{s} + 2\mathbf{k})^2 + (\mathbf{r} - \mathbf{s} + 2\mathbf{k} + 1)^2] \tag{30}$$

$$\mathbf{W} = (\mathbf{A}' + \mathbf{B}' + \mathbf{C}')/2 \tag{31}$$

$$\mathbf{A}' = (2 - \mathbf{z})[\sum_{\mathbf{j}=1}^{\mathbf{r}}(p + 1)p^{(\mathbf{j}-1)}\mathbf{j} + (1 - \mathbf{z})p^{\mathbf{r}}(\mathbf{r} + 1)] \tag{32}$$

Table 1. Topological Data for Regular Dendrimers

		MOM(D²)		W		R	
p	r	z = 0	z = 1	z = 0	z = 1	z = 0	z = 1
1	1	20	6	10	4	15	5
	2	105	50	35	20	70	35
	3	336	196	84	56	210	126
	4	825	540	165	120	495	330
	5	1716	1210	286	220	1001	715
2	1	65	15	29	9	47	12
	2	1049	357	285	117	667	237
	3	10409	4161	1981	909	6195	2535
	4	80713	35193	11645	5661	46179	20427
	5	540297	248553	62205	31293	301251	139923
3	1	136	28	58	16	97	22
	2	4537	1324	1147	400	2842	862
	3	94528	31672	16564	6304	55546	18988
	4	1562977	563032	207157	82336	885067	322684
	5	22580776	8499412	2392942	975280	12486859	4737346

$$\mathbf{B}' = (2 - \mathbf{z})(p + 1)^{\mathbf{z}}\sum_{\mathbf{s}=1}^{\mathbf{r}-2}[p^{(\mathbf{s}-\mathbf{z})}(\sum_{\mathbf{j}=1}^{\mathbf{r}-\mathbf{s}}(p + 1)p^{(\mathbf{j}-1)}\mathbf{j} + \mathbf{E}')] \tag{33}$$

$$\mathbf{C}' = (2 - \mathbf{z})(p + 1)^{\mathbf{z}} \sum_{\mathbf{s}=\mathbf{r}-1}^{\mathbf{r}} p^{(\mathbf{s}-\mathbf{z})}[(\mathbf{r} - \mathbf{s})(p + 1) + \mathbf{E}'] \tag{34}$$

$$\mathbf{E}' = p^{(\mathbf{r}-\mathbf{s})}(\mathbf{r} - \mathbf{s} + 1) + \mathbf{z}p^{\mathbf{r}}(\mathbf{r} + \mathbf{s}) + \sum_{\mathbf{k}=1}^{\mathbf{s}-\mathbf{z}}p^{(\mathbf{r}-\mathbf{s}+\mathbf{k})}[(\mathbf{r} - \mathbf{s} + 2\mathbf{k}) + (\mathbf{r} - \mathbf{s} + 2\mathbf{k} + 1)] \tag{35}$$

The evaluation of sums in eqs 26−35 results in the following analytical relations for $\mathbf{D}_{p,r}$ ($\mathbf{z} = 1$) and $\mathbf{DD}_{p,r}$ ($\mathbf{z} = 0$), respectively

$$\mathbf{MOM}(\mathbf{D}^2(\mathbf{D}_{p,r})) = [2p^{2r}(p^2 - 1)^2\mathbf{r}^2 - 4p^{2r}(2p + 1)(p^2 - 1)\mathbf{r} + (p + 1)^2 - p^{r}(p + 1)(p + 3)(3p + 1) + p^{2r}(p + 1)(3p^2 + 9p + 2)]/(p - 1)^4 \tag{36}$$

$$\mathbf{MOM}(\mathbf{D}^2(\mathbf{DD}_{p,r})) = [8p^{(2r+2)}(p - 1)^2\mathbf{r}^2 + 4p^{(2r+2)}(p - 1)(\mathbf{p} - 7)\mathbf{r} + (p + 1)^2 - 2p^{(r+1)}(p + 3)(3p + 1) + \mathbf{p}^{(2r+2)}(p^2 + 2p + 25)]/(p - 1)^4 \tag{37}$$

$$\mathbf{W}(\mathbf{D}_{p,r}) = (p + 1)[p^{2r}(p^2 - 1)\mathbf{r} - p^{2r}(2p + 1) + 2p^{r}(p + 1) - 1]/(p - 1)^3 \tag{38}$$

$$\mathbf{W}(\mathbf{DD}_{p,r}) = [4p^{(2r+2)}(p - 1)\mathbf{r} + (4p^{(r+1)} - 1)(p + 1) + p^{(2r+2)}(p - 7)]/(p - 1)^3 \tag{39}$$

By substituting eqs 36−39 in eq 8, results in **R** values which are identical with those given by eqs 16 and 17. Table 1 offers **MOM(D²)**, **W**, and **R** values for dendrimers with $\mathbf{p} = 1-3$ and $\mathbf{r} = 1-5$.

In the case of *n*-alkanes, the evaluation of the sums in eqs 26−35 offers the following simple relations for the parameters of eq 8

$$\mathbf{MOM}(\mathbf{D}^2(\mathbf{P}_\mathbf{N})) = \mathbf{N}^2(\mathbf{N}^2 - 1)/12 \tag{40}$$

$$\mathbf{W}(\mathbf{P}_N) = N(N^2 - 1)/6 \quad (41)$$

whose substitution in eq 8 results in the same relation as given in eq 18 and the same numerical values (see Table 1).

Note that the relations for **W** (eqs 38 and 39) are equivalent with the relations reported by Gutman et al.[41] and Diudea[25] and give identical numerical values.

Analytical relations and their numerical evaluation were made by using the MAPLE V Computer Algebra System (Release 2).

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