Molecular topology
24.* Wiener and hyper-Wiener indices in spiro-graphs**

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General formulas for calculating the Wiener index (W)[2] and the hyper-Wiener index (R)[3] in spiro-graphs containing three- to six-membered rings are proposed. They are derived on the basis of Hosoya's formula[4] and the Klein—Lukovitz—Gutman[5] formula for evaluating W and R, respectively, in cycle-containing graphs, by using the layer matrix of cardinality (LC).[6] An extension of the Wiener number, the W^* number of Gutman[7] is also evaluated for these spiro-graphs.

Key words: molecular topology; Wiener indices, spiro-graphs.

Wiener[2] has introduced the first structurally related number, W, for correlating with the thermodynamic properties of saturated hydrocarbons.[2,8] He calculated W as the sum of contributions, W_e, of all edges in an acyclic chemical graph, G:

$$W = W(G) = \sum_e W_e = \sum_e N_{L,e} \cdot N_{R,e} \ , \qquad (1)$$

where $N_{L,e}$ and $N_{R,e}$ 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[4] gave the well-known formula for evaluating W (also holding for cycle-containing graphs) as the half sum of all centers in the distance matrix, D:

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

Other formulas relate W to the distance sums, DS_i,[9—12] or to the distance walk degrees,[1] $DW_i^{(1)}$ (Eq. (3)) or also to the Laplacian eigenvalues,[13—15] x_i (Eq. (4)).

$$W = \frac{1}{2}\sum_i DS_i = \frac{1}{2}\sum_i DW_i^{(1)} \qquad (3)$$

$$W = N\sum_{i=2}^{N} 1/x_i \qquad (4)$$

In resuming Eq. (1) let us express edge e by its end vertices: $e = (l, r)$ (*i.e.*, the left end-point and the right end-point, respectively). Thus the subgraph lying to the left of edge e contains $N_{L,e}$ vertices whose distance to l is smaller than the distance to r. The same is true for the vertices belonging to the right subgraph, which are closer to r than to l.

In other words:

$$N_{L,e} = \left|\{i:\ i \in V(G);\ d_{li} < d_{ri}\}\right| \ , \qquad (5)$$

$$N_{R,e} = \left|\{i:\ i \in V(G);\ d_{ri} < d_{li}\}\right| \ . \qquad (6)$$

In full analogy with Eq. (1), Gutman[7] proposed an extension of the number W^*, calculable for any connected graph according to Eq. (7).

$$W^* = W^*(G) = \sum_e N_{L,e} \cdot N_{R,e} \qquad (7)$$

In cycle-containing graphs, there are, however, vertices equidistant from l and r, and according to Eqs. (5) and (6) they are not counted. Thus if G is acyclic, then

$$W^*(G) = W(G) \ . \qquad (8)$$

For every edge of the cyclic graph Cy_N, $N_{L,e} = N_{R,e} = N/2$ (where $N = N_{L,e} + N_{R,e}$) and consequently, if N is even: $W^*(Cy_N) = (1/4)N^3$, and if N is odd: $W^*(Cy_N) = (1/4)N(N-1)^2$. Note that in the case of even N, $W^*(Cy_N) = 2W(Cy_N)$. In general, $W^*(Cy_N) \geq W(Cy_N)$.

Another extension of Eq. (1) was made by Randić,[3] for all paths in G (acyclic), thus resulting the so-called "hyper-Wiener" number, R.

$$R = R(G) = \sum_p N_{L,p} \cdot N_{R,p} \qquad (9)$$

R can be evaluated from the entries of the Wiener matrix W according to Eq. (10).[16]

$$R = \frac{1}{2}\sum_i\sum_j [W]_{ij} \qquad (10)$$

* For Part 23, see Ref. 1.
** Dedicated to Academician of the RAS N. S. Zefirov (on his 60th birthday).

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Very recently, Klein, Lukovitz, and Gutman[5] extended the definition of R to account for cycle-containing structures:

$$R = \frac{1}{2}\sum_i\sum_j(MOM[D^2]+W)/2 , \quad (11)$$

where $MOM[D^2]$ denotes the second moment of distances in G,

$$MOM[D^2] = \frac{1}{2}\sum_i[D^2]_{ii} = \frac{1}{2}\sum_i\sum_j([D]_{ij})^2 . \quad (12)$$

In this paper, formulas for the Wiener index, W, and the hyper-Wiener index, R, are derived according the Eqs. (2) and (11), by using the layer matrix of cardinality, LC.[6] The W* number is calculated by the aid of a TURBO-PASCAL CWS Program.

LC matrix and Wiener-type indices

A layer matrix, LM, collects the properties of vertices u located in concentric shells (layers) at a distance j around each vertex $i \in G$. The jth layer of vertex i, $G(u)_j$, and the matrix entries can be written as

$$G(u)_j = \{u\colon d_{iu} = j\} , \quad (13)$$

$$[LM]_{ij} = \sum_{u \in G(u)_j} M_u , \quad (14)$$

where M denotes a given property. Thus the LM will be

$$LM = \{[LM]_{ij};\ i \in V(G);\ j \in [0, 1, \ldots , d]\} , \quad (15)$$

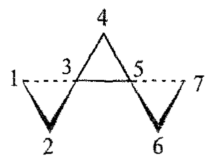
where d is the diameter of G, *i.e.*, the longest distance in G. The dimensions of such a matrix are $N(d + 1)$. For more details about the LM, see Ref. 6.

When M equals unity, the layer matrix just counts the vertices lying in each layer around i, until the distance $j = ecc_i$ (eccentricity of vertex i, *i.e.*, the longest distance from i to all other vertices G). We denoted this matrix by LC (layer matrix of cardinality). By the layer counter, $j = d_{iu}$, the matrix LC is related to the distance matrix, D, their entries being just the distance degrees and simultaneously a collection of distance degree sequences. Figure 1 illustrates the construction of an LC for the [3]-triangulane.

From the LC entries one can calculate the distance sums, DS_i.

$$DS_i = \sum_{j=1}^{d(G)}([LC]_{ij} \cdot j) \quad (16)$$

Thus LC can serve as a basis for evaluating the Wiener-related numbers, W and R, according to Eqs. (2), (3), (11), and (12).



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

LC

Fig. 1. Layer matrix of cardinality (LC) for the [3]-triangulane.

Analytical relations for W and R in spiro-graphs

A spiro-graph is obtained from simple rings by fusing a single vertex of one ring with a single vertex of another ring, giving a single vertex (of degree four) in the resultant coalesced graph.[17] The process can be repeated, thus resulting in spiro-chains.

For rings larger than three vertices, the construction of spiro-graphs have to take into account all the possibilities of connection. Thus, for four- and five-membered rings, 1,2- and 1,3-structures are considered whereas for six-membered rings, a third 1,4-structure is taken into account (Fig. 2).

The analytical relations for evaluating the W and R indices were derived on the ground of LC matrices, with the aid of the MAPLE V Computer Algebra System (Release 2). Other graph-theoretical aspects in spiro-graphs were discussed by Balasubramanian[17] and by Zefirov *et al.*[18]

In the following the relations are given in pairs: first, the relation expressed as a sum and, second, the corresponding analytical relation for each index, each type of rings, and each type of connection in spiro-graphs; n denotes the number of single cycles connected in a spiro-graph.

Three-membered rings

1. Wiener number:

$$W_n = 2\sum_{i=1}^{n} i(i+1) - n \quad (17)$$

$$W_n = \frac{n}{3}(2n^2 + 6n + 1) \quad (18)$$

2. R number:

$$MOM[D^2]_n = \frac{2}{3}\sum_{i=1}^{n} i(i+1)(2i+1) - n \quad (19)$$

$$MOM[D^2]_n = \frac{n}{3}(n^3 + 4n^2 + 5n - 1) \quad (20)$$

$$R_n = \frac{2}{3}\sum_{i=1}^{n} i(i+1)(i+2) - n \quad (21)$$

$$R_n = \frac{n^2}{6}(n^2 + 6n + 11) \quad (22)$$

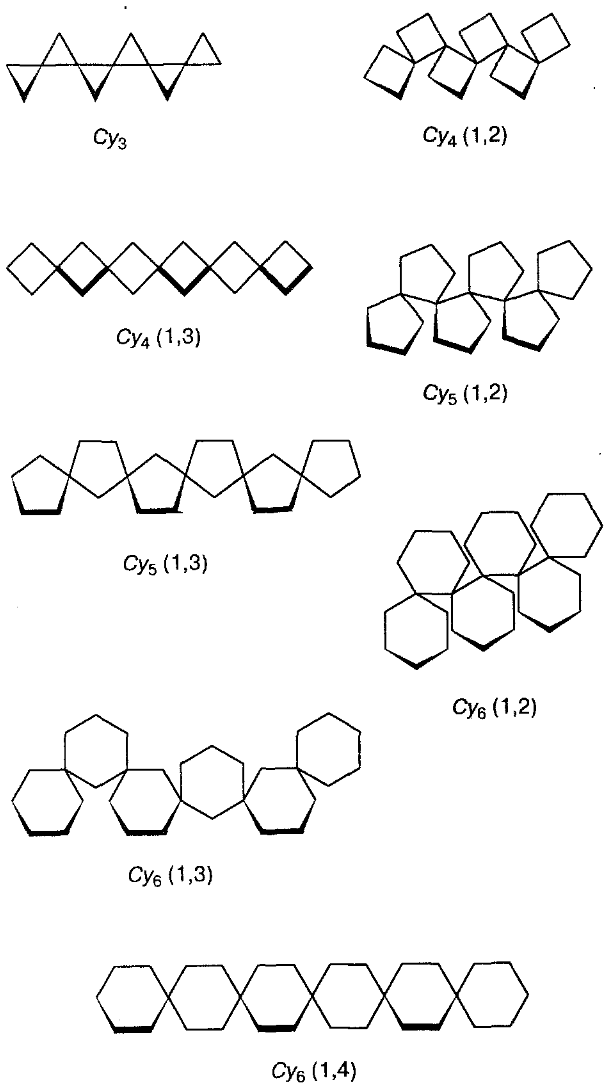


Fig. 2. Spiro-graphs with three- (Cy_3) to six-membered (Cy_6) rings.

Four-membered rings

1,3-Spiro-graphs

1. Wiener number:

$$W_n = 8(2n-1) + 4\sum_{i=1}^{n-1}(n-i)(2i+1) + 2\sum_{i=1}^{n-1}(i+1)(5n-5i-4) \quad (23)$$

$$W_n = n(3n^2+3n+2) \quad (24)$$

2. R number:

$$MOM[D^2]_n = 4(7n-4) + 4\sum_{i=1}^{n-1}(n-i)(2i+1)^2 + 4\sum_{i=1}^{n-1}(i+1)^2(5n-5i-4) \quad (25)$$

$$MOM[D^2]_n = n(3n^3+4n^2+n+4) \quad (26)$$

$$R_n = 2(11n-6) + 4\sum_{i=1}^{n-1}(n-i)(2i+1)(i+1) + \sum_{i=1}^{n-1}(i+1)(2i+3)(5n-5i-4) \quad (27)$$

$$R_n = \frac{n}{2}(3n^3+7n^2+4n+6) \quad (28)$$

1,2-Spiro-graphs

1. Wiener number:

$$W_n = 41n - 42 + \sum_{i=1}^{n-2}(i+3)[6+9(n-i-2)] \quad (29)$$

$$W_n = \frac{n}{2}(3n^2+15n-2) \quad (30)$$

2. R number:

$$MOM[D^2]_n = n^2 + 104n - 120 + \sum_{i=1}^{n-2}(i+3)^2[6+9(n-i-2)] \quad (31)$$

$$MOM[D^2]_n = \frac{n}{4}(3n^3+20n^2+55n-30) \quad (32)$$

$$R_n = \frac{1}{2}\{n^2 + 145n - 162 + \sum_{i=1}^{n-2}(i+3)(i+4)[6+9(n-i-2)]\} \quad (33)$$

$$R_n = \frac{n}{8}(3n^3+26n^2+85n-34) \quad (34)$$

Five-membered rings

1,3-Spiro-graphs

1. Wiener number:

$$W_n = 23n - 8 + 8\sum_{i=1}^{n-1}(2i+1)(n-i) + 8\sum_{i=1}^{n-1}(i+1)[1+2(n-i-1)] \quad (35)$$

$$W_n = \frac{n}{3}(4n+1)(4n+5) \quad (36)$$

2. R number:

$$MOM[D^2]_n = 41n - 16 + 8\sum_{i=1}^{n-1}(2i+1)^2(n-i) + 16\sum_{i=1}^{n-1}(i+1)^2[1+2(n-i-1)] \quad (37)$$

$$MOM[D^2]_n = \frac{n}{3}(16n^3+32n^2+20n+7) \quad (38)$$

$$R_n = 32n - 12 + 4\sum_{i=1}^{n-1}(2i+1)(2i+2)(n-i) + 4\sum_{i=1}^{n-1}(i+1)(2i+3)[1+2(n-i-1)] \quad (39)$$

$$R_n = \frac{2n}{3}(n+1)(2n+1)(2n+3) \quad (40)$$

1,2-Spiro-graphs

1. Wiener number:

$$W_n = 63n - 48 + 16\sum_{i=1}^{n-2}(i+3)(n-i-1) \quad (41)$$

$$W_n = \frac{n}{3}(8n^2 + 48n - 11) \quad (42)$$

2. R number:

$$MOM[D^2]_n = 4n^2 + 165n - 144 + 16\sum_{i=1}^{n-2}(i+3)^2(n-i-1) \quad (43)$$

$$MOM[D^2]_n = \frac{n}{3}(4n^3 + 32n^2 + 104n - 65) \quad (44)$$

$$R_n = 2n^2 + 114n - 96 + 8\sum_{i=1}^{n-2}(i+3)(i+4)(n-i-1) \quad (45)$$

$$R_n = \frac{2n}{3}(n^3 + 10n^2 + 38n - 19) \quad (46)$$

Six-membered rings

1,4-Spiro-graphs

1. Wiener number:

$$W_n = 59n - 32 + 8\sum_{i=1}^{n-1}(3i+1)(n-i) + 4\sum_{i=1}^{n-1}(3i+2)[1+2(n-i-1)] + 3\sum_{i=1}^{n-1}(i+1)[1+9(n-i-1)] \quad (47)$$

$$W_n = \frac{n}{3}(25n^2 + 15n + 14) \quad (48)$$

2. R number:

$$MOM[D^2]_n = 145n - 88 + 8\sum_{i=1}^{n-1}(3i+1)^2(n-i) + 4\sum_{i=1}^{n-1}(3i+2)^2[1+2(n-i-1)] + 9\sum_{i=1}^{n-1}(i+1)^2[1+9(n-i-1)] \quad (49)$$

$$MOM[D^2]_n = \frac{n}{4}(75n^3 + 60n^2 - n + 94) \quad (50)$$

$$R_n = 102n - 60 + 4\sum_{i=1}^{n-1}(3i+1)(3i+2)(n-i) + 2\sum_{i=1}^{n-1}(3i+2)(3i+3)[1+2(n-i-1)] + \frac{1}{2}\sum_{i=1}^{n-1}(i+1)(9i+12)[1+9(n-i-1)] \quad (51)$$

$$R_n = \frac{n}{8}(75n^3 + 110n^2 + 29n + 122) \quad (52)$$

1,3-Spiro-graphs

1. Wiener number:

$$W_n = 109n - 94 + \sum_{i=1}^{n-1}(2n-2i+3)[4+12(i-1)] + 2\sum_{i=1}^{n-2}(n-i-1)[10+13(i-1)] \quad (53)$$

$$W_n = \frac{n}{3}(25n^2 + 60n - 4) \quad (54)$$

2. R number:

$$MOM[D^2]_n = 4n^2 + 345n - 340 + \sum_{i=1}^{n-1}(2n-2i+3)^2[4+12(i-1)] + 4\sum_{i=1}^{n-2}(n-i-1)^2[10+13(i-1)] \quad (55)$$

$$MOM[D^2]_n = \frac{n}{3}(25n^3 + 80n^2 + 113n - 47) \quad (56)$$

$$R_n = 2n^2 + 227n - 217 + \sum_{i=1}^{n-1}(2n-2i+3)(2n-2i+4)[2+6(i-1)] + \sum_{i=1}^{n-2}(n-i-1)(2n-2i+3)[10+13(i-1)] \quad (57)$$

$$R_n = \frac{n}{6}(25n^3 + 105n^2 + 173n - 51) \quad (58)$$

1,2-Spiro-graphs

1. Wiener number:

$$W_n = 172n - 140 + \sum_{i=1}^{n-3}(n-i+2)[40+25(i-1)] \quad (59)$$

$$W_n = \frac{n}{6}(25n^2 + 195n - 58) \quad (60)$$

2. R number:

$$MOM[D^2]_n = 26n^2 + 596n - 590 + \sum_{i=1}^{n-3}(n-i+2)^2[40+25(i-1)] \quad (61)$$

Table 1. Wiener-type indices for spiro-graphs with three- (Cy_3) to six-membered (Cy_6) rings

n	Cy_3	Cy_4 (1,2)	Cy_4 (1,3)	Cy_5 (1,2)	Cy_5 (1,3)	Cy_6 (1,2)	Cy_6 (1,3)	Cy_6 (1,4)
				W number				
2	14	40	40	78	78	144	144	144
3	37	105	114	205	221	376	401	426
4	76	212	248	412	476	748	848	948
5	135	370	460	715	875	1285	1535	1785
6	218	588	768	1130	1450	2012	2512	3012
7	329	875	1190	1673	2233	2954	3829	4704
8	472	1240	1744	2360	3256	4136	5536	6936
				R number				
2	18	66	66	140	140	305	305	305
3	57	201	243	424	504	904	1044	1209
4	136	457	652	952	1320	1979	2614	3399
5	275	885	1440	1820	2860	3695	5470	7745
6	498	1545	2790	3140	5460	6242	10167	15342
7	833	2506	4921	5040	9520	9835	17360	27510
8	1312	3846	8088	7664	15504	14714	27804	45794
				*W** number				
2	14	80	80	104	104	288	288	288
3	37	210	228	268	300	752	802	852
4	76	424	496	528	656	1496	1696	1896
5	135	740	920	900	1220	2570	3070	3570
6	218	1176	1536	1400	2040	4024	5024	6024
7	329	1750	2380	2044	3164	5908	7658	9408
8	472	2480	3488	2848	4640	8272	11072	13872

Note. The type of ring connection is shown in parentheses.

$$MOM[D^2]_n = \frac{n}{12}(25n^3 + 260n^2 + 1157n - 758) \quad (62)$$

$$R_n = 13n^2 + 384n - 365 + \frac{1}{2}\sum_{i=1}^{n-3}(n-i+2)(n-i+3)[40+25(i-1)] \quad (63)$$

$$R_n = \frac{n}{24}(25n^3 + 310n^2 + 1547n - 874) \quad (64)$$

Numerical results

Values of the Wiener-type indices discussed herein were calculated in the spiro-graphs with three- to six-membered rings for $n = 2$ to 8. They were performed by applying the analytical relations listed above. For calculating the W^* number, a TURBO PASCAL CWS program was used. Data are collected in Table 1.

From Table 1 one can see that as the ring connection goes from 1,2- to 1,3- and then to 1,4-type, the values for all these Wiener-related indices increase. This is in agreement with the finding[5] that these express the expansiveness of graphs: a spiro-graph is more expanded as the connection of three successive rings involves more edges. Conversely, a spiro-graph is more "branched" as the number of separating edges is lower.

Our results extend the Gutman's finding that $W^* = 2W$ for even N-membered cycles (actually for spiro-graphs containing even N-membered cycles). Different results are obtained for odd N-membered cycles: for three-membered cycle spiro-graphs $W^* = W$, while for five-membered cycle spiro-graphs $W^* > W$.

The values of R are far more larger than the corresponding ones of W and W^*, a result entirely expected.

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