Three Methods for Calculation of the Hyper-Wiener Index of Molecular Graphs

Gordon Cash

Risk Assessment Division (7403), Office of Pollution Prevention and Toxics, U.S. Environmental Protection Agency, 1200 Pennsylvania Avenue, N.W., Washington, DC 20460

Sandi Klavžar*

Department of Mathematics, University of Maribor, Koroška cesta 160, SI-2000 Maribor, Slovenia

Marko Petkovšek

Department of Mathematics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia

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The hyper-Wiener index *WW* of a graph *G* is defined as $WW(G) = (\sum d\ (u, v)^2 + \sum d\ (u, v))/2$, where $d\ (u, v)$ denotes the distance between the vertices u and v in the graph *G* and the summations run over all (unordered) pairs of vertices of *G*. We consider three different methods for calculating the hyper-Wiener index of molecular graphs: the cut method, the method of Hosoya polynomials, and the interpolation method. Along the way we obtain new closed-form expressions for the WW of linear phenylenes, cyclic phenylenes, poly(azulenes), and several families of periodic hexagonal chains. We also verify some previously known (but not mathematically proved) formulas.

INTRODUCTION

The hyper-Wiener index *WW* is one of the recently conceived distance-based graph invariants, used as a structure-descriptor for predicting physicochemical properties of organic compounds (often those significant for pharmacology, agriculture, environment-protection, etc.). The hyper-Wiener index was introduced by Randić[1] and has been extensively studied; see, for instance, refs 2−11. The formula below suggests that *WW* clearly encodes the "compactness" of a structure. Furthermore, the squared term gives relatively more weight to extended structures, and *WW* should therefore be a good predictor of effects that depend more than linearly on the physical size of a molecule.

Randić's original definition of the hyper-Wiener index is applicable to trees only. Klein, Lukovits, and Gutman[4] put forward that for both trees and cycle-containing structures

$$WW(G) = \frac{1}{2}(\sum d\ (u, v)^2 + \sum d\ (u, v))$$

where $d\ (u, v)$ denotes the usual shortest path distance between the vertices u and v in the graph *G* and the summations run over all (unordered) pairs of vertices of *G*. The right-hand side of this equality is now accepted as the definition of the hyper-Wiener index of a connected graph.

In this paper we consider three different methods for calculating the hyper-Wiener index of molecular graphs: the cut method, the method of Hosoya polynomials, and the interpolation method. We discuss their advantages, drawbacks, and obtain several new closed-form expressions for the WW of infinite families of molecular graphs. We also verify some previously known (but not mathematically proved) formulas.

A *benzenoid graph* is constructed in the following manner.[12] Let **H** be the hexagonal (graphite) lattice and let *Z* be a cycle on it. Then a benzenoid graph is formed by the vertices and edges of **H**, lying on *Z* and in the interior of *Z*. Viewing a benzenoid graph *G* as a geometric figure in the plane, an *elementary cut* is defined as follows. Choose an edge *e* of *G* and draw a straight line through the center of *e*, orthogonal to *e*. This line intersects the perimeter of *G* in (at least) two points P_1 and P_2. The straight line segment *C*, the end-points of which are P_1 and P_2, is the elementary cut pertaining to the edge *e*. The set of edges intersected by an elementary cut will be called an *elementary edge-cut*.

Berris et al.[13] introduced [*N*]*phenylenes* by analogy with the catacondensed benzenoids, where *N* is the number of benzene rings. In [N]phenylenes, each benzene ring is separated from each neighboring benzene ring by a cyclobutadiene. Figure 3 depicts the hydrogen-suppressed graph representing[4] phenylene. Pericondensed benzenoids do not have analogous [N]phenylenes, but the catacondensed chain may close on itself to form a super-ring. Thus, Figure 4 depicts *cyc*[6]phenylene, the phenylene analogue of coronene.

THE CUT METHOD

The cut method is based on the results from Klavžar, Gutman, and Mohar[14] and was first introduced for calculation of the Wiener index of benzenoid graphs.[15] Subsequently it was applied in Klavžar, Gutman, and Rajapakse.[16] Moreover, it was shown that the same approach can be used for calculation of the Wiener index for the so-called Λ_1-graphs.[17]

As the cut method for the calculation of the hyper-Wiener index works for all partial cubes, we next briefly recall some basic facts about this class of graphs.

* Corresponding author phone: +386-2-2293-604; e-mail: Sandi.Klavzar@uni-lj.si.

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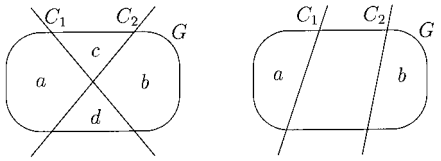

Figure 1. Different positions between two elementary cuts.

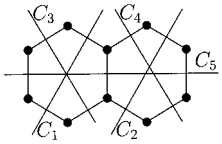

Figure 2. Naphthalene and its elementary cuts.

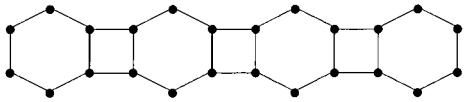

Figure 3. The linear phenylene F_4.

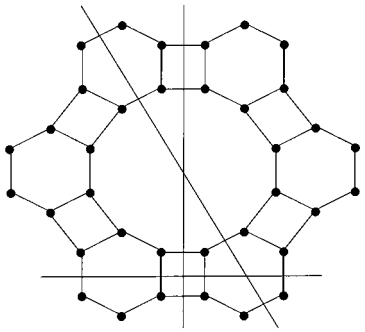

Figure 4. The cyclic phenylene R_6.

A graph is a *partial cube* if it is isomorphic to an isometric subgraph of a hypercube. (For an extensive study of partial cubes see Chapter 2 of Imrich and Klavžar.[18]) Partial cubes were also called binary Hamming graphs[14] where it was observed that benzenoid graphs are partial cubes, a fact that turned out to be very useful for investigations of the Wiener number of benzenoid graphs, see refs 15, 17, 20, and 21.

Clearly, partial cubes are bipartite, as they are subgraphs of (bipartite) hypercubes. We say that edges xy and ab of a graph G are in relation Θ if $d(x, a) + d(y, b) \neq d(x, b) + d(y, a)$. Using this definition Winkler[21] proved that a connected graph is a partial cube if and only if G is a bipartite graph in which Θ is transitive. In other words, G must be bipartite and for any triplets of edges e, f, and g of G, e, and g are in relation Θ ($e\Theta g$) whenever $e\Theta f$ and $f\Theta g$. As Θ is trivially reflexive and symmetric, it is thus an equivalence relation on a partial cube G and partitions the edge set of G into equivalence classes. The main insight for our consideration is that the Θ-equivalence classes of a benzenoid graph G coincide with its elementary edge-cuts. By extending the concept of elementary cuts to include sets of edges that are in relation Θ, a similar observation holds for the phenylenes and cyclic phenylenes to be considered later. A key result here is that, for even-membered (isometric) cycles, opposite edges are in relation Θ.

Let G be a benzenoid graph on n vertices. Then an elementary cut C divides G into two components, say $G_1(C)$ and $G_2(C)$. Let $n_1 = n_1(C)$ and $n_2 = n_2(C)$ be the number of vertices of $G_1(C)$ and $G_2(C)$, respectively, where, of course, $n_1 + n_2 = n$. Then the Wiener index of G can be calculated as

$$W(G) = \sum_i n_1(C_i) n_2(C_i)$$

where the summation goes over all elementary cuts of G. Klavžar[22] proved that this method can be extended for the calculation of the hyper-Wiener index. The method was later further elaborated in the paper by Klavžar, Žigert, and Gutman.[23] We do not wish to recall here all the details but rather describe the method intuitively. First, the hyper-Wiener index of a benzenoid graph G can be written as

$$WW(G) = W(G) + WW^*(G), \qquad (1)$$

where $WW^*(G)$ consists of a summation over all pairs of elementary cuts obtained as follows. Let C_1 and C_2 be two elementary cuts of a benzenoid graph G. There are two different cases, as shown in Figure 1. With a, b, c, and d we denote the number of vertices in the corresponding parts of G. Then the contribution of the pair C_1, C_2 to $WW^*(G)$ is $ab + cd$ in the first case and ab in the second one.

For instance, naphthalene (Figure 2) contains five elementary cuts C_1, C_2, C_3, C_4, and C_5. The contributions of pairs of cuts

$$C_1, C_2;\ C_1, C_3;\ C_1, C_4;\ C_1, C_5;\ C_2, C_3;\ C_2, C_4;\ C_2, C_5;\ C_3, C_4;\ C_3, C_5;\ C_4, C_5$$

are, respectively

$$3\cdot3 + (1\cdot1 + 2\cdot6) + 3\cdot3 + (2\cdot4 + 1\cdot3) + 3\cdot3 + (1\cdot1 + 2\cdot6) + (1\cdot3 + 2\cdot4) + (1\cdot1 + 2\cdot6) + 3\cdot3 + (1\cdot3 + 2\cdot4) = 108$$

Therefore $WW(G) = W(G) + 108 = 109 + 108 = 217$.

In Klavžar, Žigert, and Gutman[23] this method was applied to obtain the general expression for the hyper-Wiener index of the linear polyacenes L_h, and in Žigert, Klavžar, and Gutman[24] for the coronene/circumcoronene series H_k

$$WW(L_h) = \frac{1}{3}(8h^4 + 32h^3 + 46h^2 + 37h + 3)$$

and

$$WW(H_k) = \frac{548}{15}k^6 + \frac{82}{5}k^5 - \frac{55}{6}k^4 - 3k^3 + \frac{17}{15}k^2 + \frac{1}{10}k$$

NEW APPLICATIONS OF THE CUT METHOD

We now demonstrate the use of the cut method on two infinite classes of molecular graphs, linear phenylenes and cyclic phenylenes.

We first consider linear phenylenes F_h, where h denotes the number of its hexagons;[13] an example is shown in Figure 3.

A linear phenylene F_h has four types of elementary cuts, namely, a single lengthwise cut; $h - 1$ cuts across a square; h cuts across a hexagon from upper left to lower right; and h cuts across a hexagon from lower left to upper right. Thus, there are seven possible combinations of two elementary cuts that contribute to $WW^*(F_h)$: (1) lengthwise and across a square, (2) lengthwise and across a hexagon, (3) across two squares, (4) across a square and across a hexagon, (5) across

two hexagons in the same direction, (6) across the same hexagon in both directions, and (7) across different hexagons in different directions.

Contributions of the seven types to $WW^*(F_h)$ are the following. Number 3 (5 and 7) assumes cuts through the ith and jth squares (hexagons), $j > i$. Number 4 assumes the ith hexagon and the jth square but does not assume $j > i$. Note that (5) and (7) are the same, indicating that cuts across two different hexagons make the same contribution regardless of direction.

$$2\sum_{i=1}^{h-1} 3i(3h-3i) = 3h^3 - 3h, \quad (1)$$

$$2\sum_{i=1}^{h} ((3i-1)(3h-3i+2) + (3i-2)(3h-3i+1)) = 6h^3 + 4h, \quad (2)$$

$$\sum_{i=1}^{h-2}\sum_{j=i+1}^{h-1} (36ih - 36ij) = \frac{1}{2}(3h^4 - 6h^3 - 3h^2 + 6h), \quad (3)$$

$$2\left(\sum_{i=2}^{h}\sum_{j=1}^{i-1} 6j(6h-6i+3) + \sum_{i=1}^{h-1}\sum_{j=i}^{h-1} (6i-3)(6h-6j)\right) = 6h^4 - 6h^2, \quad (4)$$

$$2\sum_{i=1}^{h-1}\sum_{j=i+1}^{h} (6i-3)(6h-6j+3) = 3h^4 - 6h^3 + 6h^2 - 3h, \quad (5)$$

$$\sum_{i=1}^{h} ((6i-4)(6h-6i+2)+1) = 6h^3 - 6h^2 + 5h, \quad (6)$$

and

$$2\sum_{i=1}^{h-1}\sum_{j=i+1}^{h} (6i-3)(6h-6j+3) = 3h^4 - 6h^3 + 6h^2 - 3h \quad (7)$$

The sum of these seven expressions is

$$WW^*(F_h) = (1/2)(27h^4 - 3h^2 + 6h)$$

Gutman[25] showed that

$$W(F_h) = 18h^3 + 9h^2$$

therefore

$$WW(F_h) = W(F_h) + WW^*(F_h) = \frac{1}{2}(27h^4 + 36h^3 + 15h^2 + 6h)$$

Indeed, this is identical to the polynomial obtained by Cash[26] using the interpolation method described below, except that the polynomial in ref 27 was expressed in terms of n, which is $h - 1$ in the present notation.

As the second example let us consider cyclic phenylenes R_h, $h \geq 2$. The cyclic phenylene R_h consist of h subunits of a hexagon and a square arranged in a cycle (see Figures 4 and 5).

It is not difficult to verify that cyclic phenylenes R_h are partial cubes, thus the cut method can be applied. The

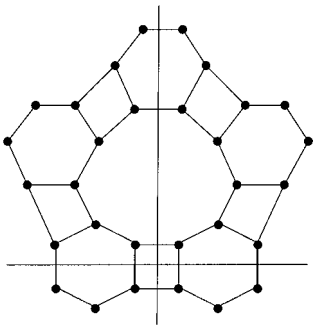

Figure 5. The cyclic phenylene R_5.

elementary cuts corresponding to Θ equivalence classes are somewhat different for h even and h odd. The h-even structures have $h/2$ cuts across the cycle that each bisect two hexagons and $h/2$ more that each bisect two squares. The h-odd structures have h cuts across the cycle that each bisect a hexagon and a square. All structures also have h "tangential" cuts that pass through a contiguous hexagon-square-hexagon component.

The sets of two cuts that contribute to $WW^*(R_h)$ are of six types: (1) two across the cycle, (2) one tangential and one across, intersecting in a hexagon, (3) one tangential and one across, intersecting in a square, (4) one tangential and one across, not intersecting at all, (5) two tangential, intersecting, and (6) two tangential, not intersecting.

For h even, type 1 is further divided into three subtypes, namely, (1a) two cuts passing through hexagons i and j, or squares i and j, $j > i$, (1b) one cut passing through hexagon i and one passing through square j, $j \geq i$, and (1c) one cut passing through hexagon i and one passing through square j, $j < i$.

Using the method of Gutman and Klavžar,[15] it is not difficult to determine that

$$W(R_h) = 9h^3 + 36h^2 - 36h$$

Contributions of the six types of cut pairs to $WW^*(R_h)$ are (1) $(1/2)(6h^4 - 9h^3 + 3h^2)$, (2) $36h^2 - 20h$, (3) $18h^2 - 18h$, (4) $18h^3 - 54h^2$, (5) $12h^2 - 4h$, and (6) $18h^2 - 54h$.

The sum of these is

$$WW^*(R_h) = \frac{1}{2}(6h^4 + 27h^3 + 63h^2 - 192h)$$

Therefore,

$$WW(R_h) = W(R_h) + WW^*(R_h) = \frac{1}{2}(6h^4 + 45h^3 + 135h^2 - 264h)$$

THE METHOD OF HOSOYA POLYNOMIALS

For a connected graph G we denote by $d(G, k)$ the number of pairs of its vertices that are at distance k. Then the *Hosoya polynomial* $H(G)$ of G is defined as[27]

$$H(G) \equiv H(G, x) = \sum_{k\geq 0} d(G, k)\, x^k$$

The method of Hosoya polynomials for obtaining the hyper-Wiener index of a graph is based on the following relation between the two concepts[28]

$$WW(G) = H'(G, 1) + \frac{1}{2}H''(G, 1) \quad (2)$$

where $H'(G, 1)$ and $H''(G, 1)$ denote the first, respectively. The second derivative of $H(G, x)$ at $x = 1$. Thus, if the Hosoya polynomial of a graph is known, one can easily compute its hyper-Wiener index. For instance, the Hosoya polynomial was recently computed for several composite graphs.[29]

We illustrate this method with several examples. For Hosoya polynomials of the poly(azulenes) A_n (see Figure 6), it is not difficult to construct the recurrence

$$H(A_n) = H(A_{n-1}) + x(1 + x + x^2 + x^3)u_{n-1} + (x + x^2)v_{n-1} + 2x^3\frac{x^{4n-3} - 1}{x - 1} + 2x^4\frac{x^{4n-3} - 1}{x - 1} + 8 + 8x + 10x^2 + 8x^3 + 2x^4$$

where

$$u_n = 1 + 2x\frac{x^{4n-1}}{x - 1} + x^{4n+1}$$

$$v_n = 1 + 2x + 3x^2 + 2x^3\frac{x^{4n-2} - 1}{x - 1}$$

for $n \geq 1$, while

$$H(A_0) = x + 2,\ u_0 = v_0 = x + 1$$

Summation of geometric series yields

$$H(A_n) = [x^{4n+2}(x + 3) + 2n(x^6 - 3x^4 - x^3 + 2x^2 - 3x + 4) - x^6 + 2x^5 - 2x^3 - 2x^2 - 3x + 2]/[(x - 1)^2] \quad (n \geq 1)$$

from which we obtain

$$WW(A_n) = \frac{2}{3}(64n^4 + 112n^3 + 68n^2 + 74n - 9)\ (n \geq 1)$$

using formula (2).

This result differs from that given in the paper by Cash[26] because that reference contains an error. Namely, the diagram and the polynomial in ref 27 are for different poly(azulene) structures. Using the standard way of designating vertices and edges, the azulene subunits are fused 2, 1 − f in that diagram and here in Figure 6 (consecutive five membered rings separated by a vertex and two edges), while the polynomial, $WW(G) = 24n^4 + 84n^3 + 116n^2 - 78n + 60$, is for the poly(azulene) formed by fusing the subunits 2, 1 − e, i.e., so that consecutive five-membered rings are separated only by an edge.

For Hosoya polynomials of the [N]phenylenes P_n, $n \geq 1$, we have the following recurrence:

$$H(P_n) = H(P_{n-1}) + 6 + 6x + 6x^2 + 3x^3 + 2(x + 2\sum_{k=2}^{3n} x^k + x^{3n+1}) + 2(x^2 + 2\sum_{k=3}^{3n+1} x^k + x^{3n+2}) + 2(x^3 + 2\sum_{k=4}^{3n+2} x^k + x^{3n+3})$$

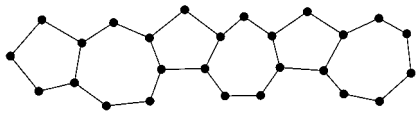

Figure 6. The poly(azulene) A_3.

with initial condition

$$H(P_1) = 12 + 14x + 20x^2 + 15x^3 + 10x^4 + 6x^5 + 2x^6$$

Again, by summation of geometric series we find

$$H(P_n) = [n(x^5 - 2x^4 - 3x^3 + 2x^2 - 4x + 6) + 2(x^{3n+4}(1 + x) + x^4 - 4x^3 + x^2 - 3x + 3)]/[(x - 1)^2]$$

whence by (2)

$$WW(P_n) = \frac{3}{2}(28 + 84n + 95n^2 + 48n^3 + 9n^4)$$

Gutman et al.[30] presented an extensive treatment of the Hosoya polynomials of periodic hexagonal chains. Most relevant to the present work is their demonstration of a method for producing the generating functions, $f(x, z)$, for the Hosoya polynomials of a periodic benzenoid chain, B_n, where n is the number of hexagons. That is

$$f(x, z) = \sum_{n=0}^{\infty} H(B_n, x)z^n$$

Periodic hexagonal chains are defined by a string of length n over the alphabet {1,2,3}, where 1, 2, and 3, respectively, signify left bend, no bend, and right bend at the corresponding hexagon in the chain. The first and last members of the string are meaningless, since no bend occurs on the first or last hexagons. Thus, {$x2y$} encodes anthracene, while {$x1y$} (or {$x3y$}) encodes phenanthrene. Chain lengths are not restricted to even multiples of the fundamental string length; a string encoding a benzenoid chain may terminate in a portion of the fundamental string. Thus, from the zigzag chain, $s = 13$, phenanthrene is {131}, chrysene is {1313}, and picene is {13131}. The Hosoya polynomial for the chain encoded by a string of length n is just the nth term of the Maclaurin series expansion of the generating function for its fundamental string. For the example just given, the fundamental string is $s = 13$, and its Hosoya-polynomial generating function is

$$f(x, z) = [(x^7 + 2x^6 - 2x^4 - x^3)z^3 + (x^5 - 2x^3)z^2 - (2x^3 + 4x^2 + 4x + 2)z - x - 2]/[(z - 1)^2(x^2z - 1)]$$

The relevance for this work is that, as stated above, $WW(G) = H'(G, 1) + H''(G, 1)/2$. Then, just as the Hosoya polynomial of the nth benzenoid chain in a series is the coefficient of the nth term of the Maclaurin expansion of the generating function, $f(x, z)$, so the hyper-Wiener index is the nth coefficient of the Maclaurin expansion of $f'(x, z) + (1/2)f''(x, z)$, evaluated at $x = 1$. (Similarly, the ordinary Wiener index, $W(G)$, of the nth benzenoid is the nth coefficient of the Maclaurin expansion of $f'(x, z)$ evaluated at $x = 1$ because $W(G) = H'(G, 1)$.) In the *Mathematica* package, if hgf is the Hosoya-polynomial generating function for some periodic benzenoid chain, then the polynomial in

n for the hyper-Wiener indices is obtained from

SeriesTerm[Factor[(D[hgf,x]+D[hgf,{x,2}]/2)/.x→1],{z,0,n}]

where SeriesTerm is a function provided by the standard package RSolve.m. Substituting a value for n into this polynomial gives the hyper-Wiener index of the nth benzenoid in the series. The advantage here is that the polynomials in n obtained in this way are guaranteed to be valid for all values of n, with the condition in some cases that $n \geq 1$ or $n \geq 2$.

For most of the fundamental strings given in ref 31, one polynomial expression for $WW(B_n)$ is sufficient for all n. In a few cases, the expressions are much simplified by computing separate $WW(B_n)$ for each possible value of n modulo the length of the fundamental string. Thus, the double-step zigzag $s = 2123$ has

$$WW(B_n) = \frac{1}{3}(8n^4 + 24n^3 + 28n^2 + 213n + 656 - 88(-1)^n)$$

for all $n \geq 2$, while the triple-step zigzag $s = 221223$ requires a separate $WW(B_n)$ for each of the six values of n mod 6. Results for the other s, for which Hosoya-polynomial generating functions are given elsewhere[30] are as follows:

$s = 2$:

$$WW(B_n) = \frac{1}{3}(8n^4 + 32n^3 + 46n^2 + 37n + 3)$$

$s = 1$, $n \geq 1$:

$$WW(B_n) = \frac{1}{3}(2n^4 + 28n^3 + 154n^2 - 169n + 111)$$

$s = 13$, $n \geq 1$:

$$WW(B_n) = \frac{1}{3}(8n^4 + 24n^3 + 28n^2 + 147n - 81)$$

$s = 221223$, $n \geq 1$:

$$WW(B_{6n}) = 3456n^4 + 1728n^3 + 336n^2 + 590n - 131$$

$$WW(B_{6n+1}) = 3456n^4 + 4032n^3 + 1776n^2 + 910n - 62$$

$$WW(B_{6n+2}) = 3456n^4 + 6336n^3 + 4368n^2 + 1902n + 155$$

$$WW(B_{6n+3}) = 3456n^4 + 8640n^3 + 8112n^2 + 3950n + 680$$

$$WW(B_{6n+4}) = 3456n^4 + 10944n^3 + 13008n^2 + 7438n + 1557$$

$$WW(B_{6n+5}) = 3456n^4 + 13248n^3 + 19056n^2 + 12750n + 3206$$

$s = 21$, $n \geq 2$:

$$WW(B_{2n}) = 24n^4 + 96n^3 + 152n^2 - 146n + 89$$

$$WW(B_{2n+1}) = 24n^4 + 144n^3 + 320n^2 + 54n + 94$$

$s = 221$, $n \geq 1$:

$$WW(B_{3n}) = 150n^4 + 340n^3 + 318n^2 - 285n + 157$$

$$WW(B_{3n+1}) = 150n^4 + 540n^3 + 718n^2 - 13n + 162$$

$$WW(B_{3n+2}) = 150n^4 + 740n^3 + 1358n^2 + 675n + 283$$

$s = 1133$, $n \geq 1$:

$$WW(B_n) = \frac{1}{2}(3n^4 + 20n^3 + 60n^2 + 18n - 54),\ n \text{ even}$$

$$WW(B_n) = \frac{1}{2}(3n^4 + 20n^3 + 54n^2 - 2n + 9),\ n \text{ odd}$$

$s = 111333$, $n \geq 1$:

$$WW(B_{6n}) = 1536n^4 + 2176n^3 + 1382n^2 - 74n - 27$$

$$WW(B_{6n+1}) = 1536n^4 + 3200n^3 + 2544n^2 + 454n + 42$$

$$WW(B_{6n+2}) = 1536n^4 + 4224n^3 + 4528n^2 + 1782n + 215$$

$$WW(B_{6n+3}) = 1536n^4 + 5248n^3 + 6896n^2 + 3654n + 636$$

$$WW(B_{6n+4}) = 1536n^4 + 6272n^3 + 9648n^2 + 6166n + 1401$$

$$WW(B_{6n+5}) = 1536n^4 + 7296n^3 + 13168n^2 + 10246n + 2862$$

THE INTERPOLATION METHOD

The third method we consider is the so-called interpolation method which is appropriate when the hyper-Wiener index of a series of graphs G_n, $n \geq 1$, is a polynomial function p of n. Now, if we know an upper bound r for the degree of p, then we compute $WW(G_n)$ for $n = 1, 2, ..., r + 1$, and construct the interpolating polynomial through the points (n, $WW(G_n)$). In this way, the closed-form expression for $WW(G_n)$ is obtained.

Note that the above method needs two assumptions in order to be exact. First, the corresponding function must be a polynomial, and second, we must have an upper bound of its degree. As to the second assumption, in practice we proceed as follows. We keep computing $WW(G_n)$ for larger and larger n, and, at each step, we construct the interpolating polynomial through all the points computed so far. Suppose that after some time the interpolating polynomial stops changing and remains the same for several consecutive steps. Then we can be quite convinced that we have indeed found the correct polynomial. This is, of course, not a proof that the polynomial will never change again, but in practice it seems quite reliable.

Cash[26] found several polynomial expressions for $WW(G)$ using this method, including some in two variables for two-dimensional benzenoid sheets. These included sheets in the shape of hexagons, parallelograms, triangles, and extended perylene-type structures. One-dimensional systems examined were the[N]phenylenes, poly(azulenes), and a set of C_{20+10n} fullerenes consisting of an all-hexagon nanotube capped on each end with a set of six pentagons. The fullerene set was the only system examined that did not give a polynomial. This was a mysterious result, since it seems that annealing another ring of hexagons into the tube should be analogous to annealing another benzene ring onto a periodic benzenoid chain. Indeed, looking at the Hosoya polynomials for this series revealed the problem: The first three members of the series (C_{20}, C_{30}, and C_{40}, corresponding to $n = 0, 1, 2$) are anomalous. This is probably due to the fact that distances

around the tube and distances along the tube are commingled when the "tube" is enough like a sphere. Removing these three members from the series gives a fourth-order polynomial in n, as might be expected:

$$WW(G_n) = \frac{1}{6}(100n^4 + 900n^3 + 2975n^2 + 14475n + 1050),\ n \geq 3$$

The polynomial for the poly(azulenes) in this reference does not match the structure given in the figure but is for a different poly(azulene). (See explanation in the preceding section.)

CONCLUDING REMARKS

The cut method, while somewhat tedious to apply, works for any family of structures that can be divided into Θ equivalence classes. This general relationship suggests that Θ classes may be related to other mathematical indices as well or perhaps directly related to physicochemical properties.

The method of Hosoya polynomials is applicable to structures that can be built up by annealing and for which recurrences satisfied by the Hosoya polynomial can be found.

The interpolation method is applicable to any series of structures that satisfy its two assumptions. A negative result, however, does not demonstrate anything, since it is impossible to tell whether $WW(G)$ is not expressible as a polynomial or the estimate of the upper bound r was merely too low.

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