Wiener Numbers of Pericondensed Benzenoid Hydrocarbons

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Using a recently developed technique for the calculation of the Wiener number (W) of benzenoid systems we determine explicit expressions for W for several homologous series of pericondensed benzenoid hydrocarbons. An elementary proof for the correctness of the used method is also included.

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INTRODUCTION

Finding explicit combinatorial expressions for the Wiener numbers (W) of particular classes of molecular graphs was initiated in 1977 by Bonchev and Trinajstić[1] and was followed by numerous subsequent researches. Especially numerous were the results obtained for acyclic molecular graphs.[2–8] Expressions for W of polycyclic systems were somewhat more difficult to deduce and, until relatively recently, significantly fewer results of this kind have been communicated. With a few exceptions,[9,10] the only polycyclic systems studied were catacondensed benzenoid hydrocarbons.[11–14]

Few years ago the situation changed.

First, Shiu and Lam, mathematicians from Hong Kong, developed a combinatorial algorithm by which they succeeded to find the formula for W of the benzene/coronene/circumcoronene series.[15] The Shiu–Lam methods divides the calculation of W into many individual steps, each based on the finding of an expression for distances between particular families of vertices of the molecular graph considered. Therefore, the method requires extensive and rather tedious computations and deals with difficult–to–handle algebraic expressions. Nevertheless, the Shiu–Lam procedure was recently successfully accomplished for several classes of pericondensed benzenoid systems.[16–19]

Second, another technique for computing W, applicable (among others) to all benzenoid systems, was recently communicated by two of the present authors and Mohar.[20,21] This method is based on a simple formula

$$W = \sum_C n_1(C)\, n_2(C) \tag{1}$$

in which C denotes an elementary edge–cut of the respective benzenoid system and the summation goes over all edge–cuts. The edge–cut C dissects the benzenoid system into two parts, having $n_1(C)$ and $n_2(C)$ vertices. (Thus, $n_1(C) + n_2(C)$ is independent of the cut C and is equal to the number N of vertices of the respective benzenoid system.)

Precise definitions of elementary edge–cuts and more details with regard to formula (1) can be found in our earlier publications.[20–22] A self–explanatory example is given in the subsequent section. An elementary proof of formula (1) is given in the Appendix.

The main purpose of this paper is to demonstrate that the method of edge–cuts is very simple to apply and that general expressions for W are easily obtained. This already has been demonstrated in the case of benzene/coronene/circumcoronene series,[21] and in this paper we offer quite a few additional formulas of the same kind. We believe that for additional benzenoid systems of interest to the readers it will not be difficult to obtain the corresponding formulas for W along the same lines. In the appendix we also give a simple, elementary proof for the validity of the used procedure.

COMPUTATIONAL DETAILS

In all benzenoid systems G considered we will partition the elementary edge–cuts of G into the sets of parallel elementary cuts C_1, C_2, C_3. Figure 1 shows an example of a benzenoid system and the corresponding partition of cuts.

Figure 1 comes about here

Throughout the paper, N will denote the number of vertices of the benzenoid system considered. In addition, expressions of the form

$$\sum_{i=1}^{k}\Big(i(2n+2)-1\Big)\Big(N-(i(2n+2)-1)\Big)\,,$$

will be written as

$$\sum_{i=1}^{k}\Big(i(2n+2)-1\Big)\Big(N-\mathcal{F}\Big)\,,$$

i.e., $\mathcal{F}$ will stand for the value of the "first bracket". In the above example we thus have $\mathcal{F}=i(2n+2)-1$. For a benzenoid system G we will also use the following notions:

$$W_1=\sum_{C\in C_1} n_1(C)\,n_2(C)\,,$$
$$W_2=\sum_{C\in C_2} n_1(C)\,n_2(C)\,,$$

and

$$W_3=\sum_{C\in C_3} n_1(C)\,n_2(C)\,.$$

Then, in view of Eq. (1), we have $W(G)=W_1+W_2+W_3$.

PARALLELOGRAMS AND TRAPEZIUMS

In this section we compute W of two relatively simple families of benzenoid systems: parallelograms and trapeziums.

Parallelograms

For $n\geq 1$ and $1\leq k\leq n$ let $P(n,k)$ be the parallelogram benzenoid system. The definition of $P(n,k)$ should be clear from the example $P(7,4)$ which is shown on Figure 2.

Figure 2 comes about here

For $P(n,k)$ we have:

$$N=(2k+2)(n+1)-2\,,$$
$$W_1=\sum_{i=1}^{k}\Big[\Big(i(2n+2)-1\Big)\Big(N-\mathcal{F}\Big)\Big]\,,$$
$$W_2=\sum_{i=1}^{n}\Big[\Big(i(2k+1)+i-1\Big)\Big(N-\mathcal{F}\Big)\Big]\,.$$

It remains to consider the C_3 cuts. We first consider the first $k-1$ cuts (from left to right) and the last $k-1$ cuts. We obtain:

$$W_3' = 2\sum_{i=1}^{k-1}\left[\left(\sum_{j=1}^{i}(3+2(j-1))\right)\left(N-\mathcal{F}\right)\right].$$

Finally, for the middle $n+3-2k$ cuts from C_3 we have

$$W_3'' = \sum_{i=1}^{n-k+1}\left[\left(\sum_{j=1}^{k-1}(3+2(j-1))+i(2k+1)+i-1\right)\left(N-\mathcal{F}\right)\right].$$

Clearly, $W_3 = W_3' + W_3''$. Simplifying the expression $W_1 + W_2 + W_3' + W_3''$ we get the following expression for $W(P(n,k))$:

$$\begin{aligned} W &= \frac{4n^3(k^2+2k+1)}{3} + \frac{2kn^2(k^2+9k+8)}{3} + \\ &\quad \frac{n(k^4+8k^3+16k^2+2k-1)}{3} - \frac{k(k^4-20k^2+4)}{15}. \end{aligned}$$

For instance, for $k=1$ the above expression reduces to

$$W(P(n,1)) = \frac{1}{3}(16n^3+36n^2+26n+3),$$

which is the well-known formula for W of polyacenes, usually denoted by L_h, i.e., $L_h = P(h,1)$.

Trapeziums

For $n \geq 1$ and $1 \leq k \leq n$ let $T(n,k)$ be the trapezium benzenoid system. The definition of $T(n,k)$ should be clear from the example $T(9,5)$ which is shown on Figure 3.

Figure 3 comes about here

For $T(n,k)$ we have:

$$N = (k+1)(2n+1) - k(k-1),$$
$$W_1 = \sum_{i=1}^{k}\left[\left(i(2n+1)-(i-1)(i-2)\right)\left(N-\mathcal{F}\right)\right].$$

Consider the first k cuts (from left to right) from C_2. We obtain:

$$W_2' = \sum_{i=1}^{k}\left[i(i+2)\right]\left[N-\mathcal{F}\right].$$

For the remaining $n-k$ cuts from C_2 we have

$$W_2'' = \sum_{i=1}^{n-k} \left[k(k+2) + i(2k+2) \right] \left[N - \mathcal{F} \right] .$$

Clearly, $W_2 = W_2' + W_2''$ and by symmetry we have, $W_3 = W_2$. Simplifying the expression $W_1 + 2(W_2' + W_2'')$ we get the following expression for $W(T(n,k))$:

$$\begin{aligned} W \quad = \quad & \frac{4n^3(k^2+2k+1)}{3} - \frac{2n^2(k+1)(2k^2-8k-3)}{3} + \\ & \frac{2n(k^4-4k^3+6k^2+9k+1)}{3} - \frac{k(8k^4+35k^2-45k-28)}{30} . \end{aligned}$$

Again, for $k = 1$, the above expression reduces to

$$W(P(n,1)) = \frac{1}{3}(16n^3 + 36n^2 + 26n + 3) .$$

PARALLELOGRAM–LIKE BENZENOID SYSTEMS

First example

For $n \geq 1$ and $1 \leq k \leq n$ let $P_1(n,k)$ be the parallelogram-like benzenoid system of type 1. The definition of $P_1(n,k)$ should be clear from the example $P_1(7,3)$ which is shown on Figure 4.

Figure 4 comes about here

For $P_1(n,k)$ we have:

$$N = 2n + 4k(n+1) ,$$
$$W_1 = \sum_{i=1}^{2k} \left[\left(i(2n+2) - 1 \right) \left(N - \mathcal{F} \right) \right] .$$

For the C_2 cuts, we first consider the first k cuts (from left to right) and the last k cuts. We obtain:

$$W_2' = 2 \sum_{i=1}^{k} \left[\sum_{j=1}^{i} \left(4j - 1 \right) \left(N - \mathcal{F} \right) \right] .$$

For the next cut just after the first k cuts from the left we have

$$W_2'' = \left[\sum_{j=1}^{k}(4j-1) + (4k+1)\right]\left(N - \mathcal{F}\right).$$

For the remaining middle $n-(k+1)$ cuts from C_2 we have

$$W_2''' = \sum_{i=1}^{n-(k+1)}\left[\sum_{j=1}^{k}(4j-1) + (4k+1) + i(4k+2)\right]\left[N - \mathcal{F}\right].$$

Clearly, $W_2 = W_2' + W_2'' + W_2'''$. Finally, for the C_3 cuts, again we consider the first k cuts (from left to right) and the last k cuts. We obtain:

$$W_3' = 2\sum_{i=1}^{k}\left[\sum_{j=1}^{i}\left(4j+1\right)\left(N - \mathcal{F}\right)\right].$$

For the middle $n-(k+1)$ cuts from C_3 we have

$$W_3'' = \sum_{i=1}^{n-(k+1)}\left[\sum_{j=1}^{k}(4j+1) + i(4k+2)\right]\left[N - \mathcal{F}\right].$$

Clearly, $W_3 = W_3' + W_3''$. Simplifying the expression $W_1 + W_2' + W_2'' + W_2''' + W_3' + W_3''$ we get for $W(P_1(n,k))$:

$$\begin{aligned} W \;=\;& \frac{4n^3(2k+1)^2}{3} + \frac{8kn^2(k+4)(2k+1)}{3} + \\ & \frac{n(8k^4+48k^3+78k^2+14k-1)}{3} - \frac{k(8k^4-20k^3-110k^2-25k+27)}{15}. \end{aligned}$$

Second example

For $n \geq 1$ and $1 \leq k \leq n$ let $P_2(n,k)$ be the parallelogram-like benzenoid system of type 2. The definition of $P_2(n,k)$ should be clear from the example $P_2(7,4)$ which is shown on Figure 5.

Figure 5 comes about here

For $P_2(n,k)$ we have:

$$N = 2k(2n+1),$$
$$W_1 = \sum_{i=1}^{2k-1}\left[i(2n+1)\right]\left[N - \mathcal{F}\right].$$

For the C_2 cuts, we first consider the first k cuts (from left to right) and the last k cuts. We obtain:

$$W_2' = 2\sum_{i=1}^{k}\left[\sum_{j=1}^{i}(4j-1)\left(N-\mathcal{F}\right)\right].$$

For the middle $n-(k+1)$ cuts from C_2 we have

$$W_2'' = \sum_{i=1}^{n-(k+1)}\left[\sum_{j=1}^{k}(4j-1)+i(4k)\right]\left[N-\mathcal{F}\right].$$

Clearly, $W_2 = W_2' + W_2''$, and by symmetry $W_3 = W_2$ Hence, simplifying the expression $W_1 + 2(W_2' + W_2'')$ we get for $W(P_2(n,k))$:

$$\begin{aligned} W &= \frac{16k^2n^3}{3} + \frac{4kn^2(4k^2+6k-1)}{3} + \\ &\quad \frac{2kn(4k^3+8k^2+3k-2)}{3} - \frac{k(8k^4-20k^3-30k^2+20k+7)}{15}. \end{aligned}$$

For instance, for $k=1$ the above expression, as previously, reduces to

$$W(P_2(n,1)) = \frac{1}{3}(16n^3+36n^2+26n+3).$$

Third example

For $n \geq 1$ and $1 \leq k \leq n+1$ let $P_3(n,k)$ be the parallelogram-like benzenoid system of type 3. The definition of $P_3(n,k)$ should be clear from the example $P_3(4,3)$ which is shown on Figure 6.

Figure 6 comes about here

For $P_3(n,k)$ we have:

$$N = 2k(2n+3)-4\,,$$

$$W_1 = \sum_{i=1}^{2k-1}\left[\left[i(2n+3)-2\right]\left(N-\mathcal{F}\right)\right].$$

For the C_2 cuts, we first consider the first $k-1$ cuts (from left to right) and the last $k-1$ cuts. We obtain:

$$W_2' = 2\sum_{i=1}^{k-1}\left[\sum_{j=1}^{i}\left(4j+1\right)\left(N-\mathcal{F}\right)\right].$$

For the next cut just after the first $k-1$ cuts from the left we have

$$W_2'' = \left[\sum_{j=1}^{k-1}(4j+1) + (4k-1)\right]\left(N - \mathcal{F}\right).$$

For the remaining middle $n-k$ cuts from C_2 we have

$$W_2''' = \sum_{i=1}^{n-k}\left[\sum_{j=1}^{k-1}(4j+1) + (4k-1) + i(4k)\right]\left[N - \mathcal{F}\right].$$

Clearly, $W_2 = W_2' + W_2'' + W_2'''$, and by symmetry $W_3 = W_2$ Hence, simplifying the expression $W_1 + 2(W_2' + W_2'' + W_2''')$ we get for $W(P_3(n,k))$:

$$\begin{aligned} W &= \frac{16k^2n^3}{3} + \frac{4kn^2(4k^2+18k-13)}{3} + \\ &\quad \frac{2n(4k^4+24k^3+27k^2-54k+12)}{3} - \\ &\quad \frac{(8k^5-60k^4-110k^3+180k^2+27k-60)}{15}. \end{aligned}$$

For instance, for $k=1$ the above expression, as previously, reduces to

$$W(P_3(n,1)) = \frac{1}{3}(16n^3 + 36n^2 + 26n + 3).$$

BITRAPEZIUMS

In this section we consider W of bitrapeziums which include the special cases of the trapeziums and the parallelograms. To consider these special cases and most importantly, to include all kinds of bitrapeziums, we need to consider two cases.

Case 1. For $n \geq 1$, $0 \leq k_1 \leq n-1$, $0 \leq k_2 \leq n-1$ and $k_1 + k_2 <= n$ let $BT(n,k_1,k_2)$ be the bitrapezium benzenoid system. The definition of $BT(n,k_1,k_2)$ should be clear from the example $BT(6,2,3)$ which is shown on Figure 7.

Figure 7 comes about here

For $BT(n,k_1,k_2)$ we have:

$$N = 2n(k_1+k_2+2) - k_1^2 - k_2^2 + 2.$$

For the first k_1+1 cuts from C_1 (from the top) we obtain

$$W_1' = \sum_{i=1}^{k_1+1} \left[i(i+2n-2k_1)\left(N - \mathcal{F} \right) \right].$$

For the last k_2 cuts from C_1 (from the bottom) we obtain

$$W_1'' = \sum_{i=1}^{k_2} \left[i(i+2n-2k_2)\left(N - \mathcal{F} \right) \right].$$

Clearly, $W_1 = W_1' + W_1''$. Now, for the first k_1+1 cuts from C_2 (from the left) we obtain

$$W_2' = \sum_{i=1}^{k_1+1} \left[i(i+2k_2+2)\left(N - \mathcal{F} \right) \right].$$

For the last k_2 cuts from C_2 (from the right) we obtain

$$W_2'' = \sum_{i=1}^{k_2} \left[i(i+2k_1+2)\left(N - \mathcal{F} \right) \right].$$

For the middle $n-(k_1+k_2+1)$ cuts from C_2 we obtain

$$W_2''' = \sum_{i=1}^{n-(k_1+k_2+1)} \left[(k_1+1)(k_1+2k_2+3) + i(2k_1+2k_2+4)\left(N - \mathcal{F} \right) \right].$$

Clearly, $W_2 = W_2' + W_2'' + W_2'''$ and by symmetry, $W_3 = W_2$. Hence, simplifying the expression $W_1 + 2W_2$ we get for $W(BT(n,k_1,k_2))$:

$$\begin{aligned} W &= \frac{4n^3(k_1+k_2+2)^2}{3} - \\ &\quad \frac{2n^2(2k_1^3 - k_1(12k_2+17) + 2k_2^3 - 17k_2 - 18)}{3} + \\ &\quad \frac{2n(k_1^4 + k_1(11k_2+13) + k_2^4 + 13k_2 + 13)}{3} - \\ &\quad \frac{8k_1^5 + 20k_1^4(k_2+2) + 5k_1^3(16k_2+23) + 5k_1^2(23k_2+28)}{30} - \\ &\quad \frac{k_1(20k_2^4 + 80k_2^3 + 115k_2^2 + 80k_2 + 27)}{30} - \\ &\quad \frac{8k_2^5 + 40k_2^4 + 115k_2^3 + 140k_2^2 + 27k_2 - 30}{30}. \end{aligned}$$

For instance, for $k_1 = k_2 = 0$ the above expression, as previously, reduces to formula for W of polyacenes. i.e.

$$W(BT(n,0,0)) = \frac{1}{3}(16n^3 + 36n^2 + 26n + 3).$$

Moreover, for $k_1 = 0, k_2 = k-1$ (respectively, $k_2 = 0, k_1 = k-1$) we obtain the formula for W of trapeziums benzenoid systems. i.e. $W(BT(n,0,k-1))$ is:

$$\begin{aligned} W &= \frac{4n^3(k^2+2k+1)}{3} - \frac{2n^2(k+1)(2k^2-8k-3)}{3} + \\ &\quad \frac{2n(k^4-4k^3+6k^2+9k+1)}{3} - \frac{k(8k^4+35k^2-45k-28)}{30}. \end{aligned}$$

Case 2. We may without loss of generality assume that $k_1 \leq k_2$. For $n \geq 1$, $0 \leq k_1 \leq n-1$, $0 \leq k_2 \leq n-1$ and $k_1 + k_2 \geq n$ let $BT(n, k_1, k_2)$ be the bitrapezium benzenoid system. In this case, the definition of $BT(n, k_1, k_2)$ should be clear from the example $BT(7, 4, 5)$ which is shown on Figure 8.

$\boxed{\text{Figure 8 comes about here}}$

For $BT(n, k_1, k_2)$ we have:

$$N = 2n(k_1 + k_2 + 2) - k_1^2 - k_2^2 + 2\,.$$

For the first $k_1 + 1$ cuts from C_1 (from the top) we obtain

$$W_1' = \sum_{i=1}^{k_1+1} \left[i(i + 2n - 2k_1) \Big(N - \mathcal{F} \Big) \right].$$

For the last k_2 cuts from C_1 (from the bottom) we obtain

$$W_1'' = \sum_{i=1}^{k_2} \left[i(i + 2n - 2k_2) \Big(N - \mathcal{F} \Big) \right].$$

Clearly, $W_1 = W_1' + W_1''$. Now, for the first $n - k_1$ cuts from C_2 (from the left) we obtain

$$W_2' = \sum_{i=1}^{n-k_1} \left[i(i + 2k_1 + 2) \Big(N - \mathcal{F} \Big) \right].$$

For the last $n - k_2$ cuts from C_2 (from the right) we obtain

$$W_2'' = \sum_{i=1}^{n-k_2} \left[i(i + 2k_2 + 2) \Big(N - \mathcal{F} \Big) \right].$$

For the middle $(k_1 + k_2 - n)$ cuts from C_2 we obtain

$$W_2''' = \sum_{i=1}^{(k_1+k_2-n)} \left[\Big[(n - k_1)(n + k_1 + 2) + i(2n + 2) \Big] \Big[N - \mathcal{F} \Big] \right].$$

Clearly, $W_2 = W_2' + W_2'' + W_2'''$ and by symmetry, $W_3 = W_2$. Hence, simplifying the expression $W_1 + 2W_2$ we get for $W(BT(n, k_1, k_2))$:

$$\begin{aligned} W \;=\; & \frac{-2n^5}{15} + \frac{2n^4(k_1 + k_2 + 1)}{3} + \frac{4n^3(2k_1 + 2k_2 + 3)}{3} + \\ & \frac{2n^2(6k_1^2(k_2 + 1) + k_1(6k_2^2 + 24k_2 + 23) + 6k_2^2 + 23k_2 + 20)}{3} - \\ & \frac{2n(20k_1^3(k_2 + 1) + 30k_1^2(k_2^2 + 2k_2 + 1))}{15} - \end{aligned}$$

$$\frac{2n(5k_1(4k_2^3+12k_2^2+k_2-9)+20k_2^3+30k_2^2-45k_2-61)}{15}-$$
$$\frac{(4k_1^5+20k_1^4+5k_1^3(15-8k_2^2)-5k_1^2(8k_2^3+24k_2^2+k_2-20))}{30}-$$
$$\frac{(k_1(11-5k_2^2)+4k_2^5+20k_2^4+75k_2^3+100k_2^2+11k_2-30)}{30}.$$

For instance, for $k_1 = k_2 = n-1$ the above expression reduces to the formula for $W(BT(n,n-1,n-1))$:

$$W = \frac{n(34n^4+170n^3+200n^2+10n-9)}{15},$$

which is the formula for W of parallelogram benzenoid system $P(n,n)$. Notice that the above formula can also be obtained from the formula for W of parallelogram benzenoid system $P(n,k)$ by substituting $k=n$. i.e. $W(BT(n,n-1,n-1)) = W(P(n,n))$.

GENERAL CASE

In this section we consider W of general benzenoid systems which include many special cases, for instance the trapeziums, the bitrapeziums and the parallelograms.

For $n \geq 1$, $0 \leq k_1 \leq k_3 \leq n$, $0 \leq k_4 \leq k_2 \leq n$ and $k_1+k_2 = k_3+k_4$ let $GB(n,k_1,k_2,k_3,k_4)$ be the general benzenoid system. Its definition should be clear from the example $GB(7,3,4,5,2)$ which is shown on Figure 9.

Figure 9 comes about here

For $GB(n,k_1,k_2,k_3,k_4)$ we have:

$$N = 2n(k_3+k_4+2) - k_1^2 + k_1(2k_3+2k_4+2) + 2k_3 - k_4^2 + 2.$$

For the first k_1+1 cuts from C_1 (from the bottom) we obtain

$$W_1' = \sum_{i=1}^{k_1+1}\left[i(i+2n)\Big(N-\mathcal{F}\Big)\right].$$

For the last k_4+1 cuts from C_1 (from the top) we obtain

$$W_1'' = \sum_{i=1}^{k_4+1}\left[\Big(i^2+2i(n+k_1-k_4)\Big)\Big(N-\mathcal{F}\Big)\right].$$

For the middle $k_3-(k_1+1)$ cuts from C_1 we obtain

$$W_1''' = \sum_{i=1}^{k_3-(k_1+1)} \left[(k_1+1)(k_1+2n+1) + i(2k_1+2n+2)\left(N - \mathcal{F}\right) \right].$$

Clearly, $W_1 = W_1' + W_1'' + W_1'''$. For the first k_2+1 cuts from C_2 (from the left) we have

$$W_2' = \sum_{i=1}^{k_2+1} \left[i(i+2k_1+2)\left(N - \mathcal{F}\right) \right].$$

For the last k_3 cuts from C_2 (from the right) we obtain

$$W_2'' = \sum_{i=1}^{k_3} \left[i(i+2k_4+2)\left(N - \mathcal{F}\right) \right].$$

For the middle $n-(k_2+1)$ cuts from C_2 we obtain

$$W_2''' = \sum_{i=1}^{n-(k_2+1)} \left[(k_2+1)(2k_1+k_2+3) + i(2k_1+2k_2+4)\left(N - \mathcal{F}\right) \right].$$

Clearly, $W_2 = W_2' + W_2'' + W_2'''$. For the first k_1+1 cuts from C_3 (from the left) we have

$$W_3' = \sum_{i=1}^{k_1+1} \left[i(i+2k_2+2)\left(N - \mathcal{F}\right) \right].$$

For the last k_4+1 cuts from C_3 (from the right) we obtain

$$W_3'' = \sum_{i=1}^{k_4+1} \left[i(i+2k_3+2)\left(N - \mathcal{F}\right) \right].$$

For the middle $n-(k_4+2)$ cuts from C_3 we obtain

$$W_3''' = \sum_{i=1}^{n-(k_4+2)} \left[(k_1+1)(k_1+2k_2+3) + i(2k_1+2k_2+4)\left(N - \mathcal{F}\right) \right].$$

Clearly, $W_3 = W_3' + W_3'' + W_3'''$. Simplifying the expression $W_1 + W_2 + W_3$ we get for $W(GB(n,k_1,k_2,k_3,k_4))$:

$$\begin{aligned} W \quad = \quad & \frac{-4n^3(k_1+k_2+2)(2k_1+2k_2-3k_3-3k_4-2)}{3} - \\ & \frac{2n^2(6k_1^3-3k_1^2(4k_2-3k_3-5k_4+2))}{3} - \\ & \frac{2n^2(3k_1(k_2^2-2k_2(2k_3+4k_4+1)+2k_3(k_4-4)+3k_4^2-10k_4-8))}{3} - \\ & \frac{2n^2(-3k_2^3-k_3^3-3k_3^2(k_4+2)-k_3(3k_4^2+17)-k_4^3+12k_4^2-5k_4)}{3} - \\ & \frac{2n^2(3(k_2^2(k_3-k_4-2)+k_2(2k_3k_4+3k_4^2-2k_4-4)-6))}{3} - \\ & \frac{n(7k_1^4+2k_1^3(9k_2-5k_3-14k_4+1)+3k_1^2(3k_2^2-2k_2(3k_3+10k_4+4))}{3} + \end{aligned}$$

$$\frac{n(3k_1^2(k_3^2+k_3(8k_4-5)+12k_4^2-11k_4-13)+2k_1(3k_2^2k_3-3k_4-2))}{3}-$$
$$\frac{n(2k_1(3k_2^2(k_3-3k_4-2))}{3}-$$
$$\frac{n(2k_1(k_2(3k_3(4k_4+1)+27k_4^2+3k_4-20))}{3}-$$
$$\frac{n(2k_1(-2k_3^3-3k_3^2(2k_4+3)-k_3(9k_4^2-3k_4+11)-8k_4^3)}{3}-$$
$$\frac{n(2k_1(27k_4^2+25k_4-11)+3k_2^4-2k_2^3(k_3+k_4-1)}{3}-$$
$$\frac{n(k_2^2(3k_3+9k_4^2+9k_4-2)-k_2(k_3(6k_4^2-6k_4-11)+12k_4^3)}{3}-$$
$$\frac{n(-k_2(-24k_4^2-59k_4-14)-2k_3^4-k_3^3(8k_4+17)-k_3^2(9k_4^2+51k_4+55))}{3}-$$
$$\frac{n(-k_3(4k_4^3+57k_4^2+111k_4+76)-35k_4^3-57k_4^2-2(20k_4+13))}{3}-$$
$$\frac{(22k_1^5+20k_1^4(3k_2-2k_3-5k_4)+10k_1^3(4k_2^2-k_2(6k_3+24k_4+7)))}{30}-$$
$$\frac{(10k_1^3(3k_3^2+k_3(12k_4-1)+2(10k_4^2-3))+5k_1^2(2k_2^3-3k_2^2(8k_4+3)))}{30}-$$
$$\frac{(5k_1^2(k_2(24K_3k_4+72k_4^2+30k_4-17)-2k_3^3+3k_3^2(1-2k_4))}{30}-$$
$$\frac{(5k_1^2(-k_3(24k_4^2-24k_4-19)-2(16k_4^3-24k_4^2-53k_4-18))}{30}-$$
$$\frac{2k_1(5k_2^4-10k_2^3(k_3+k_4-1)-5k_2^2(3k_3-12k_4^2-9k_4-4))}{30}-$$
$$\frac{2k_1(-5k_2(k_3(6k_4^2-6k_4-5)+20k_4^3-9k_4^2-49k_4-23)-10k_3^4)4))}{30}-$$
$$\frac{2k_1(-5k_3^3(8k_4+15)-5k_3^2(9k_4^2+45k_4+40)-5k_3(4k_4^3+63k_4^2)}{30}-$$
$$\frac{2k_1(-5k_3(105k_4+53)+15k_4^4-22ok_4^3-475k_4^2-290k_4-56)}{30}-$$
$$\frac{(-4k_2^5+6k_3^5+5k_3^4(6k_4+5)+10k_3^3(5k_4^2+8k_4-2))}{30}-$$
$$\frac{(5k_3^2(14k_4^3+51k_4^2+22k_4-26)+k_3(60k_4^4+400k_4^3+625k_4^2+180k_4-121))}{30}-$$
$$\frac{2(6k_4^5+105k_4^4+230k_4^3+150k_4^2+4k_4-15)+5k_2^4-10k_2^3(2k_3-k_4^2-3))}{30}-$$
$$\frac{(-5k_2^2(6k_3+8k_4^3+9k_4^2+4k_4-8)-k_2(10k_3(6k_4^2+6k_4+1))}{30}-$$
$$\frac{k_2(-30k_4^4+130k_4^3+355k_4^2+200k_4-19)}{30}.$$

SOME SPECIAL CASES

From the formula for W of general benzenoid systems obtained above, it is possible to obtain the formulas for W of the most of the benzenoid systems considered earlier. We consider the following special cases:

Polyacenes

If we set $k_1 = k_2 = k_3 = k_4 = 0$ in the above expression, it reduces to the formula for W of polyacenes (i.e. $L_h = GB(n, 0, 0, 0, 0)$):

$$W(GB(n, 0, 0, 0, 0)) = \frac{1}{3}(16n^3 + 36n^2 + 26n + 3)\,.$$

Parallelograms

We have $P(n, k) = GB(n, 0, k-1, k-1, 0)$. Thus in this special case the above expression reduces to the formula for W of parallelograms:

$$\begin{aligned} W &= \frac{4n^3(k^2 + 2k + 1)}{3} + \frac{2kn^2(k^2 + 9k + 8)}{3} + \\ &\quad \frac{n(k^4 + 8k^3 + 16k^2 + 2k - 1)}{3} - \frac{k(k^4 - 20k^2 + 4)}{15}\,. \end{aligned}$$

Trapeziums

Trapeziums can be described as

$$T(n, k) = GB(n - k + 1, k - 1, 0, k - 1, 0) = GB(n, 0, k - 1, 0, k - 1)\,,$$

hence we can again use the general formula to obtain the expression for the trapeziums:

$$\begin{aligned} W &= \frac{4n^3(k^2 + 2k + 1)}{3} - \frac{2n^2(k + 1)(2k^2 - 8k - 3)}{3} + \\ &\quad \frac{2n(k^4 - 4k^3 + 6k^2 + 9k + 1)}{3} - \frac{k(8k^4 + 35k^2 - 45k - 28)}{30}\,. \end{aligned}$$

Bitrapeziums

Bitrapeziums can be described as $BT(n,k_1,k_2) = GB(n-k_1,k_1,k_2,k_1,k_2)$. So, in this special case the general formula reduces to

$$\begin{aligned} W &= \frac{4n^3(k_1+k_2+2)^2}{3} - \frac{2n^2(2k_1^3 - k_1(12k_2+17) + 2k_2^3 - 17k_2 - 18)}{3} + \\ &\quad \frac{2n(k_1^4 + k_1(11k_2+13) + k_2^4 + 13k_2 + 13)}{3} - \\ &\quad \frac{8k_1^5 + 20k_1^4(k_2+2) + 5k_1^3(16k_2+23) + 5k_1^2(23k_2+28)}{30} - \\ &\quad \frac{k_1(20k_2^4 + 80k_2^3 + 115k_2^2 + 80k_2 + 27)}{30} - \\ &\quad \frac{8k_2^5 + 40k_2^4 + 115k_2^3 + 140k_2^2 + 27k_2 - 30)}{30} . \end{aligned}$$

Coronene/circumcoronene series

As the final example we consider the coronene/circumcoronene series (H_k). Namely, $H_k = GB(k, k-1, k-1, k-1, k-1)$. Thus, inserting these special values into the general formula for the $W(GB)$ we obtain

$$W(H_k) = \frac{1}{5}\,(164\ k^5 -\ 30\ k^3 +\ k)\,.$$

APPENDIX: PROOF OF FORMULA (1)

Let G be a connected graph. The distance between the vertices x and y of G is the length (= number of edges) in a shortest path connecting x and y . The Wiener number of G is defined as the sum of distances between all pairs of vertices of G .

Suppose for a moment that the shortest path between any two vertex of G is unique. Then instead of summing the distances of all pairs of vertices, we may count how many shortest paths go through a given edge, and sum these counts over all edges of G. [This method for computing W is applicable for acyclic graphs and was first put forward in Wiener's pioneering paper.[23]]

The above argument is certainly not applicable to benzenoid systems since in them there are many pairs of vertices which are connected by several shortest paths.

Let B be the molecular graph of a benzenoid hydrocarbon and let x and y be its two distinct vertices. In the general case there are several shortest paths connecting x and y. Choose in an arbitrary manner one of these shortest paths. Repeat this for all pairs of vertices of B. Denote by $\pi(B)$ the collection of all chosen shortest paths. Thus, by definition, $\pi(B)$ consists of $N(N-1)/2$ elements, one shortest path for each pair of vertices. The sum of the lengths of the paths from $\pi(B)$ is just the Wiener number of B.

Let C be an elementary edge–cut of B, dissecting B into fragments B' and B'', with $n_1(C)$ and $n_2(C)$ vertices, respectively. It is easy to see that between any vertex of B' and any vertex of B'' there is a path from $\pi(B)$ which is intersected by C. Furthermore, each such path is intersected exactly once (otherwise it would not have minimal length). Thus C intersects exactly $n_1(C)\,n_2(C)$ paths from $\pi(B)$, and intersects exactly one edge in each of them.

On the other hand, the collection of all elementary cuts of B intersect all edges of B and therefore all edges of all elements of $\pi(B)$. No two elementary edge–cuts intersect the same edge.

Then, in analogy with Wiener's original argument,[23] we may obtain $W(B)$ by counting how many paths from $\pi(B)$ are intersected by an elementary cut C, and then summing these counts over all elementary cuts. Because the number of paths from $\pi(B)$, intersected by C, is just $n_1(C)\,n_2(C)$ we arrived at formula (1).

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Figure Captions

Figure 1. A benzenoid system and the corresponding elementary cuts C_1, C_2, C_3.

Figure 2. Parallelogram $P(7,4)$.

Figure 3. Trapezium $T(9,5)$.

Figure 4. Parallelogram-like benzenoid system $P_1(7,3)$.

Figure 5. Parallelogram-like benzenoid system $P_2(7,4)$.

Figure 6. Parallelogram-like benzenoid system $P_3(4,3)$.

Figure 7. Bitrapezium $BT(6,2,3)$.

Figure 8. Bitrapezium $BT(7,4,5)$.

Figure 9. General benzenoid $GB(7,3,4,5,2)$.