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Calculating the hyper-Wiener index of benzenoid hydrocarbons

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A method for the calculation of the hyper-Wiener index (*WW*) of a benzenoid system *B* is described, based on its elementary cuts. A pair of elementary cuts partitions the vertices of *B* into four fragments, possessing n_{rs} $r,s = 1,2$ vertices. *WW* is equal to the sum of terms of the form $n_{11}n_{22}+n_{12}n_{21}$. The applicability of the method is illustrated by deducing a general expression for *WW* of the coronene/circumcoronene series.

Introduction

The hyper-Wiener index *WW* is one of the newly conceived topological indices. It was proposed by Randić [1] in 1993 and is currently in the focus of interest of scholars involved in QSPR and QSAR studies [2–17].

The nowadays accepted definition of the hyper-Wiener index, applicable to both acyclic and cycle-containing (molecular) graphs, was proposed by Klein et al. [6]:

$$WW(G) = \frac{1}{2}\sum_{x<y} d(x,y;G)^2 + \frac{1}{2}\sum_{x<y} d(x,y;G) \tag{1}$$

with $d(x,y;G)$ denoting the distance between the vertices x and y in the graph G.

The calculation of *WW* directly from Eq. (1) is not easy, especially in the case of large polycyclic molecules, such as benzenoid hydrocarbons. Some time ago, however, a formula was designed [17] by which these difficulties are overcome. This formula is based on the concept of elementary cuts, a graph-theoretical technique described in due detail in our earlier papers [18–21].

Denote by B a benzenoid system and by n the number of its vertices. An *elementary cut* of B is a straight line segment, passing through the centers of some edges of B, being orthogonal to these edges, and intersecting the perimeter of B exactly two times, so that at least one hexagon lies between these two intersection points.

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An elementary cut C divides B into two fragments, say $B_1(C)$ and $B_2(C)$. Let $n_1 = n_1(C)$ and $n_2 = n_2(C)$ be the number of vertices of $B_1(C)$ and $B_2(C)$, respectively, where, of course, $n_1 + n_2 = n$. Then the Wiener index of B can be calculated by means of the formula [20]

$$W(B) = \sum_i n_1(C_i) n_2(C_i) ,$$

in which the summation goes over all elementary cuts of B.

For more details on elementary cuts of benzenoid systems the readers are referred to [18–21], were also examples and a more extensive bibliography can be found.

An elementary-cut-based formula for the calculation of the hyper-Wiener index

Consider two distinct elementary cuts C_i and C_j of B. In the general case they divide the vertices of B into four fragments, say $B_{11}(C_i,C_j)$, $B_{12}(C_i,C_j)$, $B_{21}(C_i,C_j)$ and $B_{22}(C_i,C_j)$. The numbers of vertices in these fragments are denoted by $n_{rs} = n_{rs}(C_i,C_j)$, $r,s = 1,2$. Clearly, $n_{11} + n_{12} + n_{21} + n_{22} = n$. In the general case some of the vertex counts n_{rs} may be equal to zero.

The above specified fragments will be labeled such that

$$B_{11}(C_i,C_j) \cup B_{12}(C_i,C_j) = B_1(C_i) ,$$

$$B_{21}(C_i,C_j) \cup B_{22}(C_i,C_j) = B_2(C_i) ,$$

$$B_{11}(C_i,C_j) \cup B_{21}(C_i,C_j) = B_1(C_j) ,$$

$$B_{12}(C_i,C_j) \cup B_{22}(C_i,C_j) = B_2(C_j) ,$$

in which case the hyper-Wiener index of the benzenoid system B obeys the formula [17, 21]:

$$WW(B) = \sum_i n_1(C_i) n_2(C_i) + WW^*(B) ,$$

or

$$WW(B) = W(B) + WW^*(B) , \tag{2}$$

with $WW^*(B)$ being the abbreviation for

$$\sum_{i<j} [n_{11}(C_i,C_j) n_{22}(C_i,C_j) + n_{12}(C_i,C_j) n_{21}(C_i,C_j)] , \tag{3}$$

in which the summation goes over all pairs of (mutually distinct) elementary cuts of B.

An advanced example: hyper-Wiener index of circumcoronenes

In order to illustrate the way in which Eqs (2) and (3) work, as well as their power, we solve a difficult problem: we determine the general expression for the hyper-Wiener index of the k-th member H_k of the coronene/circumcoronene homologous series (H_1 = benzene, H_2 = coronene, H_3 = circumcoronene, H_4 = circumcircumcoronene, etc), see Fig. 1. These highly symmetric benzenoid systems attract for a long time the attention of both theoretical and experimental chemists. For a recent survey on their theoretical-chemical properties see [22]. Needless to say that a formula for $WW(H_k)$ was not known so far.

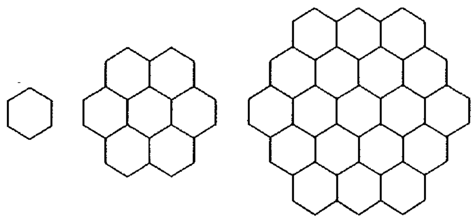
In what follows, we refer to any of the benzenoid systems H_k just as coronene.

For a pair of elementary cuts of H_h we distinguish two different arrangements as schematically depicted in Fig. 2.

Type A consists of parallel elementary cuts and type B contains pairs of intersected elementary cuts. Because of symmetry, both types of appear three times and so we can write

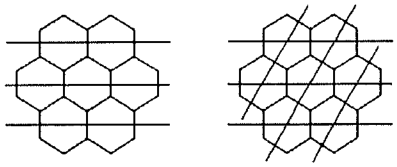
$$\mathrm{WW}^*(H_h) = 3(WW^*(A) + WW^*(B)),$$

where $WW^*(A)$ and $WW^*(B)$ denote the contributions to $WW^*(H_h)$ of parallel and intersected elementary cuts, respectively. In what follows we consider these two quantities separately. In the below calculations, for technical reasons we use indices $h = k-1$ for $h = 0, 1, \ldots$.



H_1 H_2 H_3

Fig. 1. The first three members of the coronene/circumcoronene series: H_1=benzene, H_2=coronene, H_3=circumcoronene



(a) type A (b) type B

Fig. 2. Two types of pairs of elementary cuts

Computing WW(A)*

In this case, for any two parallel elementary cuts either n_{12} or n_{21} is equal to zero. We divide parallel elementary cuts of type A into two groups, named type A_1 and type A_2 (see Figs 3 and 4). The elementary cut numbered $h+1$ in Fig. 3 divides the coronene H_h into two congruent fragments. We call them the *upper* and the *lower* fragment.

a) $WW^*(A_1)$. In this case, we calculate $n_{11}(C_i,C_j)$ and $n_{22}(C_i,C_j)$, where C_i is the elementary cut from the upper fragment or the middle elementary cut and C_j is parallel to C_i. We notice, that $i = 1,2,\ldots,h+1$ and the elementary cut C_j must lie below C_i.

Let C_i denote any of these elementary cuts, $i = 1,2,\ldots,h+1$. Then for any elementary cut C_j parallel to C_i we have:

$$n_{11}(C_i,C_j) = (2h+3) + (2h+5) + \ldots + (2h+(2i+1)) = \sum_{n=1}^{i}(2h+2n+1) = 2hi + \sum_{n=1}^{i}(2n+1)\ .$$

There are $2h+2i+1$ vertices above the elementary cut C_i, and we have to consider vertices above i elementary cuts, hence we sum from 1 to i.

In order to obtain $n_{22}(C_i,C_j)$, we have to consider h elementary cuts from the lower fragment, the middle elementary cut and h-i elementary cuts from the upper fragment. We denote the elementary cuts from the upper fragment by $C_{j'}$, where $j' = 1,2,\ldots,h$-i and the rest $C_{j''}$, where $j'' = 1,2,\ldots,h+1$. For the elementary cut $C_{j'}$ (see Fig. 3), $n_{22}(C_i,C_{j'})$ is the sum of all vertices from the lower fragment, that is

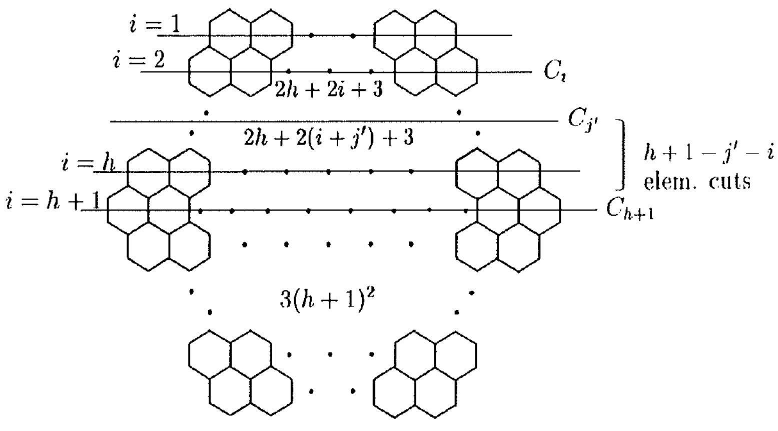


Fig. 3. Pairs of elementary cuts of type A_1

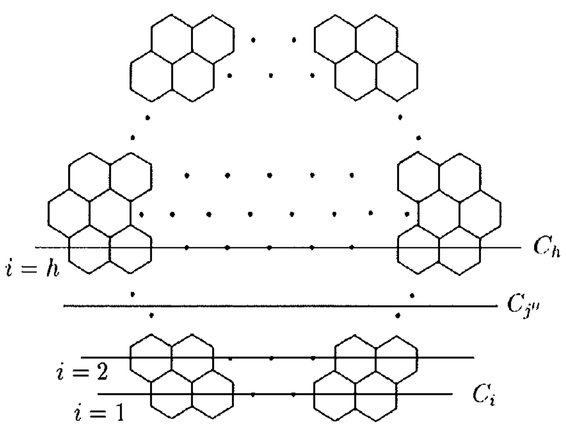


Fig. 4. Pairs of elementary cuts of type A_2

$3(h+1)^2$ vertices, and vertices between the elementary cut C_j' and the middle elementary cut C_{h+1}.

By means of Fig. 3 we determine the number of vertices below the elementary cuts C_i and C_j' (we count only the vertices which are directly below the elementary cut). Since j' goes from 1 to h-i, the number of vertices below $C_{j'}$ is $2h+2(i+j')+3$. The number of vertices below the next elementary cut is $2h+2(i+j')+5, \ldots$. So, we can write

$$n_{22}(C_i,C_j) = 3(h+1)^2 + (2(h+i+j')+3) + (2(h+i+j')+5) + \ldots +$$
$$+ (2(h+i+j') + 2(h+1-i-j')+1) = 3(h+1)^2 +$$
$$+ 2(h+i+j')(h+1-i-j') + \sum_{n=1}^{h+1-j'-i}(2n+1),$$

where $j'=1, \ldots, h-i$.

Next, we have to calculate $n_{22}(C_i,C_{j''})$. We number the elementary cuts from the bottom to the middle, as in Fig. 4. It is not difficult to see that

$$n_{22}(C_i,C_{j''}) = (2h+3) + (2h+5) + \ldots + (2h+2j''+1)$$
$$= 2hj'' + \sum_{n=1}^{j''}(2n+1),$$

where $j''= 1, \ldots, h+1$. Now we can write $WW(A_1)$ as:

$$\sum_{C_i}\sum_{C_{j'}} n_{11}(C_i,C_{j'})\, n_{22}(C_i,C_{j'}) + \sum_{C_i}\sum_{C_{j''}} n_{11}(C_i,C_{j''})\, n_{22}(C_i,C_{j''})$$

$$= \sum_{i=1}^{h+1}\sum_{j'=1}^{h-i} n_{11}(C_i,C_{j'})\, n_{22}(C_i,C_{j'}) + \sum_{i=1}^{k+1}\sum_{j''=1}^{h+1} n_{11}(C_i,C_{j''})\, n_{22}(C_i,C_{j''})$$

$$= \sum_{i=1}^{h+1} [[2hi + \sum_{n=1}^{i}(2n+1)]\cdot[\sum_{j'=1}^{h-i}[3(h+1)^2 + 2(h+i+j')\,(h+1-i-j') +$$

$$+ \sum_{n=1}^{h+1-j'-i}(2n+1)] + \sum_{j''=1}^{h+1}[2hj'' + \sum_{n=1}^{j''}(2n+1)]]]$$

$$= \frac{61}{18}h^6 + \frac{98}{5}h^5 + \frac{3151}{72}h^4 + \frac{571}{12}h^3 + \frac{1825}{72}h^2 + \frac{319}{60}h.$$

b) $WW^*(A_2)$. In this case, we calculate $n_{11}(C_i,C_j)$ and $n_{22}(C_i,C_j)$, where C_i and C_j are parallel elementary cuts from the lower fragment of H_h. As we see in Fig. 4, elementary cuts C_i are numbered from the bottom to the middle of coronene and $i = 1, \ldots, h$.

We have exactly the same situation as in the case of type A_1, when we considered elementary cuts denoted by $C_{j'}$. Bearing in mind the previous result, we obtain

$$WW^*(A_2) = \sum_{C_i}\sum_{C_j} n_{11}(C_i,C_j)\, n_{22}(C_i,C_j)$$

$$= \sum_{i=1}^{h}\sum_{j=1}^{h-i} n_{11}(C_i,C_j)\, n_{22}(C_i,C_j)$$

$$= \sum_{i=1}^{h} [[2hi + \sum_{n=1}^{i}(2n+1)]\,[\sum_{j=1}^{h-i}[3(h+1)^2 + 2(h+i+j)\,(h+1-i-j)]]$$

$$= \frac{29}{18}h^6 + \frac{74}{15}h^5 + \frac{245}{72}h^4 - \frac{13}{4}h^3 - \frac{361}{72}h^2 - \frac{101}{61}h.$$

In order to compute $WW^*(A)$, we have to add up both previous results:

$$WW^*(A) = WW^*(A_1) + WW^*(A_2) =$$

$$= 5h^6 + \frac{368}{15}h^5 + \frac{283}{6}h^4 + \frac{133}{3}h^3 + \frac{61}{3}h^2 + \frac{109}{30}h.$$

Computing WW(B)*

Our aim is to deduce an expression for $WW^*(B)$, where type B consists of intersected pairs of elementary cuts, depicted in Fig. 2(b). We can divide the pairs of elementary cuts of type B into two groups, denoted as type B_1 and type B_2 (see Figs 5 and 6). Then $WW^*(B)$ is equal to the sum $WW^*(B_1) + WW^*(B_2)$.

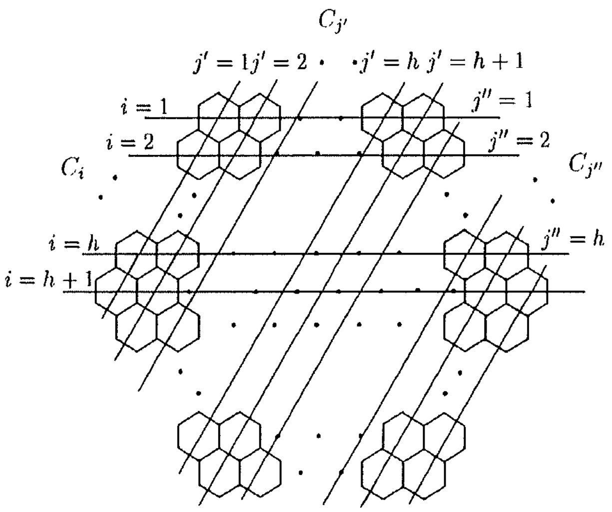


Fig. 5. Pairs of elementary cuts of type B_1

a) $\boldsymbol{WW^*(B_1)}$**.** We have to have a look at all pairs of elementary cuts (C_i,C_j), $i = 1,\ldots,h+1$, and to divide elementary cuts C_j into two classes. The elementary cuts of the first and second class are denoted by C_j and $C_{j''}$, respectively. We consider these two classes separately.

In the first subcase we are interested in all pairs (C_i,C_j), where $i = 1,\ldots,h+1$ and $j' = 1,\ldots,h+1$. We see this type of intersections in Fig. 5. The following abbreviation will be employed: $n_{11}(C_i,C_{j'}) = n'_{11}$, $n_{12}(C_i,C_{j'}) = n'_{12}$, $n_{21}(C_i,C_{j'}) = n'_{21}$

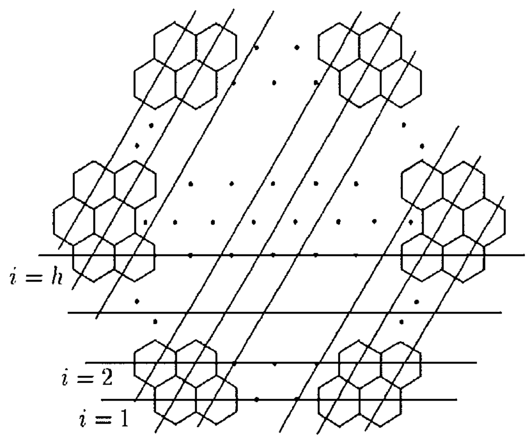


Fig. 6. Pairs of elementary cuts of type B_2

and $n_{22}(C_i,C_{j'}) = n'_{22}$. Assume that we fixed some C_i, for $i = 1,2,\ldots,h+1$. We investigate the quantities n'_{rs}, $r,s = 1,2$, where j' goes from 1 to $h+1$. Table I gives us the arrangement of quantities n_{rs}:

j'	n_{11} n_{21}	n_{12} n_{22}

We can determine n_{rs} from Fig. 5, but we do not need to calculate n_{22}, because we already have the relation $6(h+1)^2 = n'_{11}+n'_{12}+n'_{21}+n'_{22}$.
As already mentioned, n'_{22} can be calculated from the other three quantities, therefore,

$$
\begin{aligned}
n'_{22} &= 6(h+1)^2 - (n'_{11}+n'_{12}+n_{22})' \\
&= 6(h+1)^2 - (2h(i+j') + \sum_{n=1}^{i}(2n-2j'+1) + \sum_{n=1}^{j'}(2n)) .
\end{aligned}
$$

The expressions for n''_{rs}, $r,s = 1,2$, are simplified as

$$
\begin{aligned}
n'_{11} &= 2ij' , \\
n'_{12} &= 2hi + i^2 + 2i(1-j') , \\
n'_{21} &= 2hj' + j'(2i-j'-2) , \\
n'_{22} &= 6h^2 - 2h(i+j'-6) - i^2 + 2i(j'-1) - j'^2 - 2j' + 6 ,
\end{aligned}
$$

where $j'=1, \ldots, h+1$.

Table I

$j'=1$	$2i$	$(2h+1)+(2h+3)+\ldots+(2h+2i-1)=i\cdot 2h+\sum_{n=1}^{i}(2n-1)$
	$2h+3-2i$	n'_{22}
$j'=2$	$2\cdot 2i$	$(2h-1)+(2h+1)+\ldots+(2h+2i-3)=i\cdot 2h+\sum_{n=1}^{i}(2n-3)$
	$2h+3+2h+5-2\cdot 2i$	n'_{22}
$j'=3$	$3\cdot 2i$	$(2h-3)+(2h-1)+\ldots+(2h+2i-5)=i\cdot 2h+\sum_{n=1}^{i}(2n-5)$
	$2h+3+2h+5+2h+7-3\cdot 2i$	n'_{22}
⋮	⋮	⋮
j'	$2ij'$	$2i\cdot h+\sum_{n=1}^{i}(2n-2j'+1)$
	$2j'(h-i)+\sum_{n=1}^{j'}(2n+1)$	n'_{22}

Table II

$j''=1$	$(2h+3)+(i-1)(2h+4)$	$1+3+\ldots+(2(i-1)-1)$
	$3(h+1)^2+4h+3-(2h+3+(i-1)(2h+4))$	n''_{22}
$j''=2$	$(2h+3)+(2h+5)+(i-2)(2h+6)$	$1+3+\ldots+(2(i-2)+1)$
	$3(h+1)^2+4h+3+4h+1-(2h+3+2h+5+(i-2)(2h+6))$	n''_{22}
$j''=3$	$(2h+3)+(2h+5)+(2h+7)+(i-3)(2h+8)$	$1+3+\ldots+(2(i-3)+1)$
	$3(h+1)^2+4h+3+4h+1+4h-1-(2h+3+2h+5+2h+7-(i-3)(2h+8))$	n''_{22}
$\vdots$	$\vdots$	$\vdots$
j''	$j''\cdot 2h + \sum_{n=1}^{j''}(2n+1) + (i-j'')(2h+2j''+2)$	$\sum_{n=1}^{i-j''}(2n-1)$
	$3(h+1)^2+j''\cdot 4h+\sum_{n=1}^{j''}(5-2n) - j''\cdot 2h+\sum_{n=1}^{j''}(2n+1)+(i-j'')(2h+2j''+2)$	n''_{22}

We still have to determine the quantities $n_{rs}(C_i,C_{j''})$, $r,s=1,2$, for $i=1,2,\ldots,h$ and $j''=1,\ldots,h$, as shown in Fig. 5. Similarly as before, we use the abbreviation $n_{rs}(C_i,C_{j''})=n''_{rs}$, $r,s=1,2$.

We first notice that if $j''\geq i$ then $n''_{12}=0$. This means, that we have to treat elementary cuts $C_{j''}$ when $j''=1,2,\ldots,i-1$, separately from those, when $j''=i,i+1,\ldots,h$.

Let C_i be the elementary cut as in the previous case and $C_{j''}$ as in Fig. 6(a) and $j''=1,\ldots,i-1$. Then we can make Table II:

As in the previous case, n''_{22} can be calculated from the other three quantities:

$$n''_{22} = 6(h+1)^2 - (n''_{11}+n''_{12}+n''_{22}) = 6(h+1)^2 -$$
$$- \left(\sum_{n=1}^{i-j''}(2m+1) + 3(h+1)^2+j''\cdot 4h + \sum_{n=1}^{j''}(5-2n)\right) .$$

We can simplify the expressions for n''_{rs}, $r,s=1,2$, as

$$n''_{11} = 2hi+2i(j''+1) - j''^2 ,$$

$$n''_{12} = (i-j'')^2 ,$$

$$n''_{21} = 3h^2 - 2h(i-2j''-3) - 2i(j''+1)+4j''+3 ,$$

$$n''_{22} = 3h^2+2h(3-2j'') - i^2+2ij' - 4j''+3 ,$$

where $j''=1,\ldots,i-1$.

Table III

$j''=i,\quad i\le j''\le h$	
n''_{11}	$(2h+3)+(2h+5)+\ldots+(2h+(2i+1)) = i\cdot 2h + \sum_{n=1}^{i}(2n+1)$
n''_{22}	$3(h+1)^2-(4h+3+\ldots+4h+(5-2j'')) = 3(h+1)^2-j''\cdot 4h-\sum_{n=1}^{j''}(5-2n)$

The same procedure has to be repeated for pairs of elementary cuts $(C_i,C_{j''})$, where $j''=i,\ldots,h$ and C_i is an arbitrary cut, $i=1,2,\ldots,h+1$. Since for such pairs of elementary cuts either n''_{12} or n''_{21} is zero, we only have to calculate n''_{11} and n''_{22}. We collect the respective results in Table III.

Calculating the respective sums we get:

$$n''_{11} = 2hi+i^2+2i\,,$$

$$n''_{22} = 3h^2+2h(3-2j'')+j''^2-4j''+3\,,$$

where $j''=i,\ldots,h$.

Now everything has been prepared to compute $WW^*(B_1)$ as follows:

$$\sum_{C_i}\sum_{C_{j'}}[n'_{11}\cdot n'_{22}+n'_{21}\cdot n'_{12}] = \sum_{C_i}\sum_{C_{j''}}[n''_{11}\cdot n''_{22}+n''_{21}\cdot n''_{12}] =$$

$$= \sum_{i=1}^{h+1}\sum_{j'=1}^{h+1}[2j'i\cdot(6h^2-2h((i+j'-6)-i^2+2i(j'-1)-j'^2-2j'+6)+$$

$$+\ (2hi+i^2+2i(1-j')\cdot(2hj-j'(2i-j'-2))]+$$

$$+\ \sum_{i=1}^{h+1}\sum_{j''=1}^{i-1}[(2hi+2i(j''+1)-j''^2)\cdot(3h^2+2h(3-2j'')-i^2+2ij'-4j''+3)+$$

$$+\ (i-j'')^2\cdot(3h^2-2h(i-2j''-3)-2i(j''+1)+4j''+3)]+$$

$$+\ \sum_{j''=i}^{h}[(2hi+i^2+2i)\cdot(3h^2+2h(3-2j'')+j''^2-4j''+3)]] =$$

$$= \frac{323}{90}h^6+\frac{368}{15}h^5+\frac{608}{9}h^4+\frac{577}{6}h^3+\frac{6737}{90}h^2+\frac{303}{10}h+5\,.$$

b) $WW^*(B_2)$. In Fig. 6 are shown the intersected pairs of elementary cuts of the type B_2. We observe that $WW^*(B_2)$ can be calculated in a way similar as $WW^*(B_1)$. The only difference is that if (C_i,C_j) is a pair of intersected elementary cuts of type B_1, then i only goes from 1 to h and j remains the same. This means, we have to eliminate the middle cut, numbered C_{h+1}.

So, we obtain the following expression for $WW^*(B_2)$:

$$\sum_{C_i}\sum_{C_{j'}}[n'_{11}\cdot n'_{22}+n'_{12}\cdot n'_{21}] + \sum_{C_i}\sum_{C_{j''}}[n''_{11}\cdot n''_{22}+n''_{12}\cdot n''_{21}] =$$

$$= \sum_{i=1}^{h}\sum_{j'=1}^{h+1}[2j'i\cdot(6h^2-2h((i+j'-6)-i^2+2i(j'-1)-j'^2-2j'+6)+$$

$$+ (2hi+i^2+2i(1-j')\cdot(2hj-j'(2i-j'-2))]+$$

$$+ \sum_{i=1}^{h}\sum_{j''=1}^{i-1}[(2hi+2i(j''+1)-j''^2)\cdot(3h^2+2h(3-2j'')-i^2+2ij'-4j''+3)+$$

$$+ (i-j'')^2\cdot(3h^2-2h(i-2j''-3)-2i(j''+1)+4j''+3)]+$$

$$+ \sum_{j''=i}^{h}[(2hi+i^2+2i)\cdot(3h^2+2h(3-2j'')+j''^2-4j''+3)]] =$$

$$= \frac{323}{90}h^6 + \frac{278}{15}h^5 + \frac{338}{9}h^4 + \frac{223}{6}h^3 + \frac{1607}{90}h^2 + \frac{303}{10}h.$$

We thus arrive at the expression for $WW^*(B)$:

$$WW^*(B) = WW^*(B_1)+WW^*(B_2)$$

$$=\frac{323}{45}h^6 + \frac{646}{15}h^5 + \frac{946}{9}h^4 + \frac{400}{3}h^3 + \frac{4172}{45}h^2 + \frac{168}{5}h+5.$$

For coronene H_h, type A and type B embrace all possible pairs of elementary cuts. Because of symmetry, both of them appear three times. Taking this fact into account and using the results obtained above we get:

$$WW^*(H_h) = 3(WW^*(A)+WW^*(B))$$

$$=\frac{548}{15}h^6 + \frac{1014}{5}h^5 + \frac{2741}{6}h^4 + 533h^3 + \frac{5087}{15}h^2 + \frac{1117}{10}h+15.$$

Recall that we have introduced $h:=k-1$ because of technical reasons. Returning back to k we find:

$$WW^*(H_k) = \frac{548}{15}(k-1)^6 + \frac{1014}{5}(k-1)^5 + \frac{2741}{6}(k-1)^4 + 533\,(k-1)^3 + \frac{5087}{15}(k-1)^2 +$$

$$+\frac{1117}{10}(k-1)+15.$$

and, therefore,

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

In order to get the final result, we need also the expression for $W(H_k)$, cf. Eqs (2). This expression has been determined earlier [18] and reads:

$$W(H_k) = \frac{164}{5} k^5 - 6k^3 + \frac{1}{5} k .$$

Bearing this in mind, we arrive at the required formula for the hyper-Wiener index of the k-th member of the coronene/circumcoronene family:

$$\begin{aligned} WW(H_k) &= W(H_k) + WW^*(H_k) \\ &= \frac{548}{15} k^6 + \frac{82}{5} k^5 - \frac{55}{6} k^4 - 3k^3 + \frac{17}{15} k^2 + \frac{1}{10} k . \end{aligned}$$

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