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A new algorithm for computing distance matrix and Wiener index of zig-zag polyhex nanotubes

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Abstract The Wiener index of a graph G is defined as the sum of all distances between distinct vertices of G. In this paper an algorithm for constructing distance matrix of a zig-zag polyhex nanotube is introduced. As a consequence, the Wiener index of this nanotube is computed.

Keywords Zig-zag polyhex nanotube · Distance matrix · Wiener index

Introduction

Carbon nanotubes form an interesting class of carbon nanomaterials. These can be imagined as rolled sheets of graphite about different axes. These are three types of nanotubes: armchair, chiral and zigzag structures. Further nanotubes can be categorized as single-walled and multi-walled nanotubes and it is very difficult to produce the former.

Graph theory has found considerable use in chemistry, particularly in modeling chemical structure. Graph theory has provided the chemist with a variety of very useful tools, namely, the topological index. A topological index is a numeric quantity that is mathematically derived in a direct and unambiguous manner from the structural graph of a molecule. It has been found that many properties of a chemical compound are closely related to some topological indices of its molecular graph [1, 2].

Among topological indices, the Wiener index [3] is probably the most important one. This index was introduced by the chemist H. Wiener, about 60 years ago to demonstrate correlations between physico-chemical properties of organic compounds and the topological structure of their molecular graphs. Wiener defined his index as the sum of distances between two carbon atoms in the molecules, in terms of carbon–carbon bonds. Next Hosoya named such graph invariants, topological index [4]. We encourage the reader to consult Refs. [5–7] and references therein, for further study on the topic.

The fact that there are good correlations between and a variety of physico-chemical properties of chemical compounds containing boiling point, heat of evaporation, heat of formation, chromatographic retention times, surface tension, vapor pressure and partition coefficients could be rationalized by the assumption that Wiener index is roughly proportional to the van der Waals surface area of the respective molecule [8].

Diudea was the first chemist which considered the problem of computing topological indices of nanostructures [9–15]. The presented authors computed the Wiener index of a polyhex and $TUC_4C_8(R/S)$ nanotori [16–18]. In this paper, we continue this program to find an algorithm for computing distance matrix of a zig-zag polyhex nanotube. As an easy consequence, the Wiener index of this nanotube is computed.

John and Diudea [9] computed the Wiener index of zig-zag polyhex nanotube $T = T(p, q) = TUHC_6[2p,q]$, for the first times. In this paper, distance matrix of these nanotubes are computed. As an easy consequence of our results, a matrix method for computing the Wiener index of a zig-zag polyhex nanotube is introduced. We also prepare an

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algorithm for computing distance matrix of these nanotubes. Throughout this paper, our notation is standard. They are appearing as in the same way as in the following [2, 19].

Main results and discussion

In this section, distance matrix and Wiener index of the graph T = $TUHC_6[m,n]$, Fig. 1, were computed. Here m is the number of horizontal zig-zags and n is the number of columns. It is obvious that n is even and $|V(T)| = mn$.

An algorithm for constructing distance matrix of $TUHC_6[m,n]$

We first choose a base vertex b from the 2-dimensional lattice of T and assume that x_{ij} is the (i,j)th vertex of T, Fig. 2. Define $D^{(1,1)}_{m\times n} = [d^{(1,1)}_{i,j}]$, where $d^{(1,1)}_{i,j}$ is distance between (1,1) and (i,j), i = 1, 2, ..., m and j = 1, 2, ..., n. By Fig. 2, there are two separates cases for the (1,1)th vertex. For example in the case (a) of Fig. 2, $d^{(1,1)}_{1,1} = 0, d^{(1,1)}_{1,2} = d^{(1,1)}_{2,1} = 1$ and in case (b), $d^{(1,1)}_{1,1} = 0, d^{(1,1)}_{1,2} = 1, d^{(1,1)}_{2,1} = 3$. In general, we assume that $D^{(p,q)}_{m\times n}$ is distance matrix of T related to the vertex (p,q) and $s^{(p,q)}_i$ is the sum of ith row of $D^{(p,q)}_{m\times n}$. Then there are two distance matrix related to (p,q) such that $s^{(p,2k-1)}_i = s^{(p,1)}_i$; $s^{(p,2k)}_i = s^{(p,2)}_i$; $1 \le k \le n/2, 1 \le i \le m, 1 \le p \le m$.

By Fig. 2 and previous notations, if b varies on a column of T then the sum of entries in the row containing base vertex is equal to the sum of entries in the first row of $D^{(1,1)}_{m\times n}$. On the other hand, one can compute the sum of entries in other rows by distance from the position of base vertex. Therefore,

$$s^{(i,j)}_k = \begin{cases} s^{(1,1)}_{i-k+1} & 1 \le k \le i \le m, \quad 1 \le j \le n \\ s^{(1,2)}_{k-i+1} & 1 \le i \le k \le m, \quad 1 \le j \le n \end{cases} \text{If} \quad 2|(i+j)$$

$$s^{(i,j)}_k = \begin{cases} s^{(1,2)}_{i-k+1} & 1 \le k \le i \le m, \quad 1 \le j \le n \\ s^{(1,1)}_{k-i+1} & 1 \le i \le k \le m, \quad 1 \le j \le n \end{cases} \text{If} \quad 2\nmid(i+j)$$

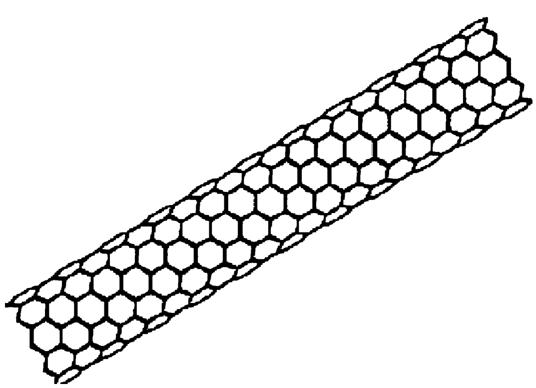

Fig. 1 The zig-zag polyhex nanotube $TUHC_6[20,n]$

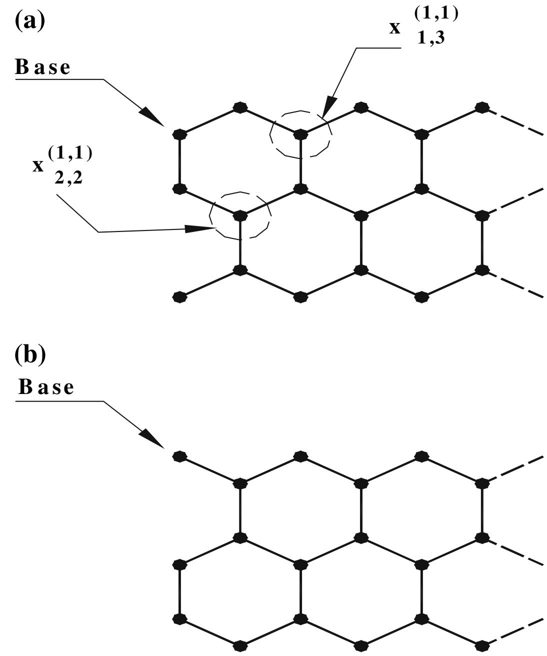

Fig. 2 Two basically different cases for the vertex b

We now describe our algorithm to compute distance matrix of a zig-zag polyhex nanotube. To do this, we define matrices $A^{(a)}_{m\times(n/2+1)} = [a_{ij}]$, $B_{m\times(n/2+1)} = [b_{ij}]$ and $A^{(b)}_{m\times(n/2+1)} = [c_{ij}]$ as follows:

$$a_{1,1}=0 \quad a_{1,2}=1 \quad a_{i,j} = \begin{cases} a_{i,1} & 2\nmid j \\ a_{i,2} & 2|j \end{cases}; \quad \begin{matrix} a_{i,1} = a_{i-1,1}+1, & a_{i,2} = a_{i,1}+1; & 2|i \\ a_{i,2} = a_{i-1,2}+1, & a_{i,1} = a_{i,2}+1; & 2\nmid i \end{matrix}$$

$$c_{1,1}=0 \quad c_{1,2}=1 \quad c_{i,j} = \begin{cases} c_{i,1} & 2\nmid j \\ c_{i,2} & 2|j \end{cases}; \quad \begin{matrix} c_{i,2} = c_{i-1,2}+1, & c_{i,1} = c_{i,2}+1; & 2|i \\ c_{i,1} = c_{i-1,1}+1, & c_{i,2} = c_{i,1}+1; & 2\nmid i \end{matrix}$$

$$b_{i,1} = i-1; \qquad b_{i,j} = b_{i,j-1}+1$$

For computing distance matrix of this nanotube we must compute matrices $D^{(a)}_{m\times n} = [d^a_{i,j}]$ and $D^{(b)}_{m\times n} = [d^b_{i,j}]$. But by our calculations, we can see that

$$d^a_{i,j} = \begin{cases} \mathrm{Max}\{a_{i,j}, b_{i,j}\} & 1 \le j \le n/2 \\ d_{i,n-j+2} & j > n/2+1 \end{cases} \quad \text{and}$$

$$d^b_{i,j} = \begin{cases} \mathrm{Max}\{a_{i,j}, c_{i,j}\} & 1 \le j \le n/2 \\ d_{i,n-j+2} & j > n/2+1 \end{cases}$$

This completes calculation of distance matrix.

Computing Wiener index of $TUHC_6[m,n]$

In previous section, distance matrix $D^{(p,q)}_{m\times n}$ related to vertex (p,q) is computed. Suppose $s^{(p,q)}_i$ is the sum of ith row of $D^{(p,q)}_{m\times n}$. Then $s^{(p,2k-1)}_i = s^{(p,1)}_i$ and $s^{(p,2k)}_i = s^{(p,2)}_i$, where $1 \le k \le n/2$, $1 \le i \le m$, $1 \le p \le m$. On the other hand, by our calculations in section ''An algorithm for constructing distance matrix of $TUHC_6[m,n]$'',

$$s_i^{(1,2k-1)} = \begin{cases} \frac{n^2}{4} + (n+i-2)(i-1) & i \le \frac{n}{2}+1 \\ \frac{n}{2}(4i-5) & i \ge \frac{n}{2}+1 \end{cases},$$
$$s_i^{(1,2k)} = \begin{cases} \frac{n^2}{4} + (n+i)(i-1) & i \le \frac{n}{2}+1 \\ \frac{n}{2}(4i-3) & i \ge \frac{n}{2}+1 \end{cases}$$
$$1 \le i \le m, \quad 1 \le k \le \frac{n}{2}.$$

Suppose $S_p^{(a)}$ and $S_p^{(b)}$ are the sum of all entries of distance matrix $D_{m\times n}^{(p,q)}$ in two cases (a) and (b). Then

$$S_1^{(a)} = \begin{cases} (mn/4)(2m+n-2)+(m/3)(m-1)(m-2) & m \le n/2+1 \\ (mn/2)(2m-3)+(n/24)(n+2)(n+4) & m \ge n/2+1 \end{cases},$$

$$S_1^{(b)} = \begin{cases} (mn/4)(2m+n-2)+(m/3)(m^2-1) & m \le n/2+1 \\ (mn/2)(2m-1)+(n/24)(n^2-4) & m \ge n/2+1 \end{cases}.$$

If p is arbitrary then one can see that:

$$S_p^{(a)} = S_1^{(a)} + \sum_{i=2}^{p} s_i^{(1,2)} - \sum_{i=m-p+2}^{m} s_i^{(1,1)}$$

$$S_p^{(b)} = S_1^{(b)} + \sum_{i=2}^{p} s_i^{(1,1)} - \sum_{i=m-p+2}^{m} s_i^{(1,2)}$$

Thus it is enough to compute $S_p^{(a)}$ and $S_p^{(b)}$. When $m \le n/2$, one can see that:

$$S_p^{(a)} = (mn/4)(2m+n+2) + (m/3)\left(m^2-1\right) - p\left(m^2+mn+n\right) + p^2(m+n)$$
$$S_p^{(b)} = (mn/4)(2m+n+2) + (m/3)(m+1)(m+2) - p\left(m^2+mn+n+2m\right) + p^2(m+n)$$

To complete our argument, we must investigate the case of $m > n/2 + 1$. To do this, we consider three cases that $p \le n/2 + 1$, $p \le m - n/2 + 1$; $m \le n + 1$, $m - n/2 + 1 < p \le n/2 + 1$ and $m > n + 1$, $p > n/2 + 1$.

(I) $p \le \frac{n}{2}+1$ and $p \le m-\frac{n}{2}+1$. In this case we have:

$$S_p^{(a)} = \frac{mn}{2}(2m+1)+\frac{n}{24}\left(n^2-4\right) + \frac{p}{12}\left(3n^2-24mn-12n-4\right)+\frac{3n}{2}p^2+\frac{p^3}{3}$$
$$S_p^{(b)} = \frac{mn}{2}(2m+3)+\frac{n}{24}(n-2)(n-4) + \frac{p}{12}\left(3n^2-24mn-24n+8\right)+\frac{p^2}{2}(3n-2)+\frac{p^3}{3}$$

(II) $m \le n + 1$ and $m-\frac{n}{2}+1 < p \le \frac{n}{2}+1$. Therefore,

$$S_p^{(a)} = \frac{mn}{4}(2m+n+2)+\frac{m}{3}\left(m^2-1\right) - p\left(m^2+mn+n\right)+p^2(m+n)$$
$$S_p^{(b)} = \frac{mn}{4}(2m+n+2)+\frac{m}{3}(m+1)(m+2) - p\left(m^2+mn+n+2m\right)+p^2(m+n)$$

(III) $m > n + 1$ and $p > \frac{n}{2}+1$. In this case,

$$S_p^{(a)} = \frac{n}{12}\left(n^2-4\right)+\frac{n}{2}(m-2p)(2m+1)+2np^2$$
$$S_p^{(b)} = \frac{n}{12}\left(n^2+8\right)+\frac{n}{2}(m-2p)(2m+3)+2np^2$$

Therefore,

$$W_{m\times n} = \begin{cases} (n/2)\left[\sum_{i=1}^{(m-1)/2}\left(S_i^{(a)}+S_i^{(b)}\right) + (1/2)\left(S_{(m+1)/2}^{(a)}+S_{(m+1)/2}^{(b)}\right)\right] & 2\nmid m \\ (n/2)\sum_{i=1}^{m/2}\left(S_i^{(a)}+S_i^{(b)}\right) & 2\mid m \end{cases}.$$

We now substitute the values of $S_p^{(a)}$ to compute the Wiener index of T, as follows:

$$W_{m\times n} = \begin{cases} \frac{mn^2}{24}\left(4m^2+3mn-4\right)+\frac{m^2n}{12}\left(m^2-1\right) & m \le \frac{n}{2}+1 \\ \frac{mn^2}{24}\left(8m^2+n^2-6\right)-\frac{n^3}{192}\left(n^2-4\right) & m > \frac{n}{2}+1 \end{cases}.$$

Constructing distance matrices of some nanotubes

In this section, distance matrices of $TUHC_6[8,10]$ and $TUHC_6[8,16]$ together with their Wiener indices are computed. To construct distance matrices of $TUHC_6[8,10]$, we must compute matrices $A_{8\times6}^{(a)}$, $A_{8\times6}^{(b)}$ and $B_{8\times6}$. By definition of these matrices, we have:

$$A_{8\times6}^{(a)} = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 2 & 1 & 2 & 1 & 2 \\ 4 & 3 & 4 & 3 & 4 & 3 \\ 5 & 6 & 5 & 6 & 5 & 6 \\ 8 & 7 & 8 & 7 & 8 & 7 \\ 9 & 10 & 9 & 10 & 9 & 10 \\ 12 & 11 & 12 & 11 & 12 & 11 \\ 13 & 14 & 13 & 14 & 13 & 14 \end{bmatrix},$$

$$A^{(b)}_{8\times 6} = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 1 \\ 3 & 2 & 3 & 2 & 3 & 2 \\ 4 & 5 & 4 & 5 & 4 & 5 \\ 7 & 6 & 7 & 6 & 7 & 6 \\ 8 & 9 & 8 & 9 & 8 & 9 \\ 11 & 10 & 11 & 10 & 11 & 10 \\ 12 & 13 & 12 & 13 & 12 & 13 \\ 15 & 14 & 15 & 14 & 15 & 14 \end{bmatrix}$$

$$B_{8\times 6} = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 5 \\ 1 & 2 & 3 & 4 & 5 & 6 \\ 2 & 3 & 4 & 5 & 6 & 7 \\ 3 & 4 & 5 & 6 & 7 & 8 \\ 4 & 5 & 6 & 7 & 8 & 9 \\ 5 & 6 & 7 & 8 & 9 & 10 \\ 6 & 7 & 8 & 9 & 10 & 11 \\ 7 & 8 & 9 & 10 & 11 & 12 \end{bmatrix}.$$

We now compute matrices $D^{(a)}_{8\times 10}$ and $D^{(b)}_{8\times 10}$. By definition, entries of the first n/2 + 1 columns of these matrices are maximum values of $\{A^{(a)}_{8\times 6}, B_{8\times 6}\}$ and $\{A^{(b)}_{8\times 6}, B_{8\times 6}\}$, respectively. Thus,

$$D^{(a)}_{8\times 10} = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 4 & 3 & 2 & 1 \\ 1 & 2 & 3 & 4 & 5 & 6 & 5 & 4 & 3 & 2 \\ 4 & 3 & 4 & 5 & 6 & 7 & 6 & 5 & 4 & 3 \\ 5 & 6 & 5 & 6 & 7 & 8 & 7 & 6 & 5 & 6 \\ 8 & 7 & 8 & 7 & 8 & 9 & 8 & 7 & 8 & 7 \\ 9 & 10 & 9 & 10 & 9 & 10 & 9 & 10 & 9 & 10 \\ 12 & 11 & 12 & 11 & 12 & 11 & 12 & 11 & 12 & 11 \\ 13 & 14 & 13 & 14 & 13 & 14 & 13 & 14 & 13 & 14 \end{bmatrix},$$

$$D^{(b)}_{8\times 10} = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 4 & 3 & 2 & 1 \\ 3 & 2 & 3 & 4 & 5 & 6 & 5 & 4 & 3 & 2 \\ 4 & 5 & 4 & 5 & 6 & 7 & 6 & 5 & 4 & 5 \\ 7 & 6 & 7 & 6 & 7 & 8 & 7 & 6 & 7 & 6 \\ 8 & 9 & 8 & 9 & 8 & 9 & 8 & 9 & 8 & 9 \\ 11 & 10 & 11 & 10 & 11 & 10 & 11 & 10 & 11 & 10 \\ 12 & 13 & 12 & 13 & 12 & 13 & 12 & 13 & 12 & 13 \\ 15 & 14 & 15 & 14 & 15 & 14 & 15 & 14 & 15 & 14 \end{bmatrix}$$

This implies that W($TUHC_6$[8,10]) = 19,700. To construct distance matrices of $TUHC_6$[8,16], we must compute matrices $A^{(a)}_{8\times 9}$ and $A^{(b)}_{8\times 9}$. Using a similar argument as above, we have:

$$A^{(a)}_{8\times 9} = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 2 & 1 & 2 & 1 & 2 & 1 & 2 & 1 \\ 4 & 3 & 4 & 3 & 4 & 3 & 4 & 3 & 4 \\ 5 & 6 & 5 & 6 & 5 & 6 & 5 & 6 & 5 \\ 8 & 7 & 8 & 7 & 8 & 7 & 8 & 7 & 8 \\ 9 & 10 & 9 & 10 & 9 & 10 & 9 & 10 & 9 \\ 12 & 11 & 12 & 11 & 12 & 11 & 12 & 11 & 12 \\ 13 & 14 & 13 & 14 & 13 & 14 & 13 & 14 & 13 \end{bmatrix},$$

$$A^{(b)}_{8\times 9} = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 3 & 2 & 3 & 2 & 3 & 2 & 3 & 2 & 3 \\ 4 & 5 & 4 & 5 & 4 & 5 & 4 & 5 & 4 \\ 7 & 6 & 7 & 6 & 7 & 6 & 7 & 6 & 7 \\ 8 & 9 & 8 & 9 & 8 & 9 & 8 & 9 & 8 \\ 11 & 10 & 11 & 10 & 11 & 10 & 11 & 10 & 11 \\ 12 & 13 & 12 & 13 & 12 & 13 & 12 & 13 & 12 \\ 15 & 14 & 15 & 14 & 15 & 14 & 15 & 14 & 15 \end{bmatrix}$$

On the other hand,

$$B_{8\times 9} = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\ 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\ 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 \\ 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \\ 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 \\ 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 \end{bmatrix},$$

Therefore,

$$D^{(a)}_{8\times 16} = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 \\ 4 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 \\ 5 & 6 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 10 & 9 & 8 & 7 & 6 & 5 & 6 \\ 8 & 7 & 8 & 7 & 8 & 9 & 10 & 11 & 12 & 11 & 10 & 9 & 8 & 7 & 8 & 7 \\ 9 & 10 & 9 & 10 & 9 & 10 & 11 & 12 & 13 & 12 & 11 & 10 & 9 & 10 & 9 & 10 \\ 12 & 11 & 12 & 11 & 12 & 11 & 12 & 13 & 14 & 13 & 12 & 11 & 12 & 11 & 12 & 11 \\ 13 & 14 & 13 & 14 & 13 & 14 & 13 & 14 & 15 & 14 & 13 & 14 & 13 & 14 & 13 & 14 \end{bmatrix},$$

$$D^{(b)}_{8\times 16} = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ 3 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 \\ 4 & 5 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 9 & 8 & 7 & 6 & 5 & 4 & 5 \\ 7 & 6 & 7 & 6 & 7 & 8 & 9 & 10 & 11 & 10 & 9 & 8 & 7 & 6 & 7 & 6 \\ 8 & 9 & 8 & 9 & 8 & 9 & 10 & 11 & 12 & 11 & 10 & 9 & 8 & 9 & 8 & 9 \\ 11 & 10 & 11 & 10 & 11 & 10 & 11 & 12 & 13 & 12 & 11 & 10 & 11 & 10 & 11 & 10 \\ 12 & 13 & 12 & 13 & 12 & 13 & 12 & 13 & 14 & 13 & 12 & 13 & 12 & 13 & 12 & 13 \\ 15 & 14 & 15 & 14 & 15 & 14 & 15 & 14 & 15 & 14 & 15 & 14 & 15 & 14 & 15 & 14 \end{bmatrix}.$$

By our calculations, it is easy to see that W($TUHC_6$[8,16]) = 59,648.

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