communications in mathematical
match
and in computer chemistry

no. 45, March 2002
MATCDY (45) 109 - 122 (2002)
ISSN 0340 - 6253

HOSOYA POLYNOMIAL IN TORI

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Abstract. The Hosoya polynomial is defined as a distance-based increasing power sequence. Analytical formulas for calculating this polynomial in several classes of toroidal nets are given. The Wiener number, derived from the first derivative of the Hosoya polynomial (in x = 1), is calculable either by close formulas or by recursions.

INTRODUCTION

A distance-based polynomial was introduced by Hosoya (1988),[1] as:

$$H(G,x) = \sum_{k=0}^{d(G)} d(G,k)x^k \tag{1}$$

with $d(G,0) = N$ and $d(G,1) = e$. In the above relations, N is the number of vertices in the graph G, e the number of edges, $d(G)$ the topological diameter (i.e., the longest topological distance in G) and $d(G,k)$ the number of pair vertices lying at distance k of each other. The polynomial (called Wiener, by its author but Hosoya, in the more recent literature[2,3]) can be expressed as a function of the vertex contributions $H(i,x)$:

Dedicated to Professor Haruo Hosoya on his 65th anniversary, in appreciation of his brilliant contribution to the Graph Theory.

$$H(i,x) = \sum_{k=0}^{d(G)} d(i,k)x^k \tag{2}$$

where $d(i,k)$ is the number of vertices at distance k from the vertex i. Since each path has two endpoints (i.e., each path is counted twice), it becomes clear that, in a vertex transitive graph, the following relation holds (see also ref. 2):

$$N \cdot H(i,x) = 2H(G,x) - N \tag{3}$$

POLYHEX HC6 AND VC6 TORI

Polyhex tori are generated by some cutting procedures,[4-8] performed on a square lattice embedded on the toroidal surface. Function of the orientation of the cut edges, HC6 (phenanthrenoid, or zig-zag) and VC6 (anthracenoid, or armchair) nets are obtained (Figures 1 and 2).

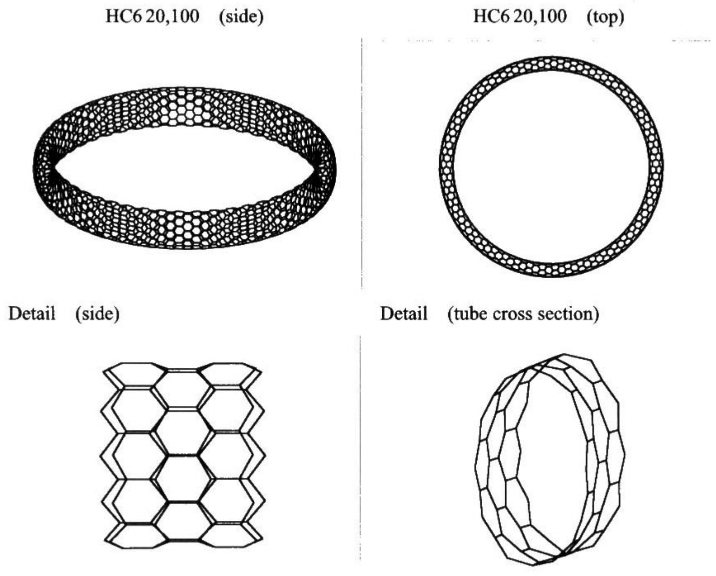

Figure 1. A HC6 lattice.

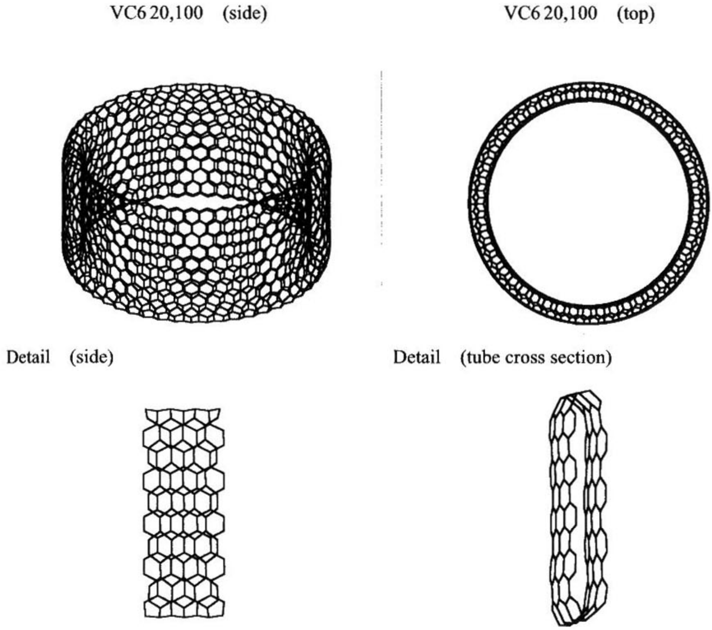

Figure 2. A VC6 lattice.

In the name of a torus, eg. HC6 *c,n* , the first letter means the type of cutting, next is the type of net and finally the dimensions: *c* is the number of points (i.e., atoms) around the tube while *n* is the number of points around the torus. Within the cutting procedure, the number of points is preserved. The actual geometry of tori in the above figures is the so-called "elongated" geometry, discussed elswhere.[9] The topology-based calculations presented in this paper are, of course, not affected by the actual geometry. Part of them have been performed by the aid of TOPOCLUJ Software Package.

* * *

The general form of the vertex Hosoya polynomials, for tori of type HC6 *c,n* and VC6 *c,n*, (regular graphs, having $N = cn$), in going from normal HC6 to normal VC6 tori, are:

HC6 c,n; $n > c$:

$$H(i,x) = 1 + 3kx^{k}{}_{,k=1,2,\dots,(c/2-1)} + (3c/2-1)x^{c/2} + (3c/2-k)x^{(c/2+k)}{}_{,k=1,2,\dots,(c/2-1)} + \\ + cx^{k}{}_{,k=c,c+1,\dots,(n-1)} + (c/2)x^{n} \tag{4}$$

HC6 c,n = VC6 c,n; $n = c$:

$$H(i,x) = 1 + 3kx^{k}{}_{,k=1,2,\dots,(c/2-1)} + (3c/2-1)x^{c/2} + (3c/2-k)x^{(c/2+k)}{}_{,k=1,2,\dots,(c/2-1)} + \\ + (c/2)x^{n} \tag{5}$$

VC6 c,n; $c+2 \le n \le 2(c-1)$:

$$H(i,x) = 1 + 3kx^{k}{}_{,k=1,2,\dots,(n/2-1)} + (3n/2-1)x^{n/2} + (3n/2-k)x^{(n/2+k)}{}_{,k=1,2,\dots,(c-1-n/2)} + \\ + (2n-3c/2-1)x^{c} + [2(n-c)-4k]x^{(c+k)}{}_{,k=1,2,\dots,((n-c)/2-1)} + x^{(c+n)/2} \tag{6}$$

VC6 c,n; $n = 2c$:

$$H(i,x) = 1 + 3kx^{k}{}_{,k=1,2,\dots,(c-1)} + (5c/2-2)x^{c} + (2c-4k)x^{(c+k)}{}_{,k=1,2,\dots,(c/2-1)} + x^{(c+n)/2} \tag{7}$$

VC6 c,n; $n \ge 2(c+1)$:

$$H(i,x) = 1 + 3kx^{k}{}_{,k=1,2,\dots,(c-1)} + (5c/2-1)x^{c} + 2cx^{k}{}_{,k=c+1,c+2,\dots,(n/2-1)} + (2c-1)x^{n/2} + \\ + (2c-4k)x^{(n/2+k)}{}_{,k=1,2,\dots,(c/2-1)} + x^{(c+n)/2} \tag{8}$$

"Normal" torus, in the above relations, means a toroidal net having the number of hexes on tube smaller than around the torus. The "normal" status is already reached at $n > c$, in HC6 tori, while $n \geq 2(c+1)$ is needed in case of VC6 tori.

Note that the coefficients of the vertex Hosoya polynomial are just the entries in the LC matrix (i.e., Layer matrix of Cardinality)[10] or the (vertex) Distance Degree Sequence DDS(i) (i.e., the number of vertices lying at distance k form the vertex i).[11] Clearly, the vertex decomposition of $H(G,x)$ would be more complicated in vertex non-transitive graphs (see below).

The polynomial coefficients can be viewed as a "distance degree" spectrum, useful in topological characterisation of graphenes. In case of the (normal) C6 20,*n* series, the spectra (per vertex d(i,k) values) are shown in Figures 3 and 4.

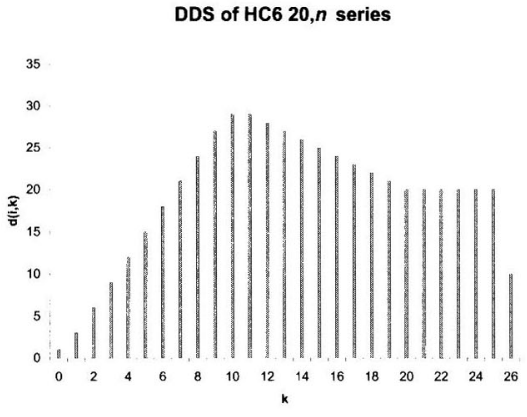

Figure 3. The distance degree spectrum of the HC6 20,*n* tori

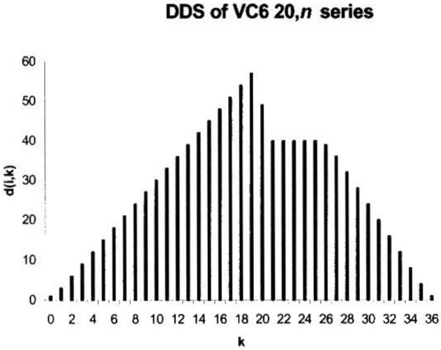

Figure 4. The distance degree spectrum of the VC6 20,*n* tori

The repeating terms : $cx^k{}_{,k=c,c+1,\dots,n-1}$ and $2cx^k{}_{,k=c+1,c+2,\dots,n/2-1}$, respectively, are the only changes, as *n* increases, in the spectrum of a given series (i.e., a series of fixed *c*). By changing the series, the spectrum will change drastically, according to the general formulas (4) -(8).

The first derivative[12] of the Hosoya polynomial (in $x = 1$) enables the calculation of the well-known Wiener[13] number *W* (i.e., the sum of all distances in *G*): $W(G) = H'(G,1)$.

In case of the normal series of tori, the first derivative of the Hosoya polynomial leads to:

HC6 c,n:

$$W = \frac{nc}{2}\left[\sum_{k=1}^{c/2-1} 3k^2 + (3c/2-1)c/2 + \sum_{k=1}^{c/2-1}(3c/2-k)(c/2+k) + \sum_{k=c}^{n\text{-}1} ck + nc/2\right] \qquad (9)$$

VC6 c,n:

$$W = \frac{nc}{2}\left[\sum_{k=1}^{c-1} 3k^2 + (5c/2-1)c + \sum_{k=c+1}^{n/2-1} 2ck + (2c-1)n/2 + \sum_{k=1}^{c/2-1}(2c-4k)(n/2+k) + (n/2+c/2)\right]$$

(10)

By expanding the sums one obtains:

HC6 c,n: $$W = \frac{1}{24} nc^2 (6n^2 + c^2 - 4) \qquad (11)$$

VC6 c,n: $$W = \frac{1}{24} nc^2 (3n^2 + c^2 + 3nc - 4) \qquad (12)$$

Expansion of eq. 6 (case VC6; $c + 2 \le n \le 2(c-1)$) also leads to relation (12). Moreover, the formulas for the other two cases:

$n = c$:

$$W = \frac{c^3}{24}(7c^2 - 4) \qquad (13)$$

and

$n = 2c$: $$W = \frac{c^3}{12}(19c^2 - 4) \qquad (14)$$

can be deduced from the first derivative of the corresponding polynomials (eqs. 5 and 7, respectively), as well as from eq. 12. Relation (13) is also a particular case of eq (11), proving the selfconsistency of the formulas (eqs. 11 and 12) for calculating the Wiener index in polyhex tori.

TWISTED VH*t*C6 *c,n* TORI

By twisting a row of squares (i.e., connecting each square with the next column), the resulting polyhex net will be also twisted. As a consequence, a chiral object will result[8] (Figure 5). The name is composed as: type of cutting, type of the twisting, number of twisted rows (in the range 1-*c*), type of net and finally the dimensions of the torus.

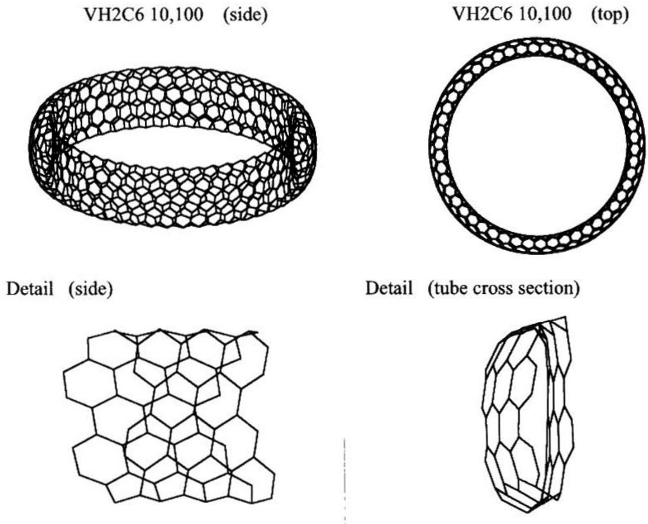

Figure 5. A twisted (chiral) VH*t*C6 lattice.

General formulas for the Hosoya polynomial and Wiener index in tori of VH*t*C6 *c,n* series are:

Case: $(n/2) > 2(c+1)$; $t < c$:

$$\begin{aligned} H(i,x) &= 1 + 3kx^{k}{}_{,k=1,2,\ldots,(c-1)} + [3c - 1 - (c-t)/2]x^{c} + (2c + t - k + 1)x^{(c+k-1)}{}_{,k=2,3,\ldots,t} \\ &+ 2cx^{k}{}_{,k=c+t,c+t+1,\ldots,(n/2-1)} + (2c-1)x^{n/2} + (2c-4k)x^{(n/2+k)}{}_{,k=1,2,\ldots,[(c-t)/2-1]} \\ &+ (t+1)x^{[n/2+(c-t)/2]} \end{aligned} \tag{15}$$

$$W_{(\mathrm{VH}t\mathrm{C6}\;c,n)} = \frac{cn}{2}\left[\sum_{k=1}^{c-1} 3k^2 + [3c-1-(c-t)/2]c + \sum_{k=2}^{t}(2c+t-k+1)(c+k-1) + \right. \\ \left. + \sum_{k=c+t}^{n/2-1} 2ck + (2c-1)n/2 + \sum_{k=1}^{(c-t)/2-1}(2c-4k)(n/2+k)\right] \qquad (16)$$

$$W_{(\mathrm{VH}t\mathrm{C6}\;c,n)} = \frac{cn}{24}\left[c^3 + 3c^2n + 3cn^2 + 3ct^2 + 4t^3 - 3nt^2 - 4c - 4t\right] \qquad (17)$$

Case: $(n/2) > 2(c+1)$; $t = c$.

$$H(i,x) = 1 + 3kx^k{}_{,k=1,2,\ldots,(c-1)} + (3c-1)x^c + (3c-k)x^{(c+k)}{}_{,k=1,2,\ldots,(c-1)} \\ + 2cx^k{}_{,k=2c,2c+1,\ldots,(n/2-1)} + cx^{n/2} \qquad (18)$$

$$W_{(\mathrm{VH},t=c,\mathrm{C6})} = \frac{cn}{2}\left[\sum_{k=1}^{c-1} 3k^2 + (3c-1)c + \sum_{k=1}^{c-1}(3c-k)(c+k) + \sum_{k=2c}^{n/2-1} 2ck + cn/2\right] \qquad (19)$$

$$W_{(\mathrm{VH},t=c,\mathrm{C6})} = \frac{c^2n}{24}(8c^2 + 3n^2 - 8) \qquad (20)$$

NAPHTYLENIC TORI

By analogy to the phenylenic alternant systems[14-16] (with C6, C4, C6, C4,...,C6 sequence), we proposed the naphtylenic systems,[17] with the sequence: C6, C6, C4, C6, C6, C4,..., C6, C6. These systems proved to be stable structures, from the energetic point of vue. One motivation in favour of naphtylenic net was the lower percent of C4 cycles (eventually showing anti-aromatic electronic properties) on the whole structure, in comparison to the phenylenic systems. Fullerenes with four membered cycles have yet been considered.[18] Another reason was a promising liquid phase synthesis of naphtylenic bracelets, tubes and finally tori. Figure 6 illustrates such a lattice.

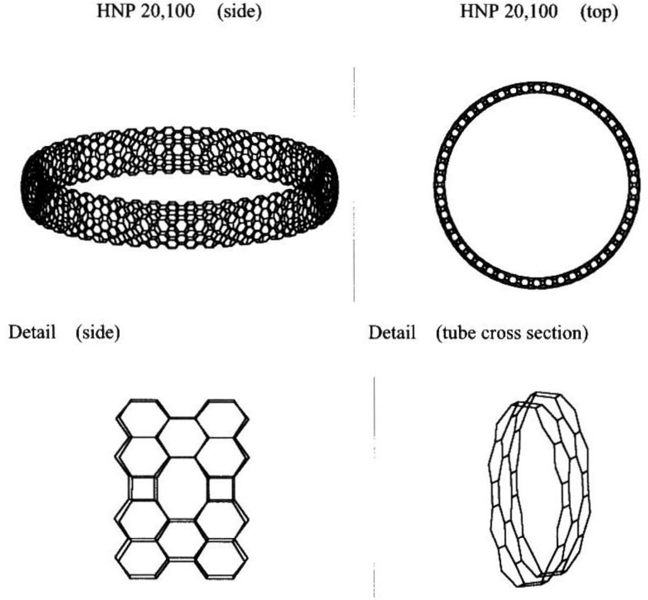

Figure 6. A naphtylenic HNP lattice

Let introduce the difference Hosoya polynomial in a homologous series of graphs (i.e., tori differing by a repeating unit in tube thickness) as:

$$\Delta H(G,x) = H(G_2,x) - H(G_1,x) \tag{21}$$

The polynomial coefficients can be factorised and thus the polynomial can be written as follows:

$$H(G,x) = A\mathbf{TX} \tag{22}$$

with $A = cn/20$ being the factor and **T** the vector (of dimension: $d(G)$) of coefficients. For two subsequent graphs relation (1) can be rewritten as:

$$\Delta H(G,x) = A_2\mathbf{T}_2\mathbf{X} - A_1\mathbf{T}_1\mathbf{X} \tag{23}$$

The vector $\mathbf{T}_2$ can be obtained by adding a (recursive) difference $\mathbf{R}$ to the vector $\mathbf{T}_1$. In naphtylenic tori $T_{c,n,hnp}$ with $c < n$, $c = 5(2m); 5(2m+1)$ and $n = 4p; 4p+2$, the factor A is calculated as follows:

(i) case c_1-even, $c = 5(2m)$: for $n = 4p$, the factor $A_1 = 2mp$ while for $n = 4p+2$ the results is $A_1 = 2mp + m$.

(ii) case c_1-odd, $c = 5(2m+1)$: for n as above, one obtains $A_1 = 2mp + p$ and $A_1 = 2mp + m + p + 1/2$

A_2 can be derived from A_1, by means of a difference ΔA; in our series, always $\Delta A = n/4$. Thus, the difference polynomial can be obtained with relation:

$$\Delta H(G,x) = \left[\mathbf{R}(A_1 + \Delta A) + \Delta A\mathbf{T}_1\right]\mathbf{X} \tag{24}$$

Keeping in mind the above values of A_1 and ΔA, the difference polynomials for the next odd and even terms, respectively, are:

$$\Delta H(G,x)_{odd} = (n/4)\left[(2m+1)\mathbf{R}_{odd} + \mathbf{T}_1\right]\mathbf{X} \tag{25}$$

$$\Delta H(G,x)_{even} = (n/4)\left[(2m+2)\mathbf{R}_{even} + \mathbf{T}_1\right]\mathbf{X} \tag{26}$$

In naphtylenic tori HNP *c,n* with $c < n$, the first two terms: HNP 5,*n* and HNP 10,*n*, and the expressions for both $\mathbf{R}_{odd}$ and $\mathbf{R}_{even}$ are as follows:

$$H(T_{5,n},x) = (cn/20)\begin{bmatrix} 20 + 30x + 56x^2 + 66x^3 + 56x^4 + 54x^5 + 52x^6 + 50x^7 + \\ (52x^{4k+8} + 50x^{4k+9} + 48x^{4k+10} + 50x^{4k+11})_{k=0,..,(y-1)} + Z \end{bmatrix}$$

$$n > 2c; \qquad y = [n - 7 - (1 + n\mathrm{mod}4)]/4 \tag{27}$$

$$Z = 26x^n \text{ (for 0mod4)}; \quad Z = 52x^{n-2} + 50x^{n-1} + 24x^n \text{ (for 2mod4)}$$

$$H(T_{10,n},x) = (cn/20)\begin{bmatrix} 20+30x+56x^2+86x^3+116x^4+136x^5+132x^6+122x^7+112x^8+ \\ 102x^9+(98x^{4k+10}+98x^{4k+11}+102x^{4k+12}+102x^{4k+13})_{k=0,..,(y-1)}+Z \end{bmatrix}$$

$$n > 2c; \qquad y = [n-8-(4-n\bmod 4)]/4$$

$$Z = 98x^{n-2}+98x^{n-1}+76x^n+26x^{n+1}(\text{for } 0\bmod 4);\ Z = 74x^n+24x^{n+1};(\text{for } 2\bmod 4)$$

(28)

$$\begin{aligned} \mathbf{R}_{odd} = {} & 10x^{5m}+40x^{5m+1}+80x^{5m+2}+100x^{5m+3}+100x^{5m+4}+ \\ & \left[100x^{5m+4k+5}+100x^{5m+4k+6}+100x^{5m+4k+7}+100x^{5m+4k+8}\right]_{k=0,..,(m-2)} \\ & 90x^{9m+1}+76x^{9m+2}+66x^{9m+3}+56x^{9m+4}+54x^{9m+5}+52x^{9m+6}+50x^{9m+7}+ \\ & \left[52x^{9m+4k+8}+50x^{9m+4k+9}+48x^{9m+4k+10}+50x^{9m+4k+11}\right]k=0,..,(y-1)+Z \\ & \quad y = [n-8m-7-(1+n\bmod 4)]/4 \\ & Z = 26x^{n+m}\ (\text{for } 0\bmod 4); \quad Z = 52x^{n+m-2}+50x^{n+m-1}+24x^{n+m}\ (\text{for } 2\bmod 4) \end{aligned} \tag{29}$$

$$\begin{aligned} \mathbf{R}_{even} = {} & 20x^{5m+3}+60x^{5m+4}+90x^{5m+5}+100x^{5m+6}+100x^{5m+7}+100x^{5m+8}+ \\ & \left[100x^{5m+4k+9}+100x^{5m+4k+10}+100x^{5m+4k+11}+100x^{5m+4k+12}\right]_{k=0,..,(m-2)} \\ & 92x^{9m+5}+80x^{9m+6}+72x^{9m+7}+60x^{9m+8} \\ & \left[52x^{9m+4k+9}+50x^{9m+4k+10}+48x^{9m+4k+11}+50x^{9m+4k+12}\right]k=0,..,(y-1)+Z \\ & \quad y = [n-8m-7-(1+n\bmod 4)]/4 \\ & Z = 26x^{n+m+1}\ (\text{for } 0\bmod 4); \quad Z = 52x^{n+m-1}+50x^{n+m}+24x^{n+m+1}\ (\text{for } 2\bmod 4) \end{aligned} \tag{30}$$

The Wiener index W is calculated as the first derivative of the Hosoya polynomial, in x = 1 (as mentioned above). According to relations (25) and (26), analytical formulas for the recursive calculation of W, are given in the following:

$$W(\text{HNP } 10,4p) = 2p(512+200p+800p^2) \tag{31}$$

$$W(\text{HNP } 10,4p+2) = (2p+1)(808+1000p+800p^2) \tag{32}$$

$$W(R_{odd\_a}) = 2\cdot(104+480m+200mp+800m^2+400p^2) \tag{33}$$

$$W(R_{odd\_b}) = 2\cdot(202+580m+400p+200mp+800m^2+400p^2) \tag{34}$$

$$W(R_{even\_a}) = 2\cdot(408+1120m+200p+200mp+800m^2+400p^2) \tag{35}$$

$$W(R_{even\_b}) = 2 \cdot (606 + 1220m + 600p + 200mp + 800m^2 + 400p^2) \quad (36)$$

$$\Delta W_{odd\_a} = p[(2m+1)W(R_{odd\_a}) + W(T_{5(2m),4p}) / 2mp] \quad (37)$$

$$\Delta W_{odd\_b} = (p+1/2)[(2m+1)W(R_{odd\_b}) + W(T_{5(2m),(4p+2)}) / (2mp+m)] \quad (38)$$

$$\Delta W_{even\_a} = p[(2m+2)W(R_{even\_a}) + W(T_{5(2m+1),(4p)}) / (2mp+p)] \quad (39)$$

$$\Delta W_{even\_b} = (p+1/2)[(2m+2)W(R_{even\_b}) + W(T_{5(2m+1),(4p+2)}) / (2mp+m+p+1/2)] \quad (40)$$

In the above relations, the subscript a and b refer to the n dimension of tori, being 0 *mod* 4 and 2 *mod* 4, respectively. The distance spectrum for the series HNP 20,n (with only five repeating quadruplets and $d(G,k)$ twice the values in the graph) is given in Figure 7.

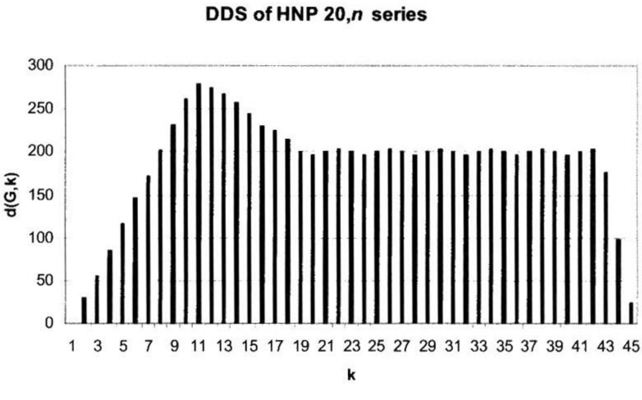

Figure 7. The distance degree spectrum of HNP 20,n tori
(normalised by n)

CONCLUSIONS

The Hosoya polynomial is calculable in toroidal maps with various tiling. Its first derivative (in x = 1) provides the Wiener invariant, with the meaning of the sum of all distances in the graph. The polynomial coefficients can be illustrated as a "distance degree spectrum".

REFERENCES

1. Hosoya, H. On some counting polynomials in chemistry. *Discrete Appl. Math.*, **1988**, *19*, 239-257.
2. Gutman, I.; Klavžar, S.; Petkovšek, M.; Žigert, P. On Hosoya polynomials of benzenoid graphs. *Commun. Math. Chem.* (*MATCH*), **2001**, *43*, 49-66.
3. Stevanović, D. Hosoya polynomial of composite graphs. *Discrete Math.* **2001**, *235*, 237-244.
4. Diudea, M. V.; Graovac, A. Generation and Graph-Theoretical Properties of C_4-Tori. *Commun. Math. Comput. Chem.* (*MATCH*), **2001**, *44*, 93-102.
5. Diudea, M. V.; Silaghi-Dumitrescu, I.; Parv, B. Toranes versus Torenes. *Commun. Math. Comput. Chem.* (*MATCH*), **2001**, *44*, 117-133.
6. Diudea, M. V.; John, P. E. Covering Polyhedral Tori. *Commun. Math. Comput. Chem.* (*MATCH*), **2001**, *44*, 103-116.
7. Diudea, M. V.; Kirby, E. C. The Energetic Stability of Tori and Single-wall Tubes. *Fullerene Sci. Technol.* **2001**, *9*, 445-465.
8. Diudea, M. V.; Silaghi-Dumitrescu, I.; Pârv, B. Toroidal Fullerenes from Square Tiled Tori. *Internet Electronic Journal of Molecular Design.* **2002**, *1*, 10-22.
9. Itoh, S.; Ihara, S. Toroidal forms of graphitic carbon. II. Elongated tori. *Phys. Rev., B*, **1993**, *48*, 8323-8328.
10. Diudea, M. V. Layer Matrices in Molecular Graphs. *J. Chem. Inf. Comput. Sci.*, **1994**, *34*, 1064-1071.
11. Diudea; M. V.; Gutman, I.; Jäntschi, L. *Molecular Topology*. Nova Science, Huntington, New York, 2001.
12. Konstantinova, E. V.; Diudea, M. V. The Wiener polynomial derivatives and other topological indices in chemical research. *Croat. Chem. Acta,* **2000**,*73*, 383-403.
13. Wiener, H. Structural determination of paraffin boiling points. *J. Am. Chem. Soc.*, **1947**, *69*, 17-20.
14. Berris, B. C.; Hovakeemian, G. H.; Lai, Y.-H.; Mestdagh, H.; Vollhardt, K. P. C. A new approach to the construction of biphenylenes by the cobalt-catalyzed cocyclization of o-diethynylbenzenes with alkynes. Application to an iterative approach to [3]phenylene, the first member of a novel class of benzocyclobutadienoid hydrocarbons. *J. Am. Chem. Soc.*, **1985**, *107*, 5670-5687.
15. Gutman, I. Easy method for the calculation of the algebraic structure count of phenylenes. *J. Chem. Soc. Faraday Trans.*, **1993**, *89*, 2413-2416.
16. Gutman, I.; Klavžar, S. A method for calculating Wiener numbers of benzenoid hydrocarbons and phenylenes. *ACH Models Chem.* **1996**, *133*, 389-399.
17. Diudea, M. V. Phenylenic and Naphtylenic Tori. *Fullerene Sci. Technol.* (submitted).
18. Gao, Y. D.; Herndon, W. C. Fullerenes with four-membered rings. *J. Amer. Chem. Soc.* **1993**, *115*, 8459-8460.