communications in mathematical
match
and in computer chemistry

no. 49, September 2003
MATCDY (49) 23- 36 (2003)

ISSN 0340 - 6253

DISTANCE COUNTING IN TORI

Mircea V. Diudea,[1,*] Basil Pârv,[2] Peter E. John[3]
Oleg Ursu,[4] and Ante Graovac[5]

[1]Babeş-Bolyai University, Faculty of Chemistry and Chemical Engineering
Babes-Bolyai University, 3400 Cluj, ROMANIA

[2]Babeş-Bolyai University, Faculty of Mathematics and Computer Science,
Department of Computer Science, Babes-Bolyai University, 3400 Cluj, ROMANIA

[3] Technical University Ilmenau, Institute of Mathematics,
PSF 100565, D-98684 Ilmenau, Germany

[4] Department of Chemistry, Cleveland State University
2121 Euclid Avenue, Cleveland OHIO 44115 USA

[4] The Rudjer Bošković Institute, HR-10002, Zagreb, POB 180, Croatia;
also at Faculty of Science, University of Split,
HR-21000, Split, Croatia

(Received February 7, 2003)

Abstract. Distance counting in closed lattices such as toroids covered by C4C8 and C5C7 faces is presented. Two related ways are considered: (i) counting the Hosoya polynomial, defined as a distance-based increasing power sequence and (ii) counting the Wiener number, the sum of all distances in a graph, available either from the first derivative of the Hosoya polynomial (at $x = 1$), or calculable from the topological distance matrix. Analytical formulas or recursive relations are given.

* Correspondence author: E-mail: diudea@chem.ubbcluj.ro

INTRODUCTION

Distance counting, *i.e.*, the numbering of all the shortest paths joining the vertices of a graph, is one of the most used graph descriptions. A distance-based polynomial was proposed by Hosoya[1] in1988 as:

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

In the above relation, N is the number of vertices in the graph G. $d(G)$ the topological diameter (*i.e.*, the longest topological distance in G) and $d(G,k)$ the number of pairs of vertices lying at distance k of each other. By definition, $d(G,0) = N$ and $d(G,1) = Q$, with Q being the number of edges in G. 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 $H(i,x)$:

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

where $d(i,k)$ is the number of vertices at distance k from the vertex i. Because of doubly counting each path has two endpoints (*i.e.*, each path is counted twice), it is clear that, in a vertex transitive graph, the following relation holds:

$$N \cdot H(i,x) = 2H(G,x) - N \qquad (3)$$

The coefficients of the vertex Hosoya polynomial are just the entries in the LC matrix (*i.e.*, Layer matrix of Counting)[4,5] or the (vertex) Distance Degree Sequence DDS(i) (*i.e.*, the number of vertices lying at distance k form the vertex i).[6] Clearly, the vertex decomposition of $H(G,x)$ would be more complicated in vertex non-transitive graphs (see below).

The first derivative[1,7] of the Hosoya polynomial (at x = 1) enables the calculation of the well-known Wiener[8] number W (*i.e.*, the sum of all distances in G):

$$W(G) = H'(G,1) \qquad (4)$$

Wiener number is accepted as a measure of molecular compactness.[8] It is calculable from the topological distance matrix, as the half sum of its entries.

Formulas for the Hosoya polynomial and Wiener number in polyhex and other tiling tori were published elsewhere.[9,10]

C_4C_8 TOROIDAL LATTICES

A C_4C_8 covering can be derived from a square C_4 covering by deleting appropriate edges.[11-17] (Figure 1).

HC_4C_8 pattern $\qquad$ HC_4C_8 net (expanded)

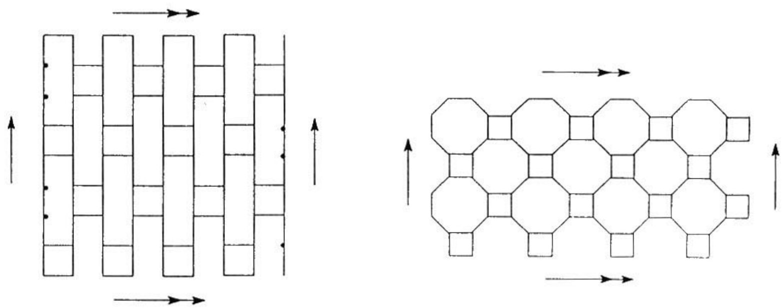


Figure 1. A C_4C_8 pattern, obtained by deleting some horizontal edges from a square C_4 covering.

The cut edge can lay either horizontally or vertically, which results in two embedding isomers However, the net is isotropic. After expanding by a molecular mechanic program, a torus (theoretically obtained by identifying the opposite edges of a quadrilateral) looks like in Figure 2. The first letter in the name of such toroidal object, *e.g.*, $HC_4C_8[c,n]$, represent the type of cutting, followed by the type of pattern (sequence and size of the covering polygons). The numbers in brackets represent the dimensions of the toroidal net: the first is the number of points (*i. e.*, atoms) on the tube cross-section while the second one is the number of slides around the large hollow of torus. The number of atoms contained by such an object is $c \times n$.

According to the building procedure, the $HC_4C_8[c,n]$ isomer contains, on dimension "c", half of the number of C_4C_8 pairs in $C_4C_8[c,n]$. Conversely, on dimension "n", $HC_4C_8[c,n]$ contains twice the number of such pairs in the $VC_4C_8[c,n]$ isomer.

$HC_4C_8[20,100]$ $VC_4C_8[20,100]$

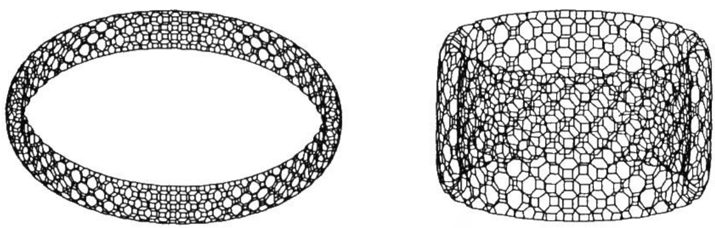


Figure 2. The two cut-embedding isomers of $C_4C_8[20,100]$, on 20x100 atoms.

DISTANCE COUNTING IN C_4C_8 TORI

General formulas for the Hosoya polynomial and Wiener index in tori $C_4C_8[c,n]$ of both H- and V-series are given in the following. Several cases can be delimited:

Tori HC_4C_8 $[c,n]$, $\mathrm{mod}(c,4) = 0$.

(1) Case: $c < n$; true HC_4C_8 $[c,n]$ torus, $c = 4p$; $n = 2r$

$$\begin{aligned} H(i,x) = 1 + m_k x^k{}_{,k=1,\ldots,(2p-1)} + (m_{2p} - 1)x^{2p} + (m_{(2p+k)} - 4k)x^{(2p+k)}{}_{,k=1,\ldots,(p-1)} \\ + 4px^k{}_{,k=3p,\ldots,(2r-1)} + (4p-1)x^{2r} + (4p-4k)x^{(2r+k)}{}_{,k=1,\ldots,(p-1)} + x^{(2r+p)} \end{aligned} \tag{5}$$

$$\begin{aligned} W_{HC4C8[4p,2r]} = 4pr\Bigg[\sum_{k=1}^{2p-1} m_k k + (m_{2p} - 1)2p + \sum_{k=1}^{p-1}(m_{(2p+k)} - 4k)(2p+k) + \sum_{k=3p}^{2r-1} 4pk \\ + (4p-1)2r + \sum_{k=1}^{p-1}(4p-4k)(2r+k) + (p+2r)\Bigg] \end{aligned} \tag{6}$$

where m_k is defined by the following recursion:

$$\begin{aligned} & m_0 = 0;\ m_1 = 3;\ m_2 = 5, \quad and \\ & m_k = m_{\left(\frac{k-\mathrm{mod}(k,2)}{2}+1\right)} + m_{\left(\frac{k+\mathrm{mod}(k,2)}{2}-1\right)} = m_{\left\lfloor \frac{k+2}{2} \right\rfloor} + m_{\left\lfloor \frac{k-1}{2} \right\rfloor} \end{aligned} \tag{7}$$

with $\lfloor x \rfloor$ being the greatest integer part of a real number x.

or, for $k = 3s + t$, $and\ t = 0, 1, 2$,

$$m_k = \frac{2 \cdot 3^{1/2} \sin\left(2k\frac{\pi}{3}\right)}{9} + 8k/3 = 8s + \begin{cases} 0, if\ t = 0 \\ 3, if\ t = 1 \\ 5, if\ t = 2 \end{cases} \tag{8}$$

With (8), recursion (7) becomes:

$$m_k = 8[(k - \mathrm{mod}(k,3))/3] + 3\,\mathrm{mod}(k,3)(2 - \mathrm{mod}(k,3)) - [(1 - \mathrm{mod}(k,3))(5\,\mathrm{mod}(k,3)/2] \tag{9}$$

Expansion of relation (6) leads to the formula:

$$W(HC_4C_8[4p,2r]) = \frac{16}{3}p^2 r(p^2 + 6r^2 + 3pr - 1) \tag{10}$$

which can be translated to c, n dimensions as:

$$W(HC_4C_8[c,n]) = c^2 n(c^2 + 24n^2 + 6cn - 16)/96 \tag{10'}$$

(2) Case: $c = n$; HC_4C_8 [c,c] = VC_4C_8 [c,c], or HC_4C_8 [$4p,4p$] = VC_4C_8 [$4p,4p$].

$$\begin{aligned} H(i,x) = 1 + m_k x^k{}_{,k=1,\ldots,(2p-1)} + (m_{2p} - 1)x^{2p} + (m_{(2p+k)} - 4k)x^{(2p+k)}{}_{,k=1,\ldots,(p-1)} \\ + 4px^k{}_{,k=3p,\ldots,(4p-1)} + (4p-1)x^{4p} + (4p-4k)x^{(4p+k)}{}_{,k=1,\ldots,(p-1)} + x^{5p} \end{aligned} \tag{11}$$

The summation of the corresponding terms, after appropriate handling, leads to the following simple relation for the Wiener index:

$$W(p) = \frac{32}{3}p^3(31p^2 - 1) \tag{12}$$

or

$$W(c) = c^3(31c^2 - 16)/96 \tag{12'}$$

(3) Case: $c > n$; HC_4C_8 [c,n]; this case turns to VC_4C_8 [n,c]

Tori VC_4C_8 [*c*,*n*]; mod(*n*,4) = 0; *c* = 2*p*; *n* = 4*r*.

(1) Case: $2p < 4r < 4p$. Two additional parameters are needed:

$$d = 3r - 2p \quad (13)$$

$$s = |2p - 2r| \quad (14)$$

Case: $d < 0$

$$H(i,x) = 1 + m_k x^k{}_{,k=1,...,(2r-1)} + (m_{2r} - 1)x^{2r} + (m_{(2r+k)} - 4k)x^{(2r+k)}{}_{,k=1,...,(r-1)} \\ + n \cdot x^k{}_{,k=3r,...,(2p-1)} + (4r-1)x^{2p} + (4r-4k)x^{(2p+k)}{}_{,k=1,...,(r-1)} + x^{(2p+r)} \quad (15)$$

Case: $d > 0$

$$H(i,x) = 1 + m_k \cdot x^k{}_{,k=1,...,(2r-1)} + (m_{2r} - 1) \cdot x^{2r} + (m_{(2r+k)} - 4k) \cdot x^{(2r+k)}{}_{,k=1,...,(2p-2r-1)} \\ + (m_{2p} - (4s+1)) \cdot x^{2p} + (m_{(2p+k)} - 4(s+2k)) \cdot x^{(2p+k)}{}_{,k=1,...,d} \\ + (4r-4k) \cdot x^{(2p+k)}{}_{,k=(d+1),...,(r-1)} + x^{(2p+r)} \quad (16)$$

(2) Case: $n = 2c$.

$$H(i,x) = 1 + m_k x^k{}_{,k=1,...,(2p-1)} + (m_{2p} - 2)x^{2p} + (m_{(2p+k)} - 8k)x^{(2p+k)}{}_{,k=1,...,(p-1)} + x^{3p} \quad (17)$$

The Wiener index corresponding to relation (17) is:

$$W(p) = \frac{p^3}{6}(436p^2 - 19) \quad (18)$$

$$W(c) = 2c^3(109c^2 - 16)/96 \quad (18')$$

(3) Case: $4p < 4r < 6p$. The additional d parameter is of the form:

$$d = 3p - 2r \quad (19)$$

while s is the same as in (14).

$$H(i,x) = 1 + m_k \cdot x^k{}_{,k=1,...,(2p-1)} + (m_{2p} - 1) \cdot x^{2p} + (m_{(2p+k)} - 4k) \cdot x^{(2p+k)}{}_{,k=1,...,(2r-2p-1)}$$
$$+ (m_{2r} - (4s+1)) \cdot x^{2r} + (m_{(2r+k)} - 4(s+2k)) \cdot x^{(2r+k)}{}_{,k=1,...,d}$$
$$+ (4r - 4k) \cdot x^{(3p+k)}{}_{,k=1,...,(r-1)} + x^{(p+2r)} \qquad (20)$$

(4) Case: $6p \le 4r$; true VC_4C_8 [$2p,4r$] torus.

$$H(i,x) = 1 + m_k x^k{}_{,k=1,...,(2p-1)} + (m_{2p} - 1)x^{2p} + (m_{(2p+k)} - 4k)x^{(2p+k)}{}_{,k=1,...,(p-1)}$$
$$+ 4x^k{}_{,k=3p,...,(2r-1)} + (4p-1)x^{2r} + (4p - 4k)x^{(2r+k)}{}_{,k=1,...,(p-1)} + x^{(p+2r)} \qquad (21)$$

$$W_{VC4C8[2p,4r]} = 4pr\left[\sum_{k=1}^{2p-1} m_k k + (m_{2p} - 1)2p + \sum_{k=1}^{p-1}(m_{(2p+k)} - 4k)(2p+k) + \sum_{k=3p}^{2r-1} 4pk\right.$$
$$\left. + (4p-1)2r + \sum_{k=1}^{p-1}(4p - 4k)(2r+k) + (p+2r)\ \right] \qquad (22)$$

By developing (22) results in the formulas:

$$W(HC_4C_8[2p,4r]) = \frac{16}{3} p^2 r(p^2 + 6r^2 + 3pr - 1) \qquad (23)$$

$$W(VC_4C_8\,[c,n]) = c^2 n(2c^2 + 3n^2 + 3cn - 8)/24 \qquad (23')$$

Observe that relations [(6), (22)] and [(10), (23)] are identical. This is a consequence of the isotropy of the C_4C_8 net. In the above, *true torus* means the torus having the number of C_4C_8 pairs around the tube smaller than around the torus. Formulas (10), (23), (10'), and (23') are applicable particularly in true tori. On domains where no close formula is given, the following relations (accounting for the involved embedding isomers) are useful:

$$W(H_{C4C8}[c,n]) = W(V_{C4C8}[c/2,2n]) \qquad (24)$$

$$W(V_{C4C8}[c,n]) = W(H_{C4C8}[2c,n/2]) = W(V_{C4C8}[n/2,2c]) \qquad (25)$$

Always an equivalent torus will be found, to verify the true result (see Table 1).

Table 1 gives examples of Wiener index calculation, along with some of the equivalent tori.

Table1. Wiener index in C_4C_8 tori

Torus	W	[p,r]	Equivalent torus
$HC_4C_8[12,12]$	80,064	[3,6]	$VC_4C_8[12,12]$* $VC_4C_8[6,24]$
$HC_4C_8[12,14]$	122,640	[3,7]	$VC_4C_8[6,28]$
$HC_4C_8[12,16]$	178,176	[3,8]	$VC_4C_8[6,32]$
$HC_4C_8[12,24]$	564,480	[3,12]	$VC_4C_8[6,48]$
$HC_4C_8[24,6]$*	80,064	[3,6]	$VC_4C_8[6,24]$
$HC_4C_8[24,8]$*	155,136	[4,6]	$VC_4C_8[8,24]$
$HC_4C_8[24,10]$*	264,000	[5,6]	$VC_4C_8[10,24]$
$HC_4C_8[24,12]$*	413,568	[6,6]	$VC_4C_8[12,24]$
$VC_4C_8[12,12]$*	80,064	[3,6]	$VC_4C_8[6,24]$
$VC_4C_8[12,20]$	264,000	[6,5]	$VC_4C_8[10,24]$
$VC_4C_8[16,20]$*	563,200	[5,8]	$VC_4C_8[10,32]$
$VC_4C_8[16,24]$*	864,768	[6,8]	$VC_4C_8[12,32]$
$VC_4C_8[16,28]$	1,254,400	[7,8]	$VC_4C_8[14,32]$
$VC_4C_8[16,32]$	1,744,896	[8,8]	$VC_4C_8[16,32]$
$VC_4C_8[8,20]$	96,000	[4,5]	$VC_4C_8[10,16]$
$VC_4C_8[8,24]$	155,136	[4,6]	$VC_4C_8[12,16]$*
$VC_4C_8[8,28]$	234,752	[4,7]	$VC_4C_8[14,16]$*
$VC_4C_8[12,36]$	1,180,224	[6,9]	$VC_4C_8[18,24]$*
$VC_4C_8[12,40]$	1,564,800	[6,10]	$VC_4C_8[20,24]$*

* values non-calculable by eqs (10), (23), (10'), and (23')

C_5C_7 TOROIDAL LATTICES

A C_5C_7 covering can be derived from a square C_4 covering by switching and deleting appropriate edges.[11-17] (Figure 3). After a Molecular Mechanics optimisation, a C_5C_7 torus looks

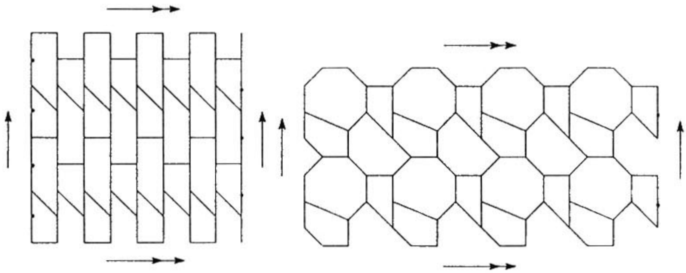


Figure 3. A C_5C_7 azulenic lattice derived from an all-C_4 net

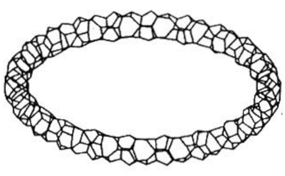
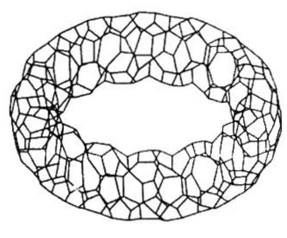
$HC_5C_7[8,44]$ $2 \times 44 = 88$ C_5C_7 pairs	$VC_5C_7[6,56]$ $6 \times 14 = 84$ C_5C_7 pairs
	

Figure 4. Optimised azulenic tori.

as in Figure 4. By reasons of energetic stability (discussed elsewhere[18]) we restrict here our considerations only to the $HC_5C_7[c,n]$ tori.

In HC_5C_7 $[c,n]$ tori, each C_5C_7 pair takes exactly four squares in the parent all-C_4 net, so that $c/4$ such pairs lie around the tube (see Figure 4). The n-dimension is, in this case, preserved. Conversely, in VC_5C_7 $[c,n]$ tori, the constant dimension is c, while the number of pairs around the torus equals $n/4$. The number of atoms is again $c \times n$.

A pentaheptite net can also be drawn by means of the Stone-Wales transformation of a hexagonal net.[19]

We were not able to find neither a closed formula nor a recursion for calculating the Wiener index in C_5C_7 tori. We have succeeded, however, to find an approximate solution, only for the series $HC_5C_7[c,n]$:

$$W(HC_5C_7[c,n]) = (cn/8)(\Delta_W + 2cn^2) \tag{26}$$

with the increment Δ_W :

$$\Delta_W = 0.3369 \cdot c^{3.0593} \tag{27}$$

Relation (27) was obtained in a regression equation, with $R^2 = 0.9999$.

Table 2 lists some W values for HC_5C_7 $[c,n]$ tori, mostly for the HC_5C_7 $[8,n]$. This choice is justified by the excellent correlation of log(W) with the Extended Huckel Theory EHT energy (in a.u.), as shown in Figure 5.

Table 2. Wiener index W in HC_5C_7 $[c,n]$ tori

c	n	W	c	n	W
8	22	174614	8	62	3825214
8	24	225816	8	64	4206656
8	26	286234	8	66	4612674
8	28	356636	8	68	5044036
8	30	437790	8	70	5501510
8	32	530464	8	72	5985864
8	34	635426	8	74	6497866

Table 2. (continued)

8	36	753444	8	76	7038284
8	38	885286	8	78	7607886
8	40	1031720	8	80	8207440
8	42	1193514	8	82	8837714
8	44	1371436	8	84	9499476
8	46	1566254	8	86	10193494
8	48	1778736	8	88	10920536
8	50	2009650	8	90	11681370
8	52	2259764	8	92	12476764
8	54	2529846	8	94	13307486
8	56	2820664	8	96	14174304
8	58	3132986	8	98	15077986
8	60	3467580	8	100	16019300
12	20	308520	16	20	574640
12	24	522288	16	24	962400
12	32	1212480	16	32	2201984

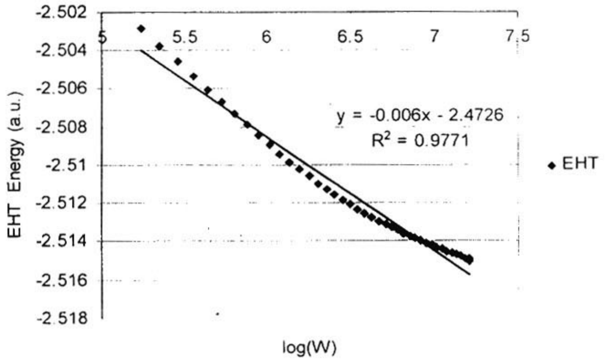


Figure 5. Plot of EHT energy *vs.* log(W)

CONCLUSIONS

The Hosoya polynomial is calculable in toroidal maps with various tiling. Its first derivative (at x = 1) provides the Wiener index, with the meaning of the sum of all distances in the graph. Wiener index was shown to correlate with EHT energy in HC_5C_7 [8,*n*] tori .

Acknwledgement. This paper is supported by the Romanian GRANT 2003. One author (M.V.D.) is grateful to DAAD for a 2002 felowship.

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. *MATCH - Commun. Math. Chem.*, **2001**, *43*, 49-66.
3. Stevanović, D. Hosoya polynomial of composite graphs. *Discrete Math.*, **2001**, *235*, 237-244.
4. Diudea, M. V. Layer Matrices in Molecular Graphs. *J. Chem. Inf. Comput. Sci.*, **1994**, *34*, 1064-1071.
5. Diudea, M. V.; Ursu O. Layer matrices and distance propety descriptors. *Indian J. Chem. A*, (in press).
6. Diudea; M. V.; Gutman, I.; Jäntschi, L. *Molecular Topology*. Nova Science, Huntington, New York, 2001.
7. Konstantinova, E. V.; Diudea, M. V. The Wiener polynomial derivatives and other topological indices in chemical research. *Croat. Chem. Acta,* 2000,*73*, 383-403.
8. Wiener, H. Structural determination of paraffin boiling points. *J. Am. Chem. Soc.*, **1947**, *69*, 17-20.
9. Diudea, M. V. Hosoya polynomial in tori. *MATCH - Commun. Math. Comput. Chem.*, **2002**, *45*, 109-122.
10. Diudea, M. V. Topology of naphthylenic tori. *Phys. Chem. Chem. Phys.*, **2002**, *4*, 4740-4746.
11. Diudea, M. V.; Graovac, A. Generation and graph-theoretical properties of C_4-tori. *MATCH - Commun. Math. Comput. Chem.*, **2001**, *44*, 93-102.

12. Diudea, M. V.; Silaghi-Dumitrescu, I.; Parv, B. Toranes versus torenes. *MATCH Commun. Math. Comput. Chem.*, **2001**, *44*, 117-133.

13. Diudea, M. V.; John, P. E. Covering polyhedral tori. *MATCH - Commun. Math. Comput. Chem.*, **2001**, *44*, 103-116.

14. Diudea, M. V.; Kirby, E. C. The energetic stability of tori and single-wall tubes. *Fullerene Sci. Technol.*, **2001**, *9*, 445-465.

15. Diudea, M. V.; Silaghi-Dumitrescu, I.; Pârv, B. Toroidal fullerenes from square tiled tori. *Internet Electronic Journal of Molecular Design*, **2002**, *1*, 10-22.

16. Diudea, M. V. Phenylenic and naphthylenic tori. *Fullerenes, Nanotubes Carbon Nanostruct.*, **2002**, *10*, 273-292

17. Diudea, M. V. Graphenes from 4-valent tori. *Bull. Chem. Soc. Japan*, **2002**, *75*, 487-492.

18. Diudea, M. V.; Parv, B.; Kirby, E. C. Azulenic tori. *MATCH – Commun. Math. Comput. Chem.*, **2003**, *47*, 53-70.

19. Deza, M.; Fowler, P. W.; Shtogrin, M.; Vietze, K. Pentaheptite modifications of the graphite sheet. *J. Chem. Inf. Comput. Sci.*, **2000**, *40*, 1325-1332