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GENERATION AND GRAPH-THEORETICAL PROPERTIES OF C_4-TORI

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Abstract. Toroidal networks are generated as rotagraphs and some of their graph theoretical properties are described.

INTRODUCTION

Numerical characterisation of cyclic molecular structures is a task more difficult in comparison to the evaluation, say, of distances in acyclic compounds. The difficulty is due to the existence of more than one way for joining two points, i and j. Some works in this respect the reader can consult refs. [1-3] We limit here to the distance-related *detour* and *Cluj-detour* descriptors, the introduction of which needs some graph theoretical background.[4]

Let $G = (V, E)$ be a connected graph, with $|V|$ vertices

and $|E|$ edges. A *walk* w is an alternating string of vertices and edges: $w_{1,n} = (v_1, e_1, v_2, e_2, ..., v_{n-1}, e_m, v_n)$, $(v_{i-1}, v_i) \in E(G)$ and $m \geq n - 1$.

Set $V(w_{1,n}) = \{v_1, v_2, ..., v_{n-1}, v_n\}$ the vertex set and $E(w_{1,n}) = \{e_1, e_2, ..., e_{m-1}, e_m\}$ the edge set of the walk $w_{1,n}$.

Dedicated to Professor A. T. Balaban on his 70[th] anniversary, in appreciation of his bright contribution to Chemical Graph Theory.

The *length* of a walk, $l(w_{1,n}) = |E(w_{1,n})| \geq |V(w_{1,n})| - 1$, equals the number of its traversed edges. Revisiting of vertices and edges is allowed. The walk is *closed* if $v_1 = v_n$ and is *open* otherwise.

A *path* p is a walk having all its vertices and edges distinct: $v_i \neq v_j$, $(v_{i-1}, v_i) \neq (v_{j-1}, v_j)$ for any $1 \leq i < j \leq n$.

As a consequence, revisiting of vertices and edges, as well as branching, is prohibited. The *length* of a path is $l(p_{1,n}) = |E(p_{1,n})| = |V(p_{1,n})| - 1$. A closed path is a *cycle* (*circuit*).

A *terminal path* $tp_{1,n}$ is the path $p = v_1, e_1, v_2, ..., v_n$ that *is no more a path* for any added vertex $v_k \in V(G)$ such that $(v_n, v_k) \in E$.

A path is *Hamiltonian* if $n = |V(G)|$. A Hamiltonian path visits once all the vertices in G. If such a path is a closed one, then it is a *Hamiltonian circuit.*

The *distance*, d_{ij}, is the length of a *shortest* path joining vertices v_i and v_j :

$d_{ij} = min\ l(p_{ij})$; otherwise $d_{ij} = \infty$. The *set of all distances* (i.e., geodesics) in G is denoted by $D(G)$.

The *detour*, δ_{ij}, is the length of a *longest* path between vertices v_i and v_j :

$\delta_{ij} = max\ l(p_{ij})$; otherwise $\delta_{ij} = \infty$. The *set of all detours* in G is denoted by $\Delta(G)$. The square array that collects the detours in a graph is called the *detour* matrix Δ: [5-11]

$$[\Delta]_{ij} = \begin{cases} e_p & ; \ l(p_{ij}) = \max \quad if\ i \neq j \\ 0 & if\ i = j \end{cases} \tag{1}$$

where e_p is the number of edges separating the vertices i and j on the longest path $p_{i,j}$.

The *Cluj Fragments* CF [12-14] represents the set of vertices defined by relation:

$$CF_{i,j,p} = \{v | v \in V(G)\, ;\, d(G_p)_{v,i} < d(G_p)_{v,j}\ ;\ p \in \Delta(G)\} \tag{2}$$

where $G_p = G - p$ is the spanning subgraph resulted from G by deleting the path p_{ij} (except its endpoints), $d(G_p)$ denotes the topological distance measured in G_p, and $\Delta(G)$ has the above mentioned meaning.

The set $CF_{i,j,p}$ represents connected subgraphs (i.e., fragments) in G, referred to i and related to j and path p.

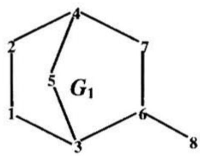
In the above definition (eq 2) the *path* p plays a central role in selecting the fragments. In cycle-containing graphs, more than one path could join the pair (i,j) thus resulting more than one fragment referred to i, so that we define the nondiagonal entries $[\mathbf{UM}]_{ij}$ in the Cluj matrix as the maximum cardinality of the sets defined by eq 2

$$[\mathbf{UM}]_{i,j} = \max_{p} \left| CF_{i,j,p} \right| \tag{3}$$

where $\mathbf{M} = \mathbf{CF\Delta}$ (Cluj-Fragmental-Detour). The diagonal entries are zero. When $p \in D(G)$, a similar definition leads to **CFD** (Cluj-Fragmental-Distance) matrix. The above definitions hold for any connected graph. The Cluj matrices are square arrays, of dimension **N** x **N**, usually *unsymmetrical* (excepting some symmetric regular graphs).

In trees, **CFΔ** and **CFD**, are identical, due to the uniqueness of the path joining the pair (i,j).

Figure 1 illustrates the construction of **CFΔ** matrix.



CFΔ(G_1)

	1	2	3	4	5	6	7	8
1	0	1	1	1	1	2	1	2
2	1	0	1	1	1	1	2	1
3	2	2	0	3	**4**	2	2	2
4	2	2	2	0	4	2	2	3
5	1	1	1	1	0	1	1	1
6	3	2	2	2	2	0	2	7
7	1	3	1	1	1	1	0	1
8	1	1	1	1	1	1	1	0

FIGURE 1. Construction of Cluj-Fragmental-Detour matrix

An interesting property is shown by the matrix **CFΔ**. Let consider the vertices 8 (of degree 1) and 5 (of degree 2) in G_1, Figure 1. The vertex 8 is an *external* vertex (with a terminal path ending in it) while the vertex 5 is an *internal* one (usually a terminal path not ending in it). An external vertex, like 8, shows all its entries in Cluj matrix equal to 1 (see Figure 1). The same entries are shown by the internal vertex 5. This unusual property is called *the internal ending of all detours* joining a vertex i and the remaining vertices in G. Such a vertex is called an *internal endpoint.* [12] There exist graphs with all the vertices internal endpoints. As a consequence, their detours are *Hamiltonian paths*. This kind of graph we call *full Hamiltonian detour graph, FHΔ*.[12] As a consequence, the index calculated as the half sum of entries in the symmetrized **CFΔ** matrix, $I(CF\Delta)$ reaches its minimum value:

$$I(CF\Delta) = \binom{v}{2} = \min = H\Delta \qquad (4)$$

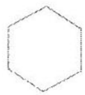
Thus, $I(CF\Delta)$ counts in $FH\Delta$ just the number of all vertex pairs, therein joined by Hamiltonian detours. A related property is shown by the detour matrix.[3,15] There exist *detour saturated graphs*, for which the elements of the detour matrix are maximal. It comes out that their detour index is maximal among the graphs of the same size. Such graphs show the same detour matrix as that of the complete graph having the same number of vertices and, of course, the maximal longest paths are Hamiltonian paths.

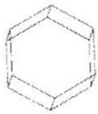
RESULTS AND DISCUSSION

In a previous paper, Diudea *et al.* [12] found that a series of cyclic structures obey a same rule in calculating the parameters given in Table 1: number of vertices v, number of edges e, detour degree sequence ΔDS (i.e., the sequence of number of vertices mutually lying at a given length of detours), detour number w (i.e., the half sum of all entries in the detour matrix), number of Hamiltonian detours $H\Delta$, entry-type in Cluj matrix $[\mathbf{CF\Delta}]_{ij}$ and the index $I(CF\Delta)$.

The series starts by the simple (n-membered) cycles $\mathbf{C}_n$, continues with stripes $\mathbf{S}_n$, goes further

$\mathbf{C}_6$ $\mathbf{S}_6$





to tubes $\mathbf{TU}_{c,n}$ and necessarily reaches the single-wall tori $\mathbf{T}_{c,n}$.

$\mathbf{TU}_{6,12,1,C4}$ $\mathbf{T}_{6,12,1,C4}$

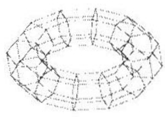


TABLE 1. Structural and Detour Data in Cycles $\mathbf{C}_n$, Stripes $\mathbf{S}_n$ and Tubes $\mathbf{TU}_{c,n}$

Graph	*v*	*e*	*ΔDS*	*W*	*HΔ*	[CFΔ]ij	*I(CFΔ)*
C3	3	3	0.3	6	3	1	3
C4	4	4	0.2.4	16	4	1	6
C5	5	5	0.0.5.5	35	5	1	10
C6	6	6	0.0.3.6.6	63	6	1; 2	24
S3	6	9	0.0.15	75	15	1	15
S4	8	12	0.12.16	184	16	1; 2	64
S5	10	15	0.0.45	405	45	1	45
S6	12	18	0.0.45	696	36	1; 2	156
$TU_{3,3}$	9	15	0.0.36	288	36	1	36
$TU_{3,4}$	12	21	0.0.66	726	66	1	66
$TU_{3,5}$	15	27	0.0.105	1470	105	1	105
$TU_{3,6}$	18	33	0.0.153	2601	153	1	153
$TU_{3,4}$	12	20	0.30.36	696	36	1; 2	156
$TU_{4,4}$	16	28	0.56.64	1744	64	1; 2	288
$TU_{4,5}$	20	36	0.90.100	3520	100	1; 2	460
$TU_{4,6}$	24	44	0.132.144	6216	144	1; 2	672
$TU_{5,3}$	15	25	0.0.105	1470	105	1	105
$TU_{5,4}$	20	35	0.0.190	3610	190	1	190
$TU_{5,5}$	25	45	0.0.300	7200	300	1	300
$TU_{5,6}$	30	55	0.0.435	12615	435	1	435
$TU_{6,3}$	18	30	0.72.81	2529	81	1; 2	369
$TU_{6,4}$	24	42	0.132.144	6216	144	1; 2	672
$TU_{6,5}$	30	54	0.210.225	12405	225	1; 2	1065
$TU_{6,6}$	36	66	0.306.324	21744	324	1; 2	1548

TOROIDAL NETWORK GENERATION

Let k be a point on a circle of radius R and copy its image n times by moving it around the circle. Considering both the images and joining edges, an n-membered cyclic graph is thus obtained. Extend now k to a graph G_k and do the same. The resulting graph is a *polygraph* and the circulant G_k is called a monomer graph, by analogy with the chemical polymerisation process. Since the monomer moved on a circle the polygraph is called a *rotagraph* [16] and is symbolised as:

$$\omega_n = \omega_n(G, X) \quad (5)$$

where X is the set of edges joining G_k with its image in position k+1, G_{k+1}. The same can be true for G_{k-1}.

Assume G is of radius $r < R$, and centred on that circle (Figure 2). If at least one point of G is located out of the plane of circle, the rotation object can be enclosed in a toroidal envelope.

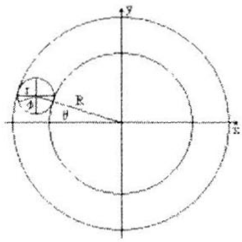


FIGURE 2. Construction of a toroidal surface

A toroidal surface can be drawn by using the well-known relations:

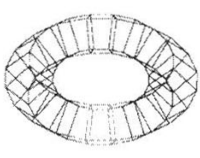
$$x = \cos(\theta)(R + r\cos\varphi) \tag{6}$$
$$y = \sin(\theta)(R + r\cos\varphi)$$
$$z = r\sin\varphi$$

Let $\boldsymbol{G}$ be a $\boldsymbol{c}$-membered cycle, and let $|X| = |V(G)|$. The rotation object is now a polyhedral (single-wall) torus, tiled by quadrilaterals (see the title of paper, that includes C_4 – the square-like boundary of the polyhedral torus). The problem can be shifted from 3D (i.e. generation of a network included in a torus) to 2D: *covering a toroidal surface*.[17] At that stage, the genuine length of r and R is not a matter.

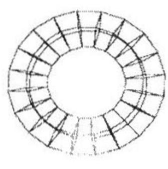
A polyhedral torus is completely defined by two topological parameters: $\boldsymbol{c}$ – membering of the circulant $\boldsymbol{G}$ and $\boldsymbol{n}$ - membering of the large circle (i.e., the number of monomer units). In the symbol thus designed: $\mathbf{T}_{c,n}$ the joining edge set X is omitted (see eq 5). Note that the two parameters can be interchanged. The name of the objects coming through this paper will be complicated, as a necessity to distinguish appearing isomers. The constitutional count will be presented below.

In case of single-wall tori, the vertex degree is 4. When the circulant G is a crown, the resulting rotation object is a double-wall torus. In such a network, each point of a toroidal layer is joined with its image in the neighbour layer. In double layer tori, $\boldsymbol{d}$ = 5 while in multi-layer tori, the network vertices have $\boldsymbol{d}$ = 6. A multi layer torus is symbolised by $\boldsymbol{T}_{c,n,s}$ with s being the number of layers (stratus – in Latin). We stress here that the objects generated by the above procedure, enclosable in a toroidal surface, are regular graphs of degree 4, 5 and 6, respectively. In the following, some mono- and multi-layer tori are illustrated:

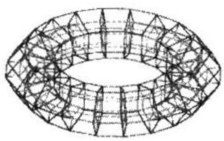
$\mathbf{T}_{4,20,1,C4}$ (a)



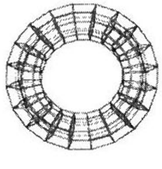
$\mathbf{T}_{4,20,1,C4}$ (b)



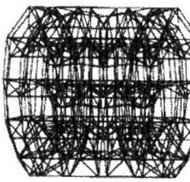
$\mathbf{T}_{5,20,2,C4}$ (a)



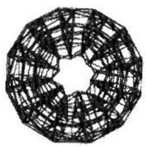
$\mathbf{T}_{5,20,2,C4}$ (b)



$\mathbf{T}_{8,12,3,C4}$ (a)

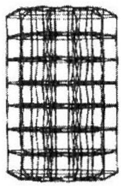


$\mathbf{T}_{8,12,3,C4}$ (b)

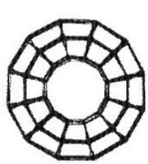


By cutting the joining edges between two images of G the open structure is, of course, a tube:

$\mathbf{TU}_{8,12,3,C4}$ (a)



$\mathbf{TU}_{8,12,3,C4}$ (b)



In studying tori, we limit here to find a basic rule, if any, that allows the calculation of detour-related parameters in toroidal networks and related structures. The rule comes out from the constitutional data:

number of vertices: $\boldsymbol{v(T)} = |V(T)| = \boldsymbol{cns}$

number of edges: $\boldsymbol{e(T)} = |E(T)| = \boldsymbol{cnsd}/2$

In single-wall, ***polyhedral tori*** $\mathbf{T}_{c,n}$ (with s = 1 and $\boldsymbol{d}$ = 4) the following rules hold (Table 2). Tubes and stripes also obey these rules.

TABLE 2. Common properties of tori, tubes and stripes.

Tori (a); c **or** n = ***odd***	**Tori** (b); $\boldsymbol{c}$ or $\boldsymbol{n}$ = *even*
structure is a $FH\Delta$ *graph*	structure is a *next-* $FH\Delta$ *graph*
entries in *Cluj detour matrix* are all **1**	entries in *Cluj detour matrix* are **1** and **2**
Number of Hamiltonian Detours $H\Delta = v(v-1)/2 = \binom{v}{2}$	*Number of Hamiltonian Detours* $H\Delta = (v/2)^2$
Detour Index (i.e., the length of all Hamiltonian detours) $w = H\Delta\,(v-1) = v(v-1)^2/2$	*Detour Index* (i.e., the length of all detours) $w = H\Delta\,(v-1) + (H\Delta - \sqrt{H\Delta})(v-2) = v(2v^2-5v+4)/4$
Cluj Detour Index $I(CF\Delta) = H\Delta = v(v-1)/2$	*Cluj Detour Index* $I(CF\Delta) = H\Delta + 2^2(H\Delta - \sqrt{H\Delta}) = 5H\Delta - 2v = v(5v-8)/4$
Tubes (as resulted form tori)	**Stripes**
v= cn; $\boldsymbol{e}(\mathbf{TU}) = \boldsymbol{cnsd}/2 - \boldsymbol{cs} = \boldsymbol{2cn} - \boldsymbol{c}$	S_n (v = $2n$; e = $3n$)
c = odd; rule (a)	n = *odd;* rule (a)
c = even; rule (b)	n = *even;* rule (b)

At the end, some data for tori are given in Table 3. It can be seen that they are either $FH\Delta$ or -next $FH\Delta$ *graphs.*

TABLE 3. Structural Counts and Detour Parameters in Tori $\mathbf{T}_{c,n}$

Graph	*v*	*E*	*ΔDS*	*w*	*HΔ*	$[CF\Delta]_{ij}$	*I*(CFΔ)
$T_{3,3}$	9	18	0.0.36	288	36	1	36
$T_{3,4}$	12	24	0.0.66	726	66	1	66
$T_{3,5}$	15	30	0.0.105	1470	105	1	105
$T_{3,6}$	18	36	0.0.153	2601	153	1	153
$T_{4,4}$	16	32	0.56.64	1744	64	1; 2	288
$T_{4,5}$	20	40	0.0.190	3610	190	1	190
$T_{4,6}$	24	48	0.132.144	6216	144	1; 2	672
$T_{5,5}$	25	50	0.0.300	7200	300	1	300
$T_{5,6}$	30	60	0.0.435	12615	435	1	435
$T_{6,6}$	36	72	0.306.324	21744	324	1; 2	1548

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