Topological Compression Factors of 2−Dimensional $TUC_4C_8(R)$ Lattices and Tori

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ABSTRACT

We derived explicit formulae for the eccentric connectivity index and Wiener index of 2−dimensional square-octagonal $TUC_4C_8(R)$ lattices with open and closed ends. New compression factors for both indices are also computed in the limit $N\to\infty$.

Keywords: 2−Dimensional square-octagonal lattice; eccentric connectivity index; Wiener index; topological compression factors.

1 INTRODUCTION

A graph G consists of a set of vertices $V(G)$ and a set of edges $E(G)$. If the vertices $u,v\in V(G)$ are connected by an edge e then we write $e = uv$. In chemical graphs, each vertex represents an atom of the molecule, and covalent bonds between atoms are represented by

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the edge between the corresponding vertices. This shape derived from a chemical compound is often called its molecular graph, and can be path, a tree, or in general a graph.

A real number that describes a molecular graph is called a topological index. The first use of a topological index for the correlation of the measured properties of molecules was made in 1947 by chemist Harold Wiener. In that year, he introduced the notion of path number of a graph as the sum of the distances between any two carbon atoms in the molecule, in terms of carbon-carbon bonds [1]. We encourage the interested readers to consult [2,3] for more information about Wiener index of trees and hexagonal systems. Hosoya [4] reformulated the Wiener index in terms of distances between vertices in an arbitrary graph. He defined W as the half-sum of distances between all pairs of vertices of the graph under consideration, $W(G) = \sum_{u>v} d(u,v)$, where $d(u,v)$ is the number of edges in a shortest path connecting the vertices u and v.

For a given vertex u of $V(G)$ its eccentricity $\varepsilon(u)$ is the largest distance between u and any other vertex v of G. The maximum eccentricity over all vertices of G is called the diameter of G and denoted here by $M(G)$ and the minimum eccentricity among the vertices of G is called radius of G and denoted by $R(G)$. The set of vertices whose eccentricity is equal to the radius of G is called the center of G. It is well known that each tree has either one or two vertices in its center. The eccentric connectivity index [5] $\xi(G)$ of a graph G is defined as $\xi(G) = \Sigma_{i\in V(G)} \delta_i \varepsilon_i$ being δ_i the number of bonds of the vertex i. In papers [6−10] the authors applied this topological index to discover some chemico-physical properties of crystallographic materials. In this paper the topological properties of a class of square-octagonal lattices, as well as the corresponding nanotubes are investigated. For more information in this topic we refer to [11−18] and references therein. We also refer to [19−23] for mathematical and physical properties of fullerenes and nanotubes.

2 TOPOLOGICAL CONSTRUCTION OF THE $TUC_4C_8(R)$ LATTICE

The unit (square or rhombic) cell U of the square-octagonal lattice **R** has been chosen having the 4 sites (vertices) represented in Figure 1. This selection allows the generation of the complete 2-dimensional infinite lattice by pure translational operation along both lattice directions. We denote the obtained lattice by $TUC_4C_8(R)$; the lattice obtained from the same basic cell by translating it along lines bisecting its sides is denoted by $TUC_4C_8(S)$. It this paper we consider only $TUC_4C_8(R)$ lattices and tori and denote them by **R** and $\mathbf{R}^C$ respectively.

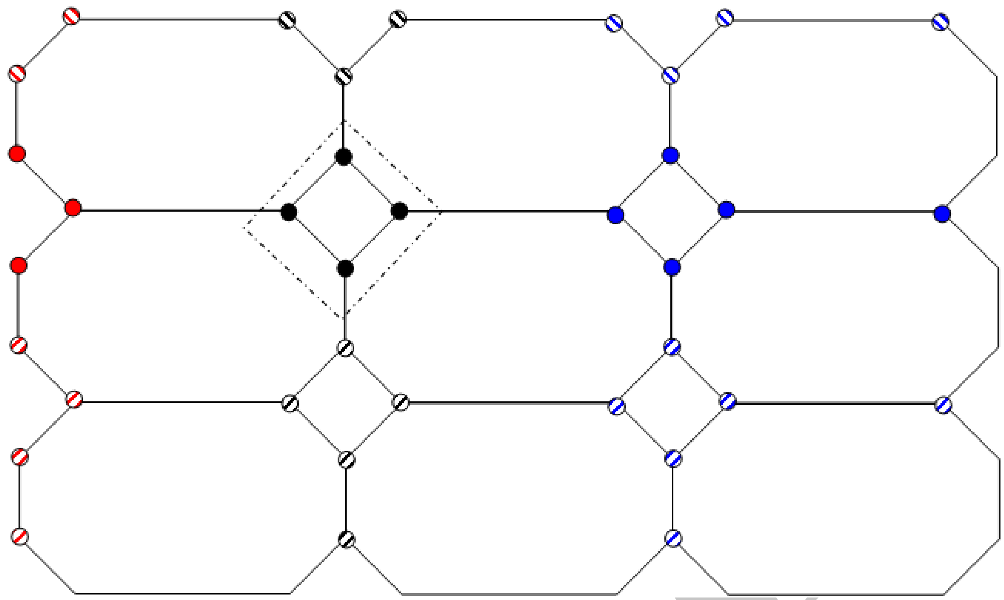

Figure 1. The 4 vertices of the unit cell *U* are depicted in the dashed rectangle. Some other unit cells are shown, also partially generated.

In the simplest case of the lattice with boundary cyclic conditions (closed ends lattice $\mathbf{R}^{\mathbf{C}}$), all vertices are equivalent with valency (degree) equals $\delta_i=3$. $\mathbf{R}^{\mathbf{C}}$ graph is then built by adding an increasing number L of unit cells *U* along both plane directions, to account for $N=4L^2$ graph vertices. The number of edges (chemical bonds) in the lattice is denoted by *B*. The 3−regularity of $\mathbf{R}^{\mathbf{C}}$ connectivity imposes that $B(N)=3/2N$, similar to the well known fullerene case.

For our lattice graph we consider several topological invariants: *W(N),* the Wiener index can be defined as the half of the sum of all distances d_{ij} in the distance matrix *D* of the graph; *M(N),* the largest distance in the graph (diameter); $\underline{w}$ the minimal sum of distances in a row (column) of *D* divided by 2. The vertex (vertices) characterized by $\underline{w}$ are the minimal vertex (vertices) $\underline{v}$ of the graph.

We recall that in a graph on *N* vertices the sum of all local eccentricities multiplied by the corresponding vertex degrees δ_i defines the topological *eccentric connectivity index*:

$$\xi(N)= \Sigma_i \, \varepsilon_i \, \delta_i$$

Previously introduced graph invariants *W, M,* $\underline{w}$*, ξ,* follow polynomial growing laws in $N^{1/2}$ according to the scheme valid for any 2−dimensional lattice:

$$W(N) = a_5N^{5/2} + a_4N^2 + a_3N^{3/2} + a_2N + a_1N^{1/2} + a_0 \quad (1)$$
$$M(N) = b_1N^{1/2} + b_0 \quad (2)$$
$$\underline{w}(N) = d_3N^{3/2} + d_2N + d_1N^{1/2} + d_0 \quad (3)$$
$$\xi(N) = f_3N^{3/2} + f_2N + f_1N^{1/2} + f_0 \quad (4)$$

Leading exponent $s=5/2$ in (1) depends from lattice dimensionality d in the following general relation [3]:

$$s = 2+d^{-1}$$

For the square-octagonal lattice in Figure 1, all coefficients in (1–4) are rational numbers and only depend on topological connectivity of its graph and they are easily numerically interpolated from different values of the quantities at growing N; see Table 1 for the case of $\mathbf{R}^C$ graph. The symmetry of the $\mathbf{R}^C$ graph forces all $\underline{w}(N)$ contributions to $W(N)$ to be equal and therefore we have $W(N)=N\underline{w}(N)$. Moreover, due to the cyclic boundary conditions, the eccentricity ε of any node equals graph diameter M. Being vertex degrees also the same $\delta = 3$ for any graph node, the local contribution to eccentric connectivity index is given by

$$e = \delta\, \varepsilon = 3M, \tag{5}$$

and therefore

$$\xi(N) = Ne(N) = 3NM(N). \tag{6}$$

In Table 1 we present numerical values of graph invariants (1−3,5,6) for $\mathbf{R}^C$ lattices for L=1,3,…,13. Explicit formulae for invariants as functions of N are:

$$W(N) = 7/24\, N^{5/2} -5/12\, N^{3/2} \tag{7}$$
$$M(N) = N^{1/2} -1 \tag{8}$$
$$\underline{w}(N) = 7/24\, N^{3/2} -5/12\, N^{1/2} \tag{9}$$
$$\xi(N) = 3(N^{3/2} - N) \tag{10}$$

The relation (8) for M has exactly the same form of the one for the square closed lattice. In addition, the eccentric connectivity index (10) shows an interesting analogy with the one of the square closed lattice ξ_S that in fact is $\xi_S=4(N^{3/2}–N)$. Having $\delta_S =4$, one may then write it as $\xi_S= \delta_S(N^{3/2}-N)$, that is similar to (10) $\xi= \delta(N^{3/2} - N)$ considering that the square-octagonal lattice has $\delta = 3$, as previously stated. We notice also that for this highly symmetric closed lattice $W(N)=N\underline{w}$

In the limit of large N, the leading term of the topological indices (6) are:

$$\underline{w}^C \to 7/24\, N^{3/2},\ W^C \to 7/24\, N^{5/2},\ \xi^C \to 3N^{3/2} \tag{11}$$

where by superscript C we emphasize the fact that we consider graphs closed on themselves, i.e. those satisfying cyclic boundary conditions. In the next paragraph, we will use the limits (11) to compare them with analogous limits for graphs with open ends to determine the so called *compression ratios* for square-octagonal infinite graphs.

Table 1. Graph Invariants for $\mathbf{R}^C$ Graphs with $N=4L^2$ Vertices.

L	N	M	W	$\underline{w}$	ξ
1	4	1	6	1.5	12
3	36	5	2178	60.5	540
5	100	9	28750	287.5	2700
7	196	13	155722	794.5	7644
9	324	17	548694	1693.5	16524
11	484	21	1498706	3096.5	30492
13	676	25	3458078	5115.5	50700

3 THE CASE OF $TUC_4C_8(R)$ GRAPH WITH OPEN ENDS

The square-octagonal lattice without cyclic boundary conditions we call the square-octagonal lattice (graph) with open ends and denote by ***R.*** The number of edges is readily obtained as $B=3/2N -N^{1/2}$. Again, the interpolation method quickly produces, starting from the values shown in Table 2, the closed forms for all previous topological lattice invariants (1-4):

$$W(N) = 2/5\ N^{5/2} - 2/3\ N^{3/2} + 4/15\ N^{1/2} \tag{12}$$
$$M(N) = 2(N^{1/2} - 1) \tag{13}$$
$$\underline{w}(N) = 7/24\ N^{3/2} - 1/6\ N^{1/2} \tag{14}$$
$$\xi(N) = 19/4\ N^{3/2} - 27/4 N + 2\ N^{1/2} + 1 \tag{15}$$

By inspection of Table 1 and Table 2, one observes that graph diameter *M* just doubles by passing to the open lattice **R**, as it is basically true also for graphenic lattices [23].

We compute now the *topological efficiency index* ρ, a topological invariant introduced recently [22] to measure the graph efficiency in filling the space when compared to its minimal vertex $\underline{v}$ (that, by definiton, may be seen as the most efficient vertex in contributing to graph overall compactness):

$$\rho = W/ N\underline{w} \qquad \text{with} \qquad \rho \geq 1. \tag{16}$$

From Equation (16), we have $\rho = 1$ for $\mathbf{R}^\mathbf{C}$ as in the C_{60} buckyball whereas for the open ends case **R** formulae (12) and (14) allow its exact determination. In the limit of large lattices $N \rightarrow \infty$:

$$\rho(\boldsymbol{R}) \rightarrow 48/35 \approx 1.371\,. \tag{17}$$

The above limit is asymptotically reached in a monotone growth as can be seen from Table 2. It is interesting to note that the open ends square lattice tends in the limit to reach slightly lower ρ value of 4/3 showing therefore an improved way to fill the plane in respect to **R**.

Asymptotic values of the Wiener index and eccentric connectivity index for **R** graphs are given by:

$$\underline{w} \to 7/24\, N^{3/2},\ W \to 2/5\, N^{5/2},\ \xi \to 19/4 N^{3/2}$$

and, by combining this with previously (11) obtained limits for $\mathbf{R}^{\mathbf{C}}$, the asymptotic values of the compression ratios for W and ξ are determined as

$$W^C / W = 35/48$$
$$\xi^C / \xi = 12/19$$

It is worth mentioning that above numerical values of both compression factors also appear in graphene lattices, as recently obtained [23].

Table 2. Graph Invariants for **R** Graphs with $N=L^2$ Vertices.

L	N	M	W	w	ξ	ρ
1	4	2	8	2	16	1
3	36	10	2968	62	796	1,330
5	100	18	39336	290	4096	1,356
7	196	26	213304	798	11740	1,364
9	324	34	751944	1698	25552	1,367
11	484	42	2054360	3102	47356	1,368
13	676	50	4740840	5122	78976	1,369

4 CONCLUSIONS

In the present note it has been demonstrated that the Wiener index, the eccentric connectivity index and other invariants (see Eqs. (1-4)), can be all represented for $d=2$ infinite lattices as polynomials in $N^{1/d}$, where N stands for the number of vertices of the lattice under study.

The asymptotic values of the Wiener index and the eccentric connectivity index for large N are given below for all lattices studied in the present note, compared to the square lattice. The leading coefficient of W is a measure of compactness of a given lattice and, as it should be expected, the lattices have to be ordered as shown below, from the most compact to the less compact. Square lattices show the largest topological efficiency for both cases, closed ends $\mathbf{S}^{\mathbf{C}}$ and open ends **S** infinite structures, as previously noticed in comment on values of topological efficiency index (17) for **R.**

Lattice type	*W(N)*	*ξ(N)*
S^C	$1/4\ N^{5/2}$	$4N^{3/2}$
R^C	$7/24N^{5/2}$	$3N^{3/2}$
S	$1/3N^{5/2}$	$6N^{3/2}$
R	$2/5N^{5/2}$	$19/4N^{3/2}$

Future computation will be done in comparing other bidimensional infinite structures.

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REFERENCES

1. Wiener H., Structural determination of the paraffin boiling points, *J. Am. Chem. Soc.*, **69** (1947) 17–20
2. Dobrynin A. A., Entringer R., Gutman I., Wiener index of trees: theory and applications, *Acta Appl. Math.*, **66** (2001) 211–249.
3. Dobrynin A. A., Gutman I., Klavžar S., Žigert P., Wiener index of hexagonal systems, *Acta Appl. Math.*, **72** (2002) 247–294.
4. Hosoya H., Topological index, a newly proposed quantity characterizing the topological nature of structure isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.,* **44** (1971) 2332–2339.
5. Sharma V., Goswami R., Madan A. K., Eccentric connectivity index: a novel highly discriminating topological descriptor for structure-property and structure-activity studies, *J. Chem. Inf. Comput. Sci.,* **37** (1997) 273–282.
6. Dureja H., Madan A. K., Superaugmented eccentric connectivity indices: new-generation highly discriminating topological descriptors for QSAR/QSPR modeling, *Med. Chem. Res.,* **16** (2007) 331–341.
7. Kumar V., Sardana S., Madan A. K., Predicting anti-HIV activity of 2,3-diary l-1,3-thiazolidin-4-ones: computational approaches using reformed eccentric connectivity index, *J. Mol. Model.*, **10** (2004) 399–407.
8. Ashrafi A. R., Došlić T., Saheli M., The eccentric connectivity index of TUC4C8(R) nanotubes, *MATCH Commun. Math. Comput. Chem.,* **65** (2011) 221–230.
9. Došlić T., Graovac A., Ori O., Eccentric connectivity index of hexagonal belts and chains, *MATCH Commun. Math. Comput. Chem.*, **65** (2011) 745–752.

10. Došlić T., Saheli M., Vukičević D., Eccentric connectivity index: extremal graphs and values, *Iranian J. Math. Chem.,* **1** (2010) 45−55.
11. John P. E., Diudea M. V., Wiener index of zig-zag polyhex nanotubes, *Croat. Chem. Acta,* **77** (2004) 127−132.
12. Diudea M. V., Stefu M., Pârv B., John P. E., Wiener index of armchair polyhex nanotubes, *Croat. Chem. Acta,* **77** (2004) 111−115.
13. Diudea M. V., Pârv B., Kirby E. C., Azulenic tori, *MATCH Commun. Math. Comput. Chem.*, **47** (2003) 53−70.
14. Diudea M. V., Toroidal graphenes from 4-valent tori, *Bull. Chem. Soc. Jpn.*, **75** (2002) 487–492.
15. Yousefi S., Ashrafi A. R., An exact expression for the Wiener index of a TUC4C8(R) nanotorus, *J. Math. Chem.*, **42** (2007) 1031−1039.
16. Yousefi S., Ashrafi A. R., An algorithm for constructing Wiener matrix of TUC4C8(R) nanotubes, *Current Nanosci.*, **4** (2008) 161−165.
17. Iranmanesh A., Ashrafi A. R., Balaban index of an armchair polyhex, TUC4C8(R) and TUC4C8(S) nanotorus, *J. Comput. Theoret. Nanosci.*, **4** (2007) 514−517.
18. Ashrafi A. R., Loghman A., Computing Padmakar-Ivan index of a TC4C8(R) nanotorus, *J. Comput. Theoret. Nanosci.*, **5** (2008) 1431−1434.
19. Cataldo F., Graovac A., Ori O., Wiener index of 1-pentagon fullerenic infinite lattice, *Int. J. Chem. Modeling.*, **2** (2010) 165−180.
20. Alipour M. A., Ashrafi A. R., A numerical method for computing the Wiener index of one-heptagonal carbon nanocone, *J. Comput. Theor. Nanosci.*, **6** (2009) 1204–1207.
21. Graovac A., Gutman I., Trinajstić N., *Topological approach to the chemistry of conjugated molecules*, Springer Verlag, Berlin, 1977.
22. Cataldo F., Ori O., Iglesias−Groth S., Topological lattice descriptors of graphene sheets with fullerene-like nanostructures, *Molecular Simulation*, **36** (2010) 341–353.
23. Cataldo F., Ori O., Graovac A., Graphene topological modifications, *Int. J. Chem. Modeling.*, **3** (2010) 45−64.