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Wiener Way to Dimensionality

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ABSTRACT

This note introduces a new general conjecture correlating the dimensionality d_T of an infinite lattice with N nodes to the asymptotic value of its Wiener Index $W(N)$. In the limit of large N the general asymptotic behavior $W(N) \approx N^s$ is proposed, where the exponent s and d_T are related by the conjectured formula $s=2+1/d_T$ allowing a new definition of dimensionality $d_W=(s-2)^{-1}$. Being related to the topological Wiener index, d_W is therefore called Wiener dimensionality. Successful applications of this method to various infinite lattices (like graphene, nanocones, Sierpinski fractal triangle and carpet) testify the validity of the conjecture for infinite lattices.

Keywords: Wiener dimensionality, Sierpinski fractals, asymptotic Wiener index.

1 INTRODUCTION

The Wiener index $W(N)$ of a lattice (or graph) with N vertices is the topological invariant defined as the half–sum of its chemical distances d_{ij}:

$$W(N) = \frac{1}{2}\sum_{ij} d_{ij} \quad with\ i, j = 1,...,N;\ \ d_{ii} = 0. \tag{1}$$

This topological invariant measures in practice the compactness of the lattice. In case of similar molecular structures with N atoms, the Wiener index assumes its minimum values in correspondence of the most compact isomers that appears quite often among the most stable ones. This is indeed the case of the C_{60} fullerene [1,3] where the physically stable icosahedral $C_{60}(I_h)$ ''buckyball'' shows the minimum $W=8340$ value among 1812 non–isomorphic isomers. Similarly, stable isomers of the C_{40}, C_{28}, C_{76}, C_{78} fullerenes present low values Wiener index, see articles [1,2,3,4].

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Considering graphs of infinite structures as polymers, Equation (1) is still applicable and the resulting integer *W(N)* shows divergent values. The infinite growth of the Wiener index has the remarkable property, originally discovered by Bonchev and Mekenyan [5] in their studies of the energy gap in conjugated polymers, of being exactly described by cubic polynomials of the number of atoms *N*.

a) $N = 4$, W = 8

b) $N = 6$, W = 27

c) $N = 8$, W = 64

d) $N = 10$, W = 125

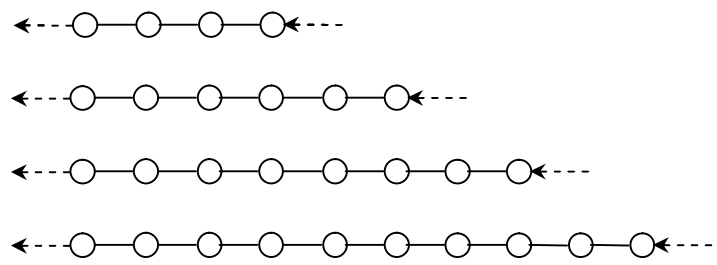


Figure 1. Graphs of $d_T=1$ torus with growing even number of nodes *N*; Wiener index values W are reported.

The general form of the Wiener index for mono–dimensional ($d_T=1$) infinite periodic lattices, i.e. lattices generated by translations of a given unit cell in one dimension, is expressed by:

$$W(N) = a_3N^3 + a_2N^2 + a_1N + a_0 \qquad \text{for } d_T = 1 \text{ lattices} \qquad (2)$$

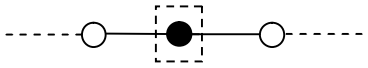
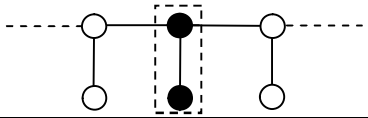
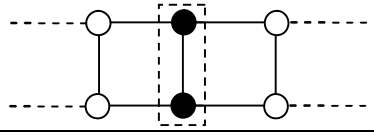
In the limit $N\rightarrow\infty$ mono–dimensional lattices follow the general asymptotic behavior $W(N) \approx N^3$. The rational coefficients a_i strictly depend from the specific lattice under study and may be determined by interpolation methods. For example, Figure 1 shows four growing steps of the closed-ends linear lattice with even number of nodes and the relative Wiener index values; coefficients a_i are easily computed from the *(N,W)* pairs: $a_3=2^{-3}$, $a_2=a_1=a_0=0$; Wiener index (2) is then $W^C_{LIN}(N) = N^3/8$.

Some other few examples of open-ends mono–dimensional lattices are listed in Table 1, where black circles identify the n_0 nodes belonging to the lattice unit cells. Their Wiener index polynomials evidence the ability of the Wiener index (1) to assume lower values in correspondence to the most compact topological structure. Then, the Wiener index values of the lattices in Table 1 should, by structural reason, respect the sequences $W_{LIN} > W^C_{LIN}$ and $W_{LIN} > W_{COMB} > W_{RAIL}$ and this is indeed the case as one may verify by the polynomial closed forms reported in the same table. For example, with $N=64$ one has as expected W_{LIN}=43680, W^C_{LIN} = 32768, W_{COMB}= 23840, W_{RAIL}= 22848 being the railway lattice the topological most compact ones,.

More generally, above sequences suggest that the Wiener index (1) of a graph with a given number of nodes *N* diminishes by increasing graph connectivity or, equivalently, by

augmenting the number of bonds in the graph, a topological operation that may be obtained by increasing the dimensionality d_T of the graph itself.

Table 1: The Wiener index cubic polynomials $W(N)$ for some open-ends $d_T=1$ lattices. Unit cells are framed by the dotted rectangle and their n_0 nodes are depicted in black.

Lattice	Unit cell	n_0	Wiener Index
Linear lattice		1	$W(N) = (N^3 - N)/6$
Comb lattice		2	$W(N) = (N^3 + 6N^2 - 10N)/12$
Railway lattice		2	$W(N) = (N^3 + 3N^2 - 4N)/12$

This mechanism becomes evident by studying the Wiener index of lattices with different dimensionalities. Figure 2 shows in fact the decreasing values of the Wiener index (1) for the $d_T=1$ linear chain ($W=43680$), the $d_T=2$ square lattice ($W=10752$) and the $d_T=3$ cubic lattice ($W=7680$) keeping fixed the number of nodes N ($N=64$ in this example). The plotted descent of W at augmenting lattice dimensionality d_T basically arises from the increasing number of bonds of each node, from 2 bonds (in the case of $d_T=1$), to 4 ($d_T=2$) and finally to 6 in the case cubic lattice, the most compact structure of these three lattices.

In the case of higher dimensionality $d_T \to \infty$ one may expect that each nodes is bounded to the remaining $N-1$ ones, the Wiener index [6] assuming values proportional to N^2 as in the case of the complete graphs K_N in Figure 3:

$$W(N) = (N^2 - N)/2 \qquad \text{for } K_N \text{ lattices} \qquad (3)$$

This structure represents indeed a very compact graph. Numerically, the K_{64} case has a value of $W=2016$ that is much lower than the $W=7680$ value of the cubic lattice with $N=64$ vertices previously computed.

Above heuristic considerations imply that Wiener index polynomial (2) of an infinite lattices with dimensionality $d_T \geq 1$ should asymptotically follow the $W(N) \approx N^s$ law with the leading exponent s constrained between two integers:

$$3 \geq s \geq 2 \qquad \text{for any values of } d_T \geq 1 \qquad (4)$$

In the inequality (4) the upper limit $s=3$ corresponds to the case of infinite mono–dimensional lattices (2) whereas the lower boundary value $s=2$ holds for infinite lattices with dimensionality $d_T \rightarrow \infty$.

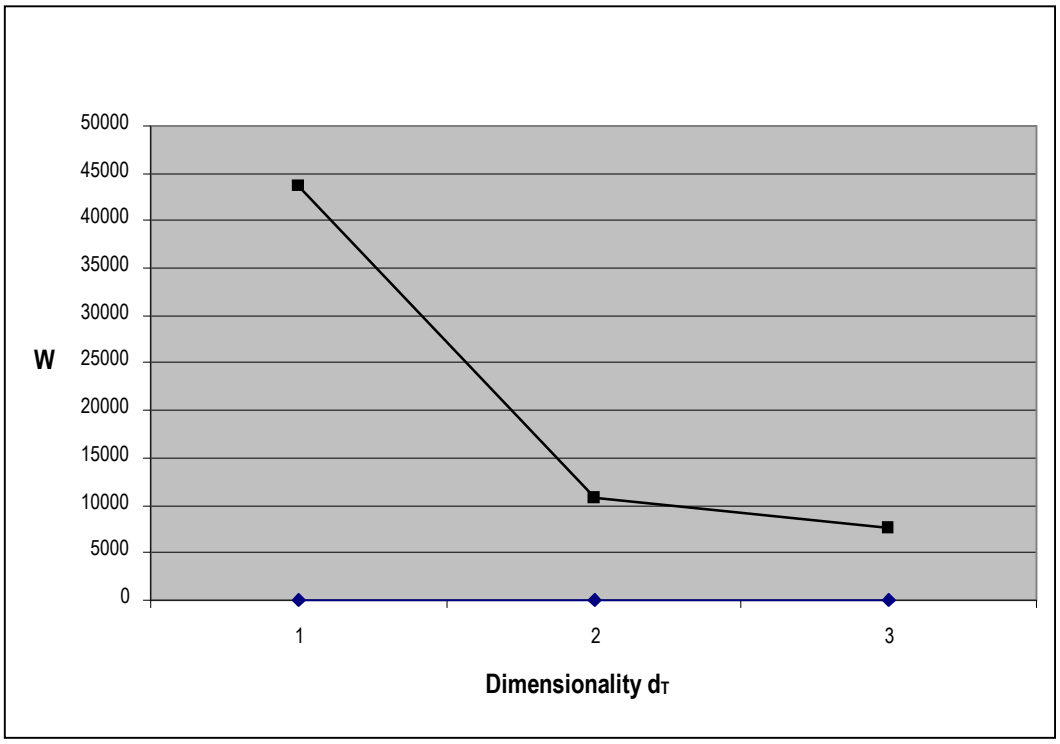


Figure 2. Wiener index values decrease for $d_T=1$ linear chain ($W=43680$), $d_T=2$ square lattice ($W=10752$) and $d_T=3$ cubic lattice ($W=7680$) with fixed number of nodes, being in this example $N=64$.

Next paragraph is devoted to the generalization of the Wiener index formula (2) to chemical structures with dimensions larger than one. A general expression for the leading exponent s in $W(N) \approx N^s$ in term of d_T values will be in fact introduced together with a new, general definition of lattice dimensionality d_T that show an intimate relationship with the topological compactness of the lattice.

Some cases confirming the validity of the new method will be given for different lattices with $d_T=2$, also fractal.

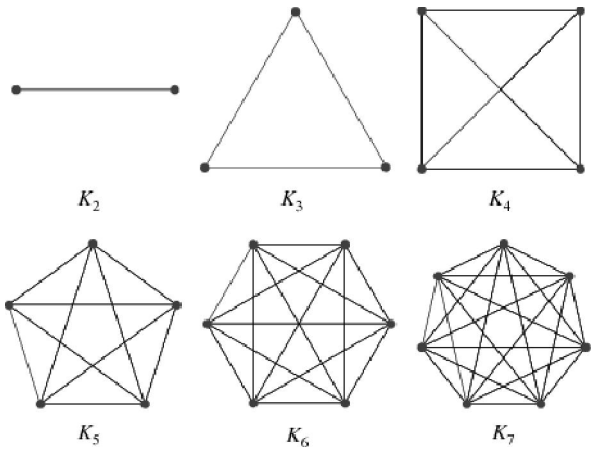


Figure 3. Complete graphs K_N for $N=2, 3, 4, 5, 6, 7$ nodes; their Wiener index values show the N^2 dependency.

2 WIENER INDEX AND DIMENSIONALITY CONJECTURED RELATIONSHIP

The attempt to generalize the Wiener index polynomial rule (2) to chemical structures with higher dimensions d_T (as graphene, diamond or zeolites) has been undertaken by the authors, leading to the following *conjecture* applicable to transitionally invariant d_T–dimensional lattices (e.g. lattices generated by a unit cell with n_0 atoms in Euclidean spaces with d_T dimensions):

- Given a d_T–dimensional lattice, being L the number of unit cells along each *edges* (e.g. the lattice is made of L^{dT} cells), the Wiener index of the lattice is polynomial in L thus $W(L)\approx L^k$ with the leading exponent k given by:

$$k = (2d_T+1) \qquad \text{for any values of } d_T \geq 1 \qquad (5)$$

Consequently, being $N=n_0L^{dT}$, the Wiener index has a polynomial-like form $W(N) \approx N^s$ where s is given in terms of d_T:

$$s = k/d_T = 2 + 1/d_T \qquad \text{for any values of } d_T \geq 1 \qquad (6)$$

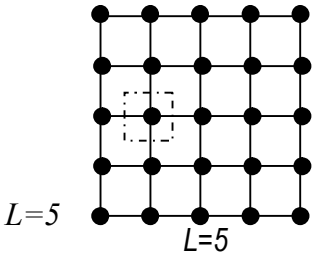
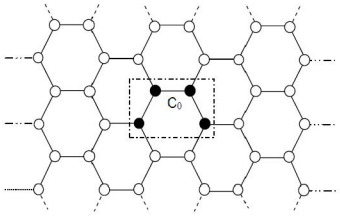
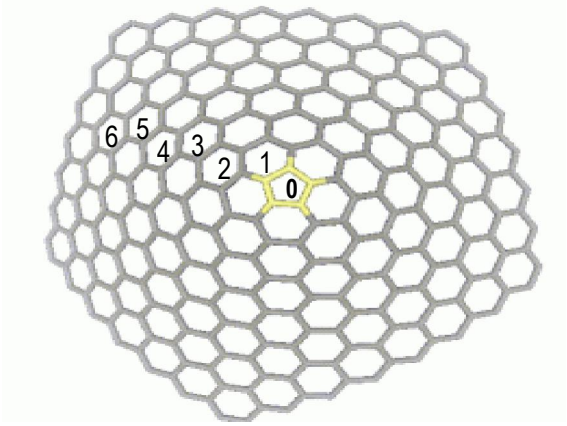
It is easy to verify that formula (6) for s agrees with previously proposed limits (4) on the leading exponent for the Wiener index closed form $W(N)\approx N^s$, ranging from $s=3$ when $d_T=1$ to $s=2$ for $d_T \rightarrow \infty$. Finally, expression (6) may be inverted to derive the new, searched general definition of dimensionality d_W:

$$d_W = (s-2)^{-1} \qquad (7)$$

Formula (7) represents the conjectured bridge between lattice topological compactness, expressed by topological invariant $W(N)\approx N^s$ and the lattice dimensionality

d_W. This new definition of d_W is supposed to have broad applicability as the next paragraph will show; being related to the asymptotic values of the Wiener index topological invariant, d_W is called Wiener dimensionality.

Table 2 The polynomial–like forms *W(L)* and *W(N)* for some open–ends infinite $d_T=2$ lattices. The unit cell, when present, is framed.

Lattice	**Unit cell**	n_0	**Wiener Index**
Square lattice		1	$W(L) = (L^5 - L^3)/3$ $W(N) = (N^{5/2} - N^{3/2})/3$ being $N = L^2$
Graphene lattice		4	$W(L)=(192L^5 -40L^3-2L)/15$ $W(N)=(6N^{5/2} -5N^{3/2} - N^{1/2})/15$ being $N=4L^2$
Pentagonal nanocone $f \geq 0$		Na	$W(f) = (124f^5+620f^4+1205f^3+1135f^2+516f+90)/6$ $W(N)\approx N^{5/2}$ being $N=5f^2+10f+5$

Before presenting some examples about the general validity of the conjectured formulae (5,6,7), a couple of comments should be given. First of all, equations (5,6)

describe the Wiener index as a grade k polynomial-like of N^{-dT}; computationally, the Wiener index assumes therefore the following general closed forms, with $k=(2d_T+1)$:

$$W(L) = b_kL^k + b_{(k-1)}L^{(k-1)} + \ldots + b_1L + b_0 \qquad \text{for any } d_T \geq 1 \text{ lattices} \qquad (8a)$$

$$W(N) = a_kN^{k/dT} + a_{(k-1)}N^{(k-1)/dT} + \ldots + a_1N^{1/dT} + a_0 \qquad \text{for any } d_T \geq 1 \text{ lattices} \qquad (8b)$$

It is worth noticing that Equations (7,8) work also for infinite lattices without unit cell; for example, the $W(N) \approx N^{5/2}$ leading term applies to the translationally invariant $d_T=2$ lattices of the graphene as well to nanocones. The Table 2 presents the polynomial-like forms $W(L)$ and $W(N)$ for some open-ends $d_T=2$ lattices with leading exponent $k=5$ and $s=5/2$ respectively. The graph nodes in the lattice unit cell n_0 are framed when present. The last graph represents a pentagonal nanocone with $f=6$ concentric rings, a relevant case of an infinite lattice *without* unit cell for which equations (7,8) are still valid.

3 RESULTS AND DISCUSSION

Mono-dimensional graphs show the direct proportionality $N \approx L$, thus the polynomials in Table 1 may be easily converted in terms of L, for example $W_{LIN}(L) = (L^3-L)/6$, confirming the general applicability of Equations (8) to infinite graphs with $d_T=1$, $k=s=3$.

In case of bi–dimensional lattices $d_T=2$, $k=5$, $s=5/2$, the Wiener index expressions (8) become:

$$W(L) = b_5L^5 + b_4L^4 + b_3L^3 + b_2L^2 + b_1L + b_0 \qquad \text{for any } d_T = 2 \text{ lattices} \qquad (9a)$$

$$W(N) = a_5N^{5/2} + a_4N^2 + a_3N^{3/2} + a_2N + a_1N^{1/2} + a_0 \qquad \text{for any } d_T = 2 \text{ lattices} \qquad (9b)$$

being $N=n_0L^2$.

The Table 2 provides some applications of the Equations (9) to square lattice and graphene, whose unit cells are shown surrounded by dotted rectangles. Present calculations on translationally invariants bi–dimensional lattices are coherent with the proposed Equations (9) for the Wiener index, being $s=5/2$ the leading exponent of $W(N)$ in the asymptotic limit $N \to \infty$.

The first remarkable extension of the present model is the prediction of the asymptotic $W(N) \approx N^{5/2}$ behavior of the Wiener index of the pentagonal nanocone (Table 2). Its lattice that in fact does not possess any unit cell, being made of f concentric circles of hexagons placed around the central pentagon. The case $f=0$ corresponds to the graph made by the sole pentagon and the nanocone with six complete concentric rings $f=6$ of hexagons is shown at the bottom of Table 2. This infinite nanocone is in effect a bi–dimensional

structure and its Wiener index should then comply with Equation (9b) $W(N)\approx N^{5/2}$ as present topological calculations in effect confirm. Therefore Equation (9b) holds for fullerenic pentagonal nanocone; article [7,8] provide detailed features of the Wiener index of this structure.

Heptagonal nanocones have a similar Wiener index closed form $W(f)=(1428f^5 - 175f^3 + 7f)/30$ as is derivable from the numerical values published in the recent paper [9]. Above detailed studies on infinite surfaces, confirm the conjectured Equations (5,6,7) with $k=5$, $s=5/2$ and the asymptotic behavior $W(N)\approx N^{5/2}$ for any $d_T=2$ structure studied so far.

A more challenging test about Equations (6,7) it has been carried out to derive the correct Wiener d_W dimensionality of the Sierpinski gasket (*SG*) starting from the asymptotic values of the Wiener index of its lattice (Figure 4). This fractal triangle has a Hausdorff dimension $d_H= log3/log2$ intermediate between a line and a surface. Figure 4 shows the appealing, self-similar structure of *SG* after a few growing *t* steps, the seed of this fractal being a simple equilateral triangle (step $t=1$). This triangle at the second iteration $t=2$ splits itself in four, with one empty part; the fractal dimension of *SG* originates from this void space left in the lattice. Iteratively, this fractal grows until the whole plane is covered. Table 3 gives the topological descriptors of the SG graph, including its Wiener index *W(N)*. In the list, *T* is the number of elementary triangles in the structure, *B* is the number of chemical bonds on the graph, *M* is the maximum distance or graph diameter. *M* equals in this case the number of bonds along the triangle edge. The number of lattice nodes *N* exponentially grows with *t* like all the other graph invariants in Table 3, with the noticeable exception of *W(N)*.

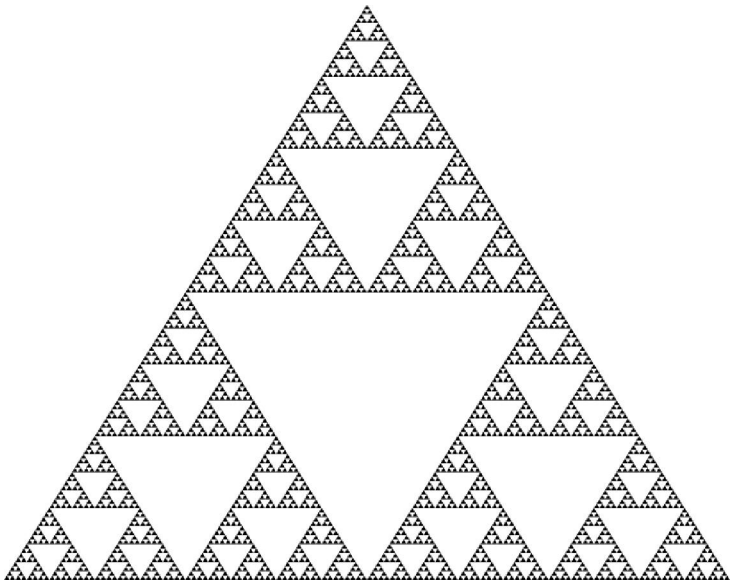


Figure 4. View of the fractal lattice *SG* after $t=7$ growing steps.

Focusing on Wiener index, the task of computing the fractal dimensionality d_H from the leading term of the Wiener index (1) in the limit $N\to\infty$ is a non-trivial application of the proposed model. If Equations (6,7) are valid, exponent s will then converge to $s=2+1/d_W=2+ln(2)/ln(3)$. This result has been in fact achieved starting from the computed W(N) values of Table 3 by assuming that:

$$\lim_{N\to\infty} W(N) = a\cdot N^s \tag{10}$$

Exponent s has to be equal to $s=2+ln(2)/ln(3)$ in order to confirm its correlation from the Wiener dimensionality d_W, Equations (6,7). In (10) both quantities a and s can be numerically interpolated from the adjacent pairs (W,N) given in Table 3, as N tends to infinity. The logarithmic diagram of $ln(W)$ vs. $ln(N)$ shows linear relationship and the intercepts of the segments joining adjacent points quickly converge to the conjectured values $s=2+ln(2)/ln(3)$.

The value of a is determined by taking $s=2+ln(2)/ln(3)$ for any (W,N) pairs, and then calculating the appropriate value for a from every (W,N) pair. This method fastly converge to the limiting value of a:

$$a = \frac{233}{885}\left(\frac{2}{3}\right)^{\ln(2)/\ln(3)} \tag{11}$$

The asymptoic leading term of $W(N)$ has then the expected general form (8b) $W(N)\approx aN^s$, with $s=2+1/d_T=2+1/d_W$:

$$\lim_{N\to\infty} W(N) = \frac{466}{885}\frac{N^2}{2}\left(\frac{2}{3}N\right)^{\ln(2)/\ln(3)} \tag{12}$$

Equation (12) has been numerically derived, but the fully analytical demonstration of the following relationships has been derived by one of the author [10] for both fractals:

$$\lim_{N\to\infty} \ln_N W(N) = 2+\frac{\ln 2}{\ln 3} \qquad \text{for } d_T=2 \text{ Sierpinski gasket} \tag{13a}$$

$$\lim_{N\to\infty} \ln_N W(N) = 2+\frac{\ln 3}{\ln 8} \qquad \text{for } d_T=2 \text{ Sierpinski carpet} \tag{13a}$$

Equation (12,13) successful testifies the existence of the conjectured bridge (6,7) between lattice topological intrinsic compactness (expressed by the lattice Wiener index)

and its dimensionality. This new connection between lattice connectivity and the Wiener dimensionality may be written in several intriguing computational ways as the following:

$$\lim_{N\to\infty} \ln_N \frac{W(N)}{N^2} = d_W^{-1} \tag{14}$$

generally applicable to any d_T-dimensional infinite graphs.

Table 3. Graph invariants for SG graphs: T, B, M, N, W are, respectively, number of elementary triangles, number of chemical bonds, graph diameter, number of nodes, Wiener index.

t	T= $3^{(t-1)}$	B= 3^t	M=$2^{(t-1)}$	N = $(3^t+3)/2$	W
1	1	3	1	3	3
2	3	9	2	6	21
3	9	27	4	15	246
4	27	81	8	42	3.765
5	81	243	16	123	64.032
6	243	729	32	366	1.130.463
7	729	2.187	64	1.095	20.215.254
8	2.187	6.561	128	3.282	363.069.729
9	6.561	19.683	256	9.843	6.530.385.420
10	19.683	59.049	512	29.526	117.517.503.027
11	59.049	177.147	1.024	88.575	2.115.137.375.634
12	177.147	531.441	2.048	265.722	38.071.401.560.949
13	531.441	1.594.323	4.096	797.163	685.278.776.820.264
14	1.594.323	4.782.969	8.192	2.391.486	12.334.979.163.295.719
15	4.782.969	14.348.907	16.384	7.174.455	222.029.391.506.636.622
16	14.348.907	43.046.721	32.768	21.523.362	3.996.527.644.152.854.793
17	43.046.721	129.140.163	65.536	64.570.083	71.937.489.166.087.238.532
18	129.140.163	387.420.489	131.072	193.710.246	1.294.874.754.367.873.060.443

4 CONCLUSIONS

A detailed discussion of the polynomial asymptotic behavior of Wiener index on infinite lattices has been presented; in all $d_T \geq 1$ cases studied so far the conjectured polynomial-like dependence $W \approx N^s$ with $s=2+1/d_T$ has been demonstrated valid also for bi-dimensional fractal structures. We moreover conjectured the intimate connection between the Wiener index of an infinite lattice and its Wiener dimensionality $d_W=(s-2)^{-1}$. This graph–theoretical

definition of dimensionality, deeply embedded in the topological compactness of the structures, applies to all bi–dimensional infinite lattices included in the present research. Further investigations will be conducted on other fractal structures, like the Koch snowflake, the Penrose tiling or the tri–dimensional SG, to better understand the validity range and the limitations of the *Wiener way to define lattice dimensionality* presented in this article.

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