DOI: 10.15643/mmcct-2023-3

Size-related graph transitiveness for Klein bottle fullerenes

Ottorino Ori

Actinium Chemical Research Srl
Via Casilina 1626/A, 00133 Roma, Italy.

Email: ottorino.ori@gmail.com

We report here about an interesting *anomaly*, recently discovered, concerning the transmission values of the vertices on the surface of a Klein bottle fullerene depicted like a hexagon-tiled graph with N vertices and $3N/2$ edges. N depends on the two graph dimensions L_C and L_M, respectively the length of "cylindrical" and Möbius zig-zag edge. Our numerical computations showed that Klein bottle cubic graphs become transitive when LCLM. As a peculiar consequence, this kind of Klein bottles are topologically indistinguishable from toroidal lattices with the same size (L_C, L_M).

Keywords: Klein bottle, graph transmission, Wiener index, Topological roundness.

German mathematician Felix Klein (1849–1925) introduced his fascinating Klein bottle (KB) in 1882 several decades after the discovery of the Möbius strip (M) independently made by August Ferdinand Möbius and Johann Listing. These two non-orientable *flächen*, with genus g =1 (M) and g = 2 (KB) are correlated: the Klein surface is obtainable by closing in a *cylindrical* way the open edges of a Möbius strip. Tori (T) and KBs, showing the same Euler characteristics equal to 0, admit a hexagonal tiling without the need of pentagons or other polygons. We call here these polyhex surfaces Klein bottle fullerenes. [1] and investigate their graph invariants, namely the transmission and the Wiener index [2]. For those willing to understand the mechanisms of transforming a simple cylinder into the popular “classical inverted sock” Klein bottle, a helpful pictorial explanation can be found in [3].

Given the building parameters of the graphs, i.e. the integer lengths L_C and L_M of the "cylindrical" and Möbius zigzag edge respectively, the number of hexagons *h*, atoms *N*, and bonds *B* are fixed. A few details about the construction of toroidal (T) and Klein bottle (KB) fullerenes graphs will be provided in the next page. An introduction to topological distance-based descriptors (also including detailed calculations for small polyhexes) is also presented, with the general results derived for both types of graphs for large *N*. Topological similarities between toroidal and Klein bottle graphenic nano-systems are discussed, and this contribution concludes with indications about symmetry properties of these hexagonal systems.

The nanostructures considered here show the zigzag Möbius edge parallel to *x* with dangling bonds closed across the direction *y*.

The topological models of the typical graphs for T and KB fullerenes are shown in Figure 1. Both graphs have the same integer dimensions $L_C = 2$, $L_M = 6$ and $h = L_M \times L_C$ hexagons, $N = 4h = 48$ trivalent atoms connected by $B = 6h = 72$ bonds (graph edges).

Let us start the walk along the graph edges. Naming b_{ik} the number of *k*-neighbors of the *i*-node, a quick calculation shows that $T_{6,2}$ is a *transitive graph* in which all nodes have the same set $\{b_{ik}\} = \{3,6,9,9,8,7,4,1\}$ and eccentricity $\epsilon = 8$ (Figure 1A). The maximum eccentricity value of the determines the graph diameter *M*, in this case then $M = 8$. Topologically, graph transitiveness makes all nodes to look the same for an observer walking along the graph. The observer in fact sees that all nodes have the same coordination numbers $\{b_k\}$.

When the nodes along the zigzag edge are glued in anti-antiparallel way, such as 25−24, 29−20, …, 45−4 bonds are formed, the $KB_{6,2}$ fullerene graph is built (Figure 1B). The most relevant effects caused by the Möbius closure are: (*i*) the graph is no longer transitive, with 4 classes of independent nodes with multiplicity 8,16,16,8; (*ii*) the graph is now more compact, with most of the nodes (40 on 48) which present a reduced eccentricity $\epsilon_i = M - 1 = 7$ (Table 1).

Graph invariants $\{b_{ik}\}$ are instrumental to compute all kinds of distance-based topological descriptors, such as the transmission w_i of the i-vertex:

$$w_i = \frac{1}{2}\sum_{k=1}^{M} b_{ik} \quad (1)$$

The Wiener index of the whole graph:

$$W = \sum_{i=1}^{N} w_i \quad (2)$$

The extreme topological roundness:

$$\rho^E = \frac{max\{w_i\}}{min\{w_i\}} \quad (3)$$

and many others.

Table 1. Topological classes for the vertices of the graph $KB_{6,2}$, including eccentricity ε_i, transmission w_i, $\{b_{ik}\}$, Wiener number W, and extreme topological efficiency ρ_E; multiplicity is given in brackets. $T_{6,2}$ descriptors hold for all nodes of the toroidal polyhex and coincide with the last class of $KB_{6,2}$.

$KB_{6,2}$ W = 4504; ρ_E =98/91 = 1.0769			
V	$\{b_{ik}\}$	ε_i	w_i
(8) *v*5 *v*8 *v*17 *v*20 *v*29 *v*32 *v*41 *v*44	3 6 9 12 11 5 1	7	91
(16) *v*6 *v*7 *v*10 *v*11 *v*18 *v*19 *v*22 *v*23 *v*30 *v*31 *v*34 *v*35 *v*42 *v*43 *v*46 *v*47	3 6 9 11 11 6 1	7	92
(16) *v*1 *v*4 *v*9 *v*12 *v*13 *v*16 *v*21 *v*24 *v*25 *v*28 *v*33 *v*36 *v*37 *v*40 *v*45 *v*48	3 6 9 10 9 7 3	7	95
(8) *v*2 *v*3 *v*14 *v*15 *v*26 *v*27 *v*38 *v*39	3 6 9 9 8 7 4 1	8	98
$T_{6,2}$ W = 4704; ρ_E = 1			
(48) *v*1, *v*2, ... , *v*47, *v*48	3 6 9 9 8 7 4 1	8	98

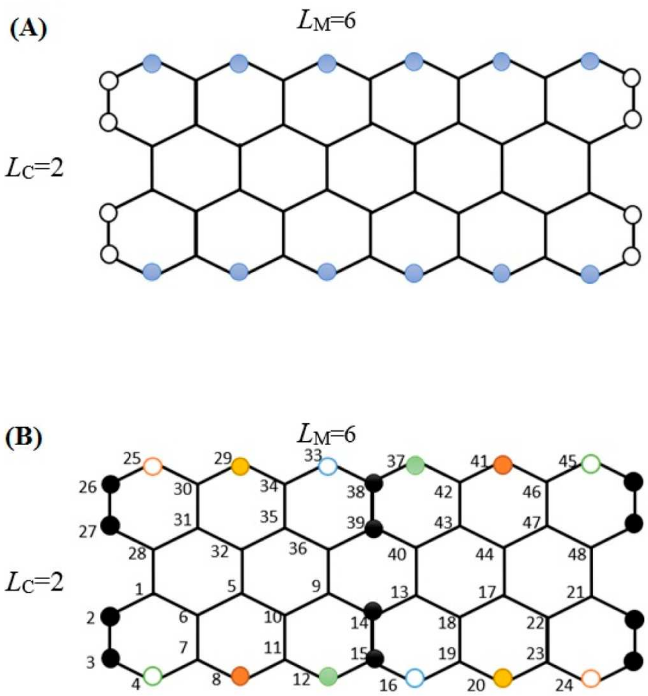

Fig. 1. Representation of $T_{6,2}$ toroidal and $KB_{6,2}$ Klein bottle fullerenes. Only the first one is transitive.

Remarkably, numerical simulations show that the Klein bottle fullerenes become transitive graphs when a certain ratio between the size of the edges is assured. Figure 2 gives a visual example of this, somehow unexpected, *symmetry* for the $L_C = 2, L_M = 3$ case. Graph $KB_{3,2}$ has the dandling bonds along x sewn in antiparallel way (13–12, 17–8, 21–4); whereas the open bonds along y are cylindrically close. This Klein bottle is formed by

N = 24 equivalent nodes all showing the same coordination numbers $\{b_k\}$ = {3,6,8,5,1}, exactly the same set shown by all nodes of the $T_{3,2}$ torus. Both graphs are transitive and indistinguishable thanks to this peculiar combination of seizes, $L_C = 2$, $L_M = 3$.

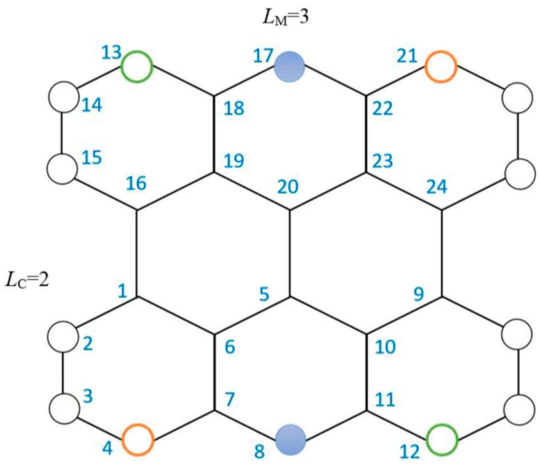

Fig. 2. Representation of $T_{3,2}$ toroidal and $KB_{3,2}$ Klein bottle fullerenes. Both graphs are transitive.

We end this short report by presenting the original results based on numerical simulations performed so far.

A) For Klein bottle fullerenes with size-ratio $L_C \geq L_M - 1$ the following topological relevant effect are observed: i) their graph becomes transitive; ii) the transmission values are the same of the same-sizes Torus.

In different words,

B) an observer measuring whatever type of topological interaction due to the graph neighbours, will never distinguish the kind of surface (orientable or non-orientable) he is exploring when the size-ratio $L_C \geq L_M - 1$ is present. A remarkable case of a new type of topological symmetry that gets broken when the ratio $L_C \geq L_M - 1$ is not respected.

The interested scholars are invited to read the original paper [4], whereby the present results are reported and discussed in details.

References

1. Deza M., Fowler P.W., Rassat A., Rogers K.M. // *J. Chem. Inf. Comput. Sci.* **2000.** V. 40. P. 550.
2. Dobrynin A.A., Ori O., Putz M.V., Vesnin A.Y. // *Fullerene Nanotube Carbon Nanostruct.* **2020.** V. 28. P. 545.
3. Freiberger M. Introducing the Klein bottle. *PlusMagazine,* 6 January **2015**. Available online: https://plus.maths.org/content/introducing-klein-bottle (accessed on 15 June 2020).
4. Putz M.V., Ori O. // *Symmetry.* **2020.** V. 12. P. 1233.