

Chapter 6

Geometry and Topology of Nanotubes and Nanotori

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Abstract A molecular graph is the graph of a molecule in which the vertices are atoms and edges are chemical bonds. We review the recent results on computing symmetry of series of armchair polyhex, zig-zag polyhex and $C_4C_8(R/S)$ nanotubes and nanotori. The topological properties of these nanostructures are also investigated.

6.1 Introduction

A *graph* G is a pair (V, E) consisting of a set $V = V(G)$ of vertices and a set $E = E(G)$ of *unordered pairs* $\{x, y\} = xy$ of distinct vertices of G called edges. Suppose M is a chemical system like a molecule (having dimensionality $\Delta = 0$), a carbon nanotube ($\Delta = 1$), a graphenic lattice ($\Delta = 2$) or a diamond crystal ($\Delta = 3$). The *molecular graph* of M is a simple graph such that *vertices are atoms* and *edges are chemical bonds*. The *degree* δ of each vertex (the number of chemical bonds) in a molecular graph is assumed to be at most four. Taking into consideration sp^2 carbon systems, we mention here that in the Hückel theory only pi electron molecular orbitals are included because these determine the general properties of these molecules and the sigma electrons are ignored. Thus, when we are talking about Hückel theory we need

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the molecule to have a pi network and therefore all molecular graphs should have max degree 3 or less—a vertex of degree 4 represents a saturated carbon atom that cannot be part of a pi system and which is typical of diamond-like bulk structures. The max degree 4 also holds for alkanes, which are not included in the present research.

Being this chapter devoted to the investigation of the structural and topological properties of some families of nanostructures, a few formal tools have to be shortly introduced here starting with a simple recap of the concept of *group*.

A *group* is a mathematical structure that is usually used to describe the symmetries characterizing a given set of mathematical objects. It is a set of elements G equipped with a binary operation of multiplication $*$: $G \times G \rightarrow G$ such that:

- i) it is associative, e.g. for all $x, y, z \in G$, $x * (y * z) = (x * y) * z$;
- ii) there exists an element $e \in G$ such that for an arbitrary element g in G , $g * e = e * g = g$;
- iii) and, for each $x \in G$ there exists $y \in G$ such that $x * y = y * x = e$.

A group is then called *finite* if the underlying set G is *finite*. The *symmetry* structure of G can be formalized by the notion of *finite group action*. To describe it, we assume G is a group and X is a set. We also assume that there is a map $\phi : G \times X \rightarrow X$ with the following two properties:

- a. for each $x \in X$, $\phi(e, x) = x$,
- b. and, for all elements $x \in X$ and $g, h \in G$, $\phi(g, \phi(h, x)) = \phi(gh, x)$.

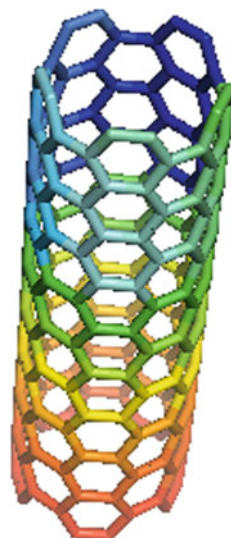
In this case, G and X are called a *transformation group* and a *G-set*, respectively. The mapping ϕ is called a *group action*. For simplicity it is convenient to define $gx = \phi(g, x)$.

Suppose now G is a group and H is a non-empty subset of G . H is said to be a *subgroup* of G , if H is closed under group multiplication. A subgroup H of G is called to be *normal* in G , if for all $g \in G$ we have $g^{-1}Hg = H$. When both H and K are subgroups of G such that H is normal in G , $H \cap K = 1$, and $G = HK$, then G is called a semi-direct product of H by K . Here, HK is the set of all elements of G in the form of xy such that $x \in H$ and $y \in K$.

An *automorphism* of G is a permutation g of $V(G)$ such that $g(u)$ and $g(v)$ are adjacent if and only if u and v are adjacent, where $u, v \in V(G)$. It is well-known that the set of all automorphisms of G , with the operation of composition of permutations, is a permutation group on $V(G)$, denoted $Aut(G)$. The name *topological symmetry* is also used for this algebraic structure. Randić (1974, 1976) showed that a graph can be depicted in different ways such that its point group symmetry or even the 3D representation may differ, but its automorphism group symmetry remains the same. The *topological symmetry* of a molecular graph is not usually the same as its point group symmetry but it corresponds to the maximal symmetry the geometrical realization of a given topological structure may possess. This very important topological feature will play an instrumental role in the present investigations.

Computationally, several software packages are may be sourced on line for solving computational problems related to finite groups. GAP is an abbreviation for Groups,

Fig. 6.1 The molecular graph of an armchair $[p, 10]$ nanotube



Algorithms and Programming (The GAP Team 1995). Since all symmetry elements of a physical object is a group under composition of functions, the package is useful for this topic. Our calculations are based however on three other packages. These are *HyperChem* (HyperChem package Release 7.5 for Windows 2002), *TopoCluj* (Diudea et al. 2002) and *MAGMA* (Bosma et al. 1997).

Calculations reported in this paper are done by using a combination of these packages. We first draw a nanotube or nanotorus by HyperChem. Then we will compute the adjacency matrix by TopoCluj. We then apply MAGMA and GAP for computing symmetry group. All notations are standard and taken from the standard book of group theory. We encourage to reader to consult the celebrated book of Trinajstić (1992) for more information on symmetry.

6.2 Nanotubes and Nanotori Topological Indices

A *carbon nanotube* is a new allotrope of carbon with a tubular structure at the nanoscale. The molecular graphs of *armchair* and *zig-zag polyhex nanotubes* are depicted in Figs. 6.1 and 6.2, respectively. We associate two parameters $[r, s]$ to each armchair and zig-zag polyhex nanotube as follows. In an armchair nanotube, Figs. 6.1 and 6.2, the parameter s denotes the number of vertical zig-zags, while in a zig-zag nanotube, Figs. 6.3 and 6.4, s denotes the number of horizontal zig-zags. On the other hand, the parameter r in an armchair polyhex is the number of rows and in a zig-zag nanotube it returns the number of hexagons in each row.

A C_4C_8 net is a trivalent (atom degree 3) decoration made by *alternating* squares C_4 and octagons C_8 . Such a plane covering can be derived from square net by the

Fig. 6.2 The 2D lattice of an armchair [11, 6] nanotube

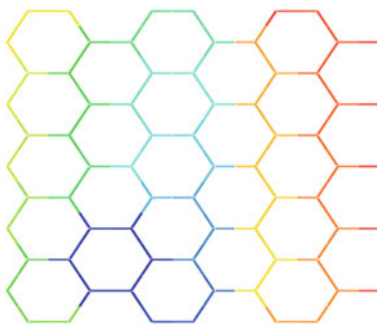


Fig. 6.3 The molecular graph of a zig-zag [13, 13] nanotube

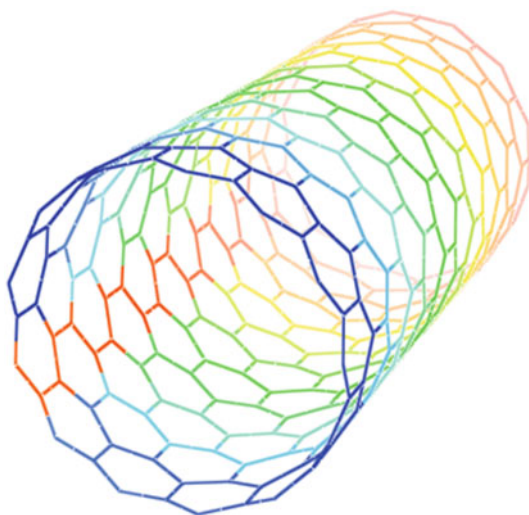


Fig. 6.4 The 2D lattice of a zig-zag [6, 8] nanotube

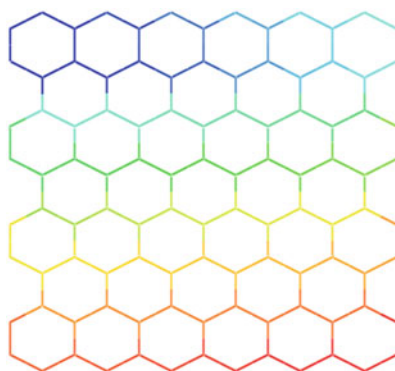


Fig. 6.5 The molecular graph of a $C_4C_8(R)$ nanotube



Fig. 6.6 The 2D lattice of a $C_4C_8(R)$ nanotube

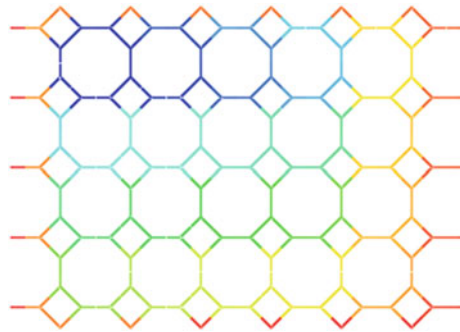
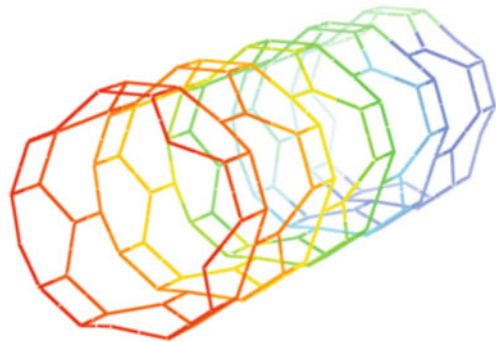


Fig. 6.7 The molecular graph of a $C_4C_8(S)$ nanotube



leapfrog operation, Figs. 6.5 and 6.6. A $C_4C_8(R)$ nanotube is another beautiful mathematical object constructed by squares and octagons. An charming example is shown in Figs. 6.7 and 6.8. A *carbon nanotorus* is geometrically obtained by connecting the two ends of a carbon nanotube into a ring, Figs. 6.9, 6.10, 6.11 and 6.12.

The symmetry properties of these nanostructures are one of the main subject of this study.

Suppose (G, \cdot_1) and (H, \cdot_2) are groups. The *cartesian product* $G \times H$ is the set of all *ordered pairs* (a, b) where $a \in G$ and $b \in H$, together with the following group

Fig. 6.8 The 2D lattice of $C_4C_8(S)$ nanotube

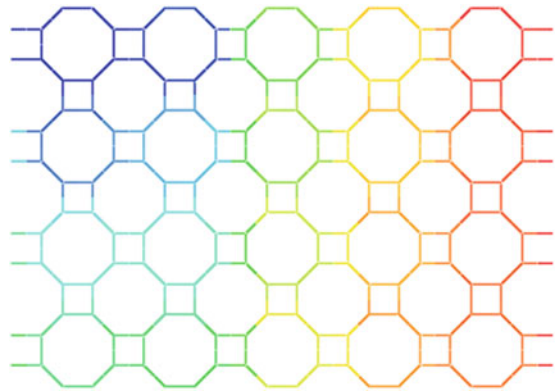


Fig. 6.9 The molecular graph of a $C_4C_8(R)$ nanotorus

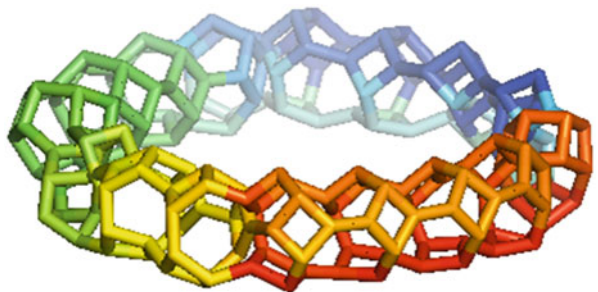
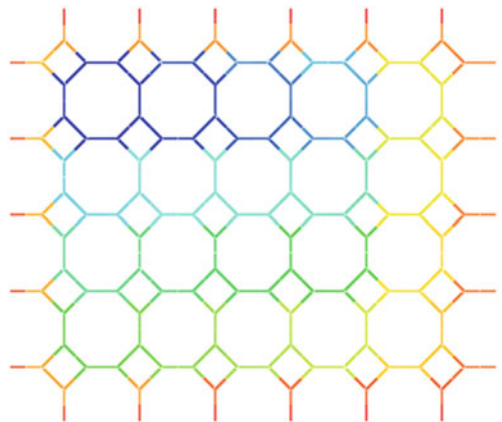


Fig. 6.10 The 2D Lattice of $C_4C_8(R)$ Nanotorus



structure:

$$(a, b) * (x, y) = (a \cdot_1 x, b \cdot_2 y) \tag{6.1}$$

The concept of *semi-direct product* is a generalization of cartesian product. In the cartesian product of two groups, each component represents in fact a normal

Fig. 6.11 The 2D lattice of $C_4C_8(S)$ nanotorus

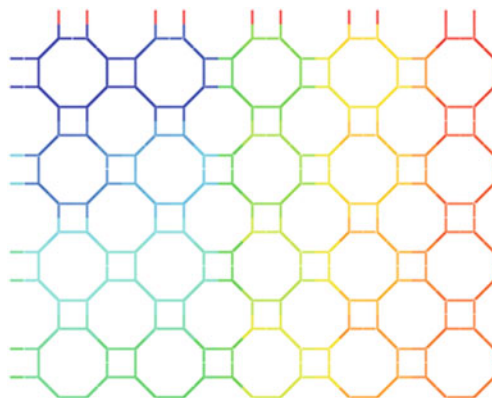
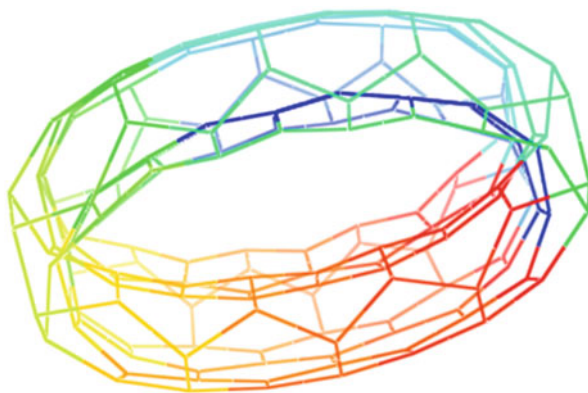


Fig. 6.12 The molecular graph of a polyhex nanotorus



subgroup, their intersection is trivial and the components generate the whole group. In the *semi-direct product* instead we admit one of the subgroup to be non-normal. In mathematical exact phrasing: *in semi-direct product a group can be constructed from two subgroups, one of which is a normal subgroup, the intersection of two subgroups is trivial and they generate the group.*

It is easy to see that if N and H are groups and φ is a homomorphism of H into the automorphism group of N then the set $N \times H$ by operation $(n_1, h_1) \cdot (n_2, h_2) = (n_1 \varphi_{h_1}(n_2), h_1 h_2)$, $n_1, n_2 \in N$ and $h_1, h_2 \in H$, has a group structure. This group is denoted by $N \times_{\varphi} H$ and called the *semi-direct product* of N by H .

A *graph invariant* is a quantity that is *invariant under all graph automorphisms*. The *topological indices* are numerical *graph invariants* used in theoretical chemistry to encode molecules for the classification and design of chemical compounds with given physico-chemical properties or given pharmacological and biological activities (Trinajstić 1992) (MIHAI). Notice that the bond relations between atoms do not fully determine the molecular geometry and so, in general, topological indices cannot uniquely determine a chemical compound, but they are usually useful to obtain information on some physico-chemical properties of compounds.

We now recall some algebraic definitions used here. Suppose G is a simple graph and $\{u, v\} \subseteq V(G)$. A *path* connecting u and v in G is a sequence:

$$u = u_0, e_1, u_1, e_2, \dots, e_n, u_n = v \quad (6.2)$$

of distinct vertices u_1, \dots, u_n and distinct edges e_1, \dots, e_n such that e_i is an edge with end vertices u_{i-1} and u_i . The *distance* $d(u, v)$ is defined to be the length of a minimal path connecting u and v . The half-summation of all distances between pairs of vertices in G is called the *Wiener index* of G which is denoted by $W(G)$. The Wiener index has been the first distance-based graph invariant and it was introduced by the American chemist Harold Wiener (1947). Suppose $e = uv$ individuates an edge in G . Define quantities $m_u(e)$ and $m_v(e)$ as follows: $m_u(e)$ is defined as the number of edges lying closer to the vertex u than the vertex v , and $m_v(e)$ is defined analogously. The edges equidistant from both ends of the edge uv are not counted. In a similar way, we define $n_u(e)$ to be the number of vertices lying closer to the vertex u than v . The *PI index* (Khadikar et al. 2001) of G is defined as

$$PI(G) = \sum_{e=uv} [m_u(e) + m_v(e)] \quad (6.3)$$

For acyclic molecular graphs G , Wiener discovered a remarkably simple algorithm for computing $W(G)$. To explain his method, we assume that $e = ij$ is an edge of G , $N(i)$ is the number of vertices of G lying closer to i than to j and $N(j)$ is defined analogously. Thus,

$$\begin{aligned} N(i) &= |\{u \in V(G) | d(u, i) < d(u, j)\}| \quad \text{and} \\ N(j) &= |\{u \in V(G) | d(u, j) < d(u, i)\}| \end{aligned} \quad (6.4)$$

Then the *Szeged index* of G is defined as the half-summation of all products $N(i)N(j)$ over all graph edges $e = ij$. This generalization was conceived by Ivan Gutman (1994) at the Attila Jozsef University in Szeged, and so it was called the Szeged index. It is useful to mention here that Gutman in his 1994 paper proposed the existence of the cyclic index and abbreviated it by W^* . In that paper he has not given any name to this index. Khadikar et al. (1995) used the name ‘‘Szeged index’’ and abbreviated as Sz. According to a long-known result in the theory of graph distances, if G is a tree then $Sz(G) = W(G)$, reproducing Wiener’s original method.

Klavžar et al. (1996) proved that for every connected graph G we have $W(G) \leq Sz(G)$. So it is natural to ask about equality of these graph invariants. To find a characterization of graphs satisfy the equality, we need some notation. A maximal 2-connected subgraph of a connected graph G is called a *block* of G . The block graphs are those in which every block is a clique. Dobrynin and Gutman (1995) investigated the structure of a connected graph G featuring the property that $Sz(G) = W(G)$. They proved that $Sz(G) = W(G)$ if and only if G is a block graph (Dobrynin et al. 1995). A new proof for this result is recently published (Khodashenas et al. 2011).

The Wiener, PI and Szeged indices are all distance based invariants of a graph. There are some other graph invariants based on degree sequence of the molecular

graph under consideration. The first such invariants are *Zagreb group indices*. The Zagreb indices have been introduced more than forty years ago by Gutman and Trinajstić (1972). They are defined as:

$$M_1(G) = \sum_{v \in V(G)} \text{deg}(v)^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} \text{deg}(u) \times \text{deg}(v) \quad (6.5)$$

where $\text{deg}(u)$ is the degree of the vertex u of G . A historical background, computational techniques and mathematical properties of Zagreb indices can be found in papers (Gutman and Das 2004; Khalifeh et al. 2009; Zhou 2004; Zhou and Gutman 2005).

The *Randić molecular connectivity index*, Randić index for short, is a second degree-based topological invariant, introduced in (Randić 1975). It is defined as:

$$\chi(G) = \sum_{uv \in E(G)} (\text{deg}(u) \text{deg}(v))^{-1/2}. \quad (6.6)$$

It reflects molecular branching and has several applications in chemistry (Klarner 1997).

The *atom-bond connectivity (ABC) index* is another degree-based topological index introduced by Estrada et al. 1998 to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{\text{deg}(u) + \text{deg}(v) - 2}{\text{deg}(u) + \text{deg}(v)}}. \quad (6.7)$$

Estrada (2008) presented a new topological approach which provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes. He also reported that the heat of formation of alkanes can be obtained as a combination of stabilizing effects coming from atoms, bonds and protobranches. Furtula et al. (2009) studied the mathematical properties of the ABC index of trees. They found chemical trees with extremal ABC values and proved that, among all trees, the star tree S_n , has the maximal ABC index. Das (2010) presented the lower and upper bounds on ABC index of graphs and trees, and characterize graphs for which these bounds are best possible. Fath-Tabar et al. (2011) obtained some inequalities for the atom-bond connectivity index of a series of graph operations and proved that the bounds are tight. They applied their result to compute the ABC indices of C_4 nanotubes and nanotori.

The relationship between degree-based topological indices of graphs is an important problem in chemical graph theory. Das and Trinajstić (2010) compared the GA and ABC indices for chemical trees and molecular graphs and proved some results.

The *Balaban index* of a molecular graph G is defined by Balaban (1982, 1983) as:

$$j(G) = m / (\mu + 1) \sum_{e=uv} [d(u)d(v)]^{-0.5} \quad (6.8)$$

where m is the number of edges of G , $\mu(G) = |E(G)| - |V(G)| + 1$ is the cyclomatic number of G and for every vertex x , $d(x)$ is the summation of topological distances between x and all vertices of G .

In the end of this section the concept of *eccentric connectivity index* of molecular graphs is presented. Let G be a molecular graph (Sharma et al. 1997; Sardana and Madan 2001). The eccentric connectivity index $\xi(G)$ is defined as:

$$\xi(G) = \sum_{u \in V(G)} \deg_G(u) \varepsilon_G(u) \quad (6.9)$$

where $\deg_G(u)$ denotes the degree of vertex u and $\varepsilon_G(u)$ is the largest distance between u and any other vertex v of the graph G .

6.3 Symmetry Considerations on Nanotubes and Nanotori

A *dihedral group* is the group of symmetries of a regular polygon, including both rotations and reflections. These groups play an important role in chemistry. Most of point group symmetry of molecules can be described by dihedral groups. It is easy to prove that a group generated by two involutions on a finite domain is a dihedral group. A dihedral group with $2n$ symmetry elements is denoted by D_n . This group can be presented as follows:

$$D_n = \{x, y | x^n = y^2 = (xy)^2 = 1\} \quad (6.10)$$

We now consider the molecular graph of a zig-zag and armchair (achiral) polyhex nanotorus. Yavari and Ashrafi (2009) proved in some special cases that the symmetry group of armchair and zig-zag polyhex nanotorus is constructed from a dihedral group and a plane symmetry group of order 2.

Arezoomand and Taeri (2009) presented a generalization of this result. They proved that:

Theorem 1 (Arezoomand and Taeri) The symmetry group of the molecular graph of a zig-zag and armchair (achiral) polyhex nanotorus is isomorphic to $D_{4m} \times Z_2$, where Z_2 denotes the cyclic group of order 2.

Hypergraphs are generalizations of graphs in which an edge can connect more than two vertices. In the graph theoretical language, a hypergraph consists of a set of vertices V and a set of hyper-edges E which is a collection of subsets in V in such a way that the union of hyper-edges are the whole vertices. A *k-hypergraph* is a hypergraph with the property that any edge connects exactly k vertices. The case of $k = 2$ corresponds to the usual graphs considered so far. The best generalization of the mentioned result was introduced by Staic and Petrescu-Nita (2013). They studied the symmetry group of two special types of carbon nanotori by using the notion of *Cayley hypergraph*. To explain this concept, we assume that G is a group and S is a non-empty subset of G such that $S = S^{-1}$ and $G = \langle S \rangle$. We define a graph $\text{Cay}(G, S)$ as follows: (i) $V(\text{Cay}(G, S)) = G$, and, (ii) two vertices a and y are adjacent if and only if $xy^{-1} \in S$. The graph $\text{Cay}(G, S)$ is called the *Cayley graph* of G constructed by S . If G is a group and T is a generator set for G containing elements of order 3 such that $a \in T$ implies that $a^{-1} \notin T$ then 3-hypergraph $\text{Cay}_3(G, T)$ can be defined

as follows: take the set of vertices to be G . A cyclically ordered 3-subset $\{g_1, g_2, g_3\}$ is a hyper-edge if there exists $a \in T$ such that $g_2 = g_1 a$ and $g_3 = g_1 a$. The main result of Staica and A. Petrescu-Nita is as follows:

Theorem 2 (Staic and Petrescu-Nita) Suppose T_n is a group presented as follows:

$$T_n = \{a; b | a^3 = 1; b^3 = 1; (ab)^3 = 1; (ab^2)^n = 1\} \tag{6.11}$$

Then T_n is a semi-direct product of $Z_n \times Z_n$ by Z_3 . Moreover, the Cayley hypergraph associated with the group T_n can be placed on a torus.

If $SL(2,3)$ denotes the set of all 2×2 matrices over a field of order 3 then a Cayley hypergraph associated with this group can be placed on a torus.

We end this section by a result on the symmetry group of nanotubes. Suppose $A[p, q]$, $B[p, q]$, $C(R)[p, q]$ and $C(S)[p, q]$ are zig-zag polyhex, armchair polyhex, $C_4C_8(R)$ and $C_4C_8(S)$ nanotubes with parameters p and q , respectively.

Theorem 3 The symmetry groups of $A[p, q]$, $B[p, q]$, $C(R)[p, q]$ and $C(S)[p, q]$ are computed as follows:

1. $Aut(A[p, q]) = \begin{cases} D_{4p} & p \neq q \\ C_2 \times D_{2p} & p = q \end{cases}$,
2. If q is even and $p \neq 3$ then $Aut(B[p, q]) = \begin{cases} D_{2q} & p \text{ is even} \\ D_{2q} & \frac{q}{2} \text{ is odd} \\ C_2 \times D_q & \frac{q}{2} \text{ is even} \end{cases}$ $p \text{ is odd}$
3. If $p \neq 2$ then $Aut(C(R)[p, q]) \cong Aut(C(S)[p, q]) \cong Z_2 \times D_{2p}$. Moreover, if $p = 2$ then $Aut(C(S)[2, 1]) \cong Z_2 \times D_8$ and $Aut(C(S)[2, q]) = C_2 \times C_2 \times C_2$, when $q \neq 1$.

Previous theorems clearly illustrate the power of topological methods in predicting geometrical properties of carbon nanostructures.

6.4 Topology of Nanotubes and Nanotori

The history of computing topological indices of nanotubes and nanotori started by publishing two paper by Diudea and his co-workers (Diudea et al. 2004; John and Diudea 2004) about Wiener index armchair and zig-zag polyhex nanotubes. After publishing these seminal papers, several scientists focus on computing such numbers for the molecular graphs of nanostructures. For the sake of completeness we record the mentioned results of Diudea and his co-workers in Theorem 4.

Theorem 4 Suppose $A = A[p, q]$ and $B = B[p, q]$ are zig-zag and armchair polyhex nanotubes, respectively. Then the Wiener index of these nanotubes can be computed by the following formulas:

$$1) W(A) = \begin{cases} \frac{qp^2}{24}(4q^2 + 3qp - 4) + \frac{q^2p}{12}(q^2 - 1) & q \leq \frac{p}{2} + 1 \\ \frac{qp^2}{24}(8q^2 + p^2 - 6) - \frac{p^3}{192}(p^2 - 4) & q > \frac{p}{2} + 1 \end{cases},$$

$$2) W(B) = \begin{cases} \frac{p}{12}[p^2(12q^2 - 2p^2 + 8) + 8pq(p^2 + q^2 - 2) + 3(-1 + (-1)^p)] & q \geq p \\ \frac{p}{12}[24p^2q^2 + 2q^4 - 8q^2 + 3(-1)^p(1 - (-1)^q)] & q \leq p \end{cases}.$$

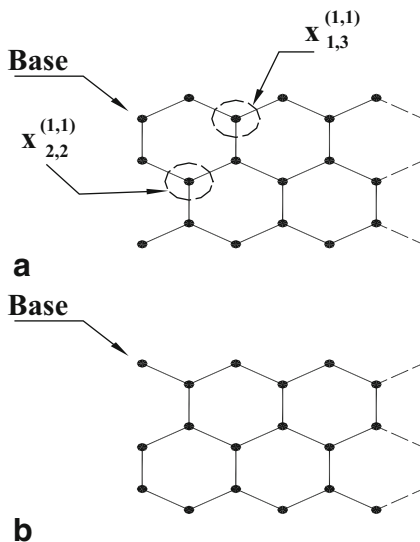
In a series of papers (Yousefi and Ashrafi 2006, 2007, 2008a, 2011; Yousefi et al. 2008c, d; Ashrafi and Yousefi 2007a, b) introduced a matrix method to recalculate the Wiener number of armchair, zig-zag polyhex nanotubes, $C_4C_8(R/S)$ nanotube, polyhex nanotorus and $C_4C_8(R/S)$ nanotorus. Choose a zig-zag polyhex nanotube T . The main idea of this matrix method is choosing a base vertex b from the 2-dimensional lattice of a T and then label vertices of hexagon by starting from the hexagon containing b . By computing distances between b and other vertices, we can obtain a distance matrix of nanotubes related to the vertex b . It is clear that by choosing different base vertices, one can find different distance matrices for T , but the summation of all entries will be the same. To explain, we assume that b is a base vertex from the 2-dimensional lattice of T and x_{ij} is the $(i, j)^{th}$ vertex of T , Fig. 6.6. Define $D_{m \times n}^{(1,1)} = [d_{ij}^{(1,1)}]$, where $d_{ij}^{(1,1)}$ is distance between $(1,1)$ and (i, j) , $i = 1, 2, \dots, m$ and $j = 1, 2, \dots, n$. There are two separates cases for the $(1,1)^{th}$ vertex, where in the first case $d_{1,1}^{(1,1)} = 0, d_{1,2}^{(1,1)} = d_{2,1}^{(1,1)} = 1$ and in the second case $d_{1,1}^{(1,1)} = 0, d_{1,2}^{(1,1)} = 1, d_{2,1}^{(1,1)} = 3$. Suppose $D_{m \times n}^{(p,q)}$ is distance matrix of T related to the vertex (p, q) and $s_i^{(p,q)}$ is the sum of i^{th} row of $D_{m \times n}^{(p,q)}$. Then there are two distance matrix related to (p, q) such that $s_i^{(p,2k-1)} = s_i^{(p,1)}$; $s_i^{(p,2k)} = s_i^{(p,2)}$; $1 \leq k \leq n/2$, $1 \leq i \leq m$, $1 \leq p \leq m$. If b varies on a column of T then the sum of entries in the row containing base vertex is equal to the sum of entries in the first row of $D_{m \times n}^{(1,1)}$. On the other hand, one can compute the summation of all entries in other rows by distance from the position of base vertex. Therefore, if $2 \mid (i + j)$ then

$$s_k^{(i,j)} = \begin{cases} s_{i-k+1}^{(1,1)} & 1 \leq k \leq i \leq m, \quad 1 \leq j \leq n \\ s_{k-i+1}^{(1,2)} & 1 \leq i \leq k \leq m, \quad 1 \leq j \leq n \end{cases}$$

and if $2 \nmid (i + j)$ then we have $s_k^{(i,j)} = \begin{cases} s_{i-k+1}^{(1,2)} & 1 \leq k \leq i \leq m, \quad 1 \leq j \leq n \\ s_{k-i+1}^{(1,1)} & 1 \leq i \leq k \leq m, \quad 1 \leq j \leq n \end{cases}$.

We now describe our algorithm to compute distance matrix of a zig-zag polyhex nanotube. To do this, we define matrices $A_{m \times (n/2+1)}^{(a)} = [a_{ij}]$, $B_{m \times (n/2+1)} = [b_{ij}]$ and $A_{m \times (n/2+1)}^{(b)} = [c_{ij}]$ as follows: (Fig. 6.13).

Fig. 6.13 Two Basically Different Cases for the Vertex b



For computing distance matrix of this nanotube we must compute matrices $D_{m \times n}^{(a)} = [d_{i,j}^a]$ and $D_{m \times n}^{(b)} = [d_{i,j}^b]$. By these calculations, one can see that

$$d_{i,j}^a = \begin{cases} \text{Max}\{a_{i,j}, b_{i,j}\} & 1 \leq j \leq n/2 \\ d_{i,n-j+2} & j > n/2 + 1 \end{cases} \text{ and } d_{i,j}^b = \begin{cases} \text{Max}\{a_{i,j}, c_{i,j}\} & 1 \leq j \leq n/2 \\ d_{i,n-j+2} & j > n/2 + 1 \end{cases}$$

By continuing this method, the mentioned authors proved that:

Theorem 5 Suppose A and B are an armchair and zig-zag polyhex nanotube, respectively, with exactly m rows and n columns, Fig. 6.2. Moreover, we assume that C is a polyhex nanotorus with similar parameters. Then,

1. (Yousefi and Ashrafi 2007)

$$W(A) = \begin{cases} \frac{m^2 n}{12} (3n^2 + m^2 - 4) + \frac{n}{8} (-1)^{\frac{n}{2}} [1 - (-1)^n] & m \leq \frac{n}{2} + 1 \\ \frac{mn^2}{24} (n^2 + 4m^2 + 3mn - 8) - \frac{n^3}{192} (n^2 - 16) + \frac{n}{8} \left[(-1)^{\frac{n}{2}} - 1 \right] & m > \frac{n}{2} + 1 \end{cases}$$

2. (Ashrafi and Yousefi 2007a)

$$W(B) = \begin{cases} \frac{mn^2}{24} (4m^2 + 3mn - 4) + \frac{m^2 n}{12} (m^2 - 1) & m \leq \frac{n}{2} + 1 \\ \frac{mn^2}{24} (8m^2 + n^2 - 6) - \frac{n^3}{192} (n^2 - 4) & m > \frac{n}{2} + 1 \end{cases}$$

3. Yousefi-Azari et al. (2008e)

$$W(C) = \begin{cases} \frac{pq^2}{24}(6p^2 + q^2 - 4) & q < p \\ \frac{p^2q}{24}(3q^2 + 3pq + p^2 - 4) & q \geq p \end{cases}$$

Suppose $E = TUC_4C_8(R)[m, n]$, $F = TUC_4C_8(S)[m, n]$ are two different types of C_4C_8 nanotubes and $G = TC_4C_8(R)[m, n]$ is a C_4C_8 nanotorus in terms of the number of rhombs in a fixed row (m) and column (n). We have

Theorem 6 The Wiener indices of E, F, G and H can be computed as follows:

1. (Yousefi and Ashrafi 2006)

$$W(E) = \begin{cases} \frac{2m}{3}(m^2 - 1) + mn(m + 3n) - k_1 & m < n \\ \frac{2n}{3}(n^2 - 1) + mn(3m + n) - k_2 & m > n \\ \frac{n}{3}(14n^2 - k_3) & m = n \end{cases}$$

$$\text{in which } k_1 = \begin{cases} 0 & 2|n \ \& \ 2|m \\ n - m & 2|n \ \& \ 2 \nmid m \\ m & 2 \nmid n \ \& \ 2|m \\ n & 2 \nmid n \ \& \ 2 \nmid m \end{cases} \quad k_2 = \begin{cases} 0 & 2|m \\ m & 2 \nmid m \end{cases} \quad k_3 = \begin{cases} 2 & 2|n \\ 5 & 2 \nmid n \end{cases}$$

2. (Ashrafi and Yousefi 2007b)

$$W(F) = \begin{cases} \frac{nm^2}{6}(6m^2 + 3nm + n^2 - 4) & n \leq m \\ \frac{mn^2}{6}(6n^2 + 3mn + m^2 - 4) & m < n \end{cases}$$

3. (Yousefi and Ashraf 2008b, 2011)

$$W(G) = \begin{cases} \frac{2mn^2}{3}(4m^2 + 9mn - 4) + \frac{m^2n}{6}[16m^2 - 7 + 3(-1)^n] & m \leq \frac{n+1}{2} \\ \frac{2mn^2}{3}(12m^2 + 3mn + 2n^2 - 5) - \frac{n^3}{6}(n^2 - 1) & \\ -\frac{n}{8}(8m^2 + n^2 - 4mn - 1)[1 - (-1)^n] & m > \frac{n+1}{2} \end{cases}$$

Suppose $e = uv$ and $M(e)$ denotes the number of edges that are equidistant to the vertices u and v (including the edge e itself), then evidently $m_u(e) + m_v(e) + M(e) = m$.

Therefore, $PI(G) = m^2 - \sum_{e=uv} M(e)$. Using this simple equation, it can be proved that if G is an acyclic graph containing n vertices then $PI(G) = (n - 1)(n - 2)$. In particular, $PI = 0$, for acyclic graphs when $n = 1$ and 2 . Since every acyclic graph with n vertices has exactly $m = n - 1$ edges, the previous result states that in every acyclic graph G with m edges $PI(G) = m(m - 1)$.

The notion of **PI partition** was introduced by Klavžar (2007) to find a formula for the PI index of product graphs. Suppose G is a graph and X is a subset of $V(G)$. The subgraph of G induced by X will be denoted $\langle X \rangle$. Moreover, let ∂X stands for the set of edges of G with one end vertex in X and the other not in X . For an edge $e = uv$ of G , we define $V_1(e)$ and $V_2(e)$ as follows:

$$V_1(e) = \{x \in V(G) \mid d(x,u) < d(x,v)\} \text{ and } V_2(e) = \{x \in V(G) \mid d(x,u) > d(x,v)\}.$$

It is easily seen that if G is bipartite then for any edge e of G , $V_1(e)$ and $V_2(e)$ form a partition of $V(G)$. We say that a partition E_1, \dots, E_k of $E(G)$ is a PI-partition of G if for any $i, 1 \leq i \leq k$, and for any $e, f \in E_i$ we have $V_1(e) = V_1(f)$ and $V_2(e) = V_2(f)$. If $e = uv$ is an edge a G then we define $V_3(e)$ to be the set of all vertices that are at equal distance from u and v . Thus $V(G) = V_1(e) \cup V_2(e) \cup V_3(e)$. Klavžar (2007) proved that if E_1, \dots, E_k is a PI-partition of a graph G then $PI(G) = |E(G)|^2 - \sum_{i=1}^k |E_i|(|E_i| + |E(\langle V_3(e) \rangle)| + |\partial V_3(e)|)$. If G is bipartite then $\partial V_3(e) = V_3(e) = \emptyset$; and consequently $PI(G) = |E(G)|^2 - \sum_{i=1}^k |E_i|^2$.

Using the mentioned method of Klavžar or a straightforward calculation by the mentioned simple equation, one can prove the following two results:

Theorem 7 The PI index of armchair polyhex, zig-zag polyhex and polyhex nanotorus nanotubes can be computed as follows:

1. (Ashrafi and Loghman 2006a)

$$PI(B[2p, q]) = \begin{cases} \begin{cases} X - p & q \leq p + 1 \\ Y - p & q \geq p + 1 \end{cases} & 2|p \ \& \ 2|q - 1 \\ \begin{cases} X & q \leq p + 1 \\ Y & q \geq p + 1 \end{cases} & \text{Otherwise} \end{cases},$$

where $X = 9p^2q^2 - 12p^2q - 5pq^2 + 8pq + 4p^2 - 4p$ and $Y = 9p^2q^2 - 20p^2q - p^2 + 4pq + 4p^3 + 8p^2 - 4p$.

2. (Ashrafi and Loghman 2006b)

$$PI(A[2p, q]) = \begin{cases} p^2(9q^2 - 7q + 2) - 4pq^2 & q \leq p \\ p^2(9q^2 - 15q + 4p - 2) + 4pq & q \geq p \end{cases}.$$

3. (Ashrafi and Rezaei 2007)

$$PI(C) = \begin{cases} 9p^2q^2 - pq^2 - 12p^2q + 4pq & q \geq 2p \\ 9p^2q^2 - 7pq^2 + 4pq & q < 2p \end{cases}$$

Theorem 8 The PI index of $TUC_4C_8(R/S)$ nanotubes and $TC_4C_8(R/S)$ nanotori can be computed as follows:

1. (Ashrafi and Loghman 2008)

$$PI(E[p,q]) = \begin{cases} \begin{cases} 36p^2q^2 - 26pq^2 - 2p^2q + 8pq & q < p \\ 36p^2q^2 - 26p^2q - 2pq^2 + 8pq & q \geq p \end{cases} & \text{if } p \ \& \ q \text{ are even} \\ \begin{cases} 36p^2q^2 - 10pq^2 - 2p^2q & q < p \\ 36p^2q^2 - 10p^2q - 2pq^2 & q \geq p \end{cases} & \text{if } p \ \& \ q \text{ are odd} \\ \begin{cases} 36p^2q^2 - 18pq^2 - 2p^2q & q < p \\ 36p^2q^2 - 18p^2q - 2pq^2 + 8pq & q > p \end{cases} & \text{if } p \text{ is even } \ \& \ q \text{ is odd} \\ \begin{cases} 36p^2q^2 - 18p^2q - 2pq^2 & q > p \\ 36p^2q^2 - 18pq^2 - 2p^2q + 8pq & q < p \end{cases} & \text{if } p \text{ is odd } \ \& \ q \text{ is even} \end{cases}$$

2. (Ashrafi and Loghman 2006c)

$$PI(F[4p, q]) = \begin{cases} X & q \leq p \\ Y & q \geq p \end{cases},$$

where $X = 36p^2q^2 - 28p^2q + 8p^2 - 8pq^2$ and $Y = 36p^2q^2 - 36p^2q - 4pq^2 + 4pq + 4p^3 + 4p^2$.

3. (Ashrafi et al. 2009)

$$PI(G[p, q]) = \begin{cases} 36p^2q^2 - 8p^2q - 10pq^2 + 4pq & q \leq 2p \\ 36p^2q^2 - 20p^2q - 4pq^2 + 4pq & q > 2p \end{cases}.$$

We are now ready to investigate the Szeged index of nanotubes and nanotori. Dobrynin and Gutman (1994) proved that if G is a connected bipartite graph with n vertices and m edges, then $Sz(G) = \frac{1}{4} \left(n^2m - \sum_{e \in E(G)} (d(u) - d(v))^2 \right)$. Using this result Yousefi et al. (2008d) proved that the Szeged index of a polyhex nanotorus is computed by $Sz(C) = \frac{3}{8}p^3q^3$. Another application of the mentioned result

of Dobrynin and Gutman is computing Szeged index of $C_4C_8(S)$ nanotubes. In (Heydari and Taeri 2009) and (Manoochehrian et al. 2008) the Szeged index of $TUC_4C_8(S)[p, q]$ and zig-zag polyhex nanotubes are computed as follows:

Theorem 9 Suppose F denotes the $TUC_4C_8(S)[p, q]$ nanotube. Then

1. If $q \leq p$, then the Szeged index of F is given by the following formula:

$$Sz(F) = \frac{pq}{3}(-2q^4 + (64p^2 + 2)q^2 - 16p^2).$$

2. If $q > p$, then Szeged index of long $TUC_4C_8(S)$ nanotubes is given by

$$Sz(F) = \begin{cases} \frac{p}{15} (12p^5 - 80qp^4 + (160q^2 - 20)p^3 + 200q^3p^2 \\ + (20q^4 - 60q^2 + 8)p - 2q(q^4 - 5q^2 + 4)) & q \leq 2p \\ \frac{p^2}{15} (-52p^4 + 80qp^3 + 60p^2 + (280q^3 - 120q)p - 8) & q > 2p \end{cases} .$$

3. The Szeged index of zig-zag polyhex nanotube is as follows.

$$Sz(A[p, q]) = \begin{cases} \frac{8}{3}p^3q^3 - \frac{2}{3}p^3q + \frac{1}{6}pq^3 - \frac{1}{6}pq^5 & q \leq p \\ \frac{5}{2}p^6 + \frac{43}{6}p^5 + \frac{35}{6}p^4 + \frac{5}{6}p^3 - \frac{1}{3}p^2 & q = p + 1 \\ \frac{2}{3}p^3q^3 + \frac{2}{3}p^3q - \frac{2}{15}pq + \frac{2}{15}p^2 - \frac{1}{5}pq^5 + \frac{4}{3}p^2q^4 & \\ -\frac{5}{3}pq^3 + \frac{8}{3}p^2q^2 - \frac{1}{3}p^4 - \frac{4}{3}p^5q + \frac{1}{5}p^6 & p + 1 < q < 2p \\ \frac{89}{5}p^6 - \frac{5}{3}p^4 - \frac{1}{15}p^2 & q = 2p \\ 2p^3q^3 - \frac{4}{3}p^3q - \frac{2}{15}p^2 + \frac{4}{3}p^5q - \frac{13}{15}p^6 + p^4 & q > 2p \end{cases} .$$

Recently, (Farahani 2012) computed some degree-based topological indices of zig-zag and armchair polyhex nanotubes. His calculations shows that $\chi(A[m, n]) = mn + 2m\left(\frac{\sqrt{6}-1}{3}\right)$, $ABC(A[m, n]) = 2mn + 2m\left(\sqrt{2} - \frac{2}{3}\right)$, $M_1(A[m, n]) = 18mn + 8$, $M_2(A[m, n]) = 27mn + 6$, $\chi(B[m, n]) = \left(n + \frac{\sqrt{6}-1}{3} + \frac{1}{2}\right)m$, $ABC(B[m, n]) = \left(2n + \frac{3\sqrt{2}}{2} - \frac{2}{3}\right)m$, $M_1(B[m, n]) = 18mn + 8$ and $M_2(B[m, n]) = 27mn + 7m$. Moreover, (Asadpour et al. 2011) proved that $\chi(E[p, q]) = 4pq$, $M_2(E[p, q]) = 108pq$, $ABC(E[p, q]) = \frac{12\sqrt{2}}{\sqrt{3}}pq$, $\chi(F[p, q]) = 6pq + \left(\frac{4}{\sqrt{6}} - 3\right)(p + q) + 4 - \frac{2}{\sqrt{6}}$, $M_2(F[p, q]) = 16(3pq + p + q - 1)$ and $ABC(F[p, q]) = \sqrt{2}(8pq - 3p - 3q + 4) + 4\sqrt{\frac{3}{5}}(p + q - 2)$.

The Balaban index J which is defined as the average distance sum connectivity is the least degenerate single topological index proposed till now. The mathematical properties of this distance-based topological index in the classes of polyhex and $TUC_4C_8(R/S)$ nanotori are investigated by (Iranmanesh and Ashrafi 2007). They proved that:

Theorem 10 Suppose $C[m, n]$, $E[m, n]$ and $F[m, n]$ are polyhex and $TUC_4C_8(R/S)$ nanotori, respectively. Then,

$$a) \quad J(C[m, n]) = \begin{cases} \frac{12m^2n}{(mn + 4)(6m^2 + n^2 - 4)} & n < m \\ \frac{12mn^2}{(mn + 4)(3n^2 + 3mn + m^2 - 4)} & n \geq m \end{cases},$$

$$b) \quad J(E[m, n]) = \begin{cases} \frac{108m^3n^3}{(mn + 1)[2m(m^2 - 1) + 3mn(m + 3n) - 3k_1]} & m < n \\ \frac{108m^3n^3}{(mn + 1)[2n(n^2 - 1) + 3mn(3m + n) - 3k_2]} & m > n \\ \frac{108m^2n^3}{(n^2 + 1)(14n^2 - k_3)} & m = n \end{cases},$$

in which

$$k_1 = \begin{cases} 0 & \text{if } 2|n \quad \& \quad 2|m \\ n - m & \text{if } 2|n \quad \& \quad 2 \nmid m \\ m & \text{if } 2 \nmid n \quad \& \quad 2|m \\ n & \text{if } 2 \nmid n \quad \& \quad 2 \nmid m \end{cases}, \quad k_2 = \begin{cases} 0 & \text{if } 2|m \\ m & \text{if } 2 \nmid m \end{cases}, \quad k_3 = \begin{cases} 2 & \text{if } 2|n \\ 5 & \text{if } 2 \nmid n \end{cases},$$

and, “|” denotes the divisibility relation.

$$c) \quad J(F[m, n]) = \begin{cases} \frac{54mn^2}{(mn + 2)(6n^2 + 3nm + m^2 - 4)} & n \leq m \\ \frac{54mn^2}{(mn + 2)(6m^2 + 3mn + n^2 - 4)} & m < n \end{cases}$$

In the end of this chapter we report two recent results in computing eccentric connectivity index of nanotubes and nanotori.

Theorem 11 The eccentric connectivity index of armchair and zig-zag polyhex nanotubes are computed as follows:

1. (Saheli and Ashrafi 2010a) The eccentric connectivity index of a zig-zag polyhex nanotube is as follows:

$$\xi(A[p, q]) = \begin{cases} -\frac{7}{2}pq + p + \frac{9}{2}pq^2 & p \leq q + 1 \\ -\frac{1}{2}pq + p + \frac{21}{4}pq^2 - 3p^2 + \frac{3}{4}p^3 - \frac{3}{2}qp^2 & \\ + \frac{1 - (-1)^q}{2} 3p \left(p - q - \frac{1}{4} \right) & q + 1 < p < 2q . \\ -4pq - 2p^2 + \frac{7}{4}p + \frac{9}{4}pq^2 + \frac{3}{2}qp^2 & \\ + \frac{1 - (-1)^q}{2} 3p(p + q + 1) & p \geq 2q \end{cases}$$

2. (Saheli and Ashrafi 2010b) The eccentric connectivity index of an armchair polyhex nanotube with parameters p and q is as follows:

$$\xi(B[p, q]) = \begin{cases} q^2(3p - 2) & p \leq \frac{q}{2} + 1 \\ \frac{3}{4}q^3 + \frac{1}{2}q^2 + 2q - 5qp + 3qp^2 & \frac{q}{2} + 1 < p \leq q . \\ \frac{9}{4}qp^2 - \frac{7}{2}qp + \frac{3}{2}q^2p - q^2 + \frac{5}{4}q & p \geq q + 1 \end{cases}$$

Theorem 12 The eccentric connectivity index of $TUC_4C_8(R/S)$ nanotubes and nanotori can be computed as follows:

1. The eccentric connectivity index of $E[p, q]$ is given by

$$\xi(E[p, q]) = \begin{cases} (p + 1)[(9q^2 + 18pq + 15p + 22q + 10) + R(p, q)] & q < \left\lceil \frac{p}{2} \right\rceil \\ (p + 1)[6p^2 - (6pq + 33q^2 + 5p + 42q + 14) + R(p, q)] & \left\lceil \frac{p}{2} \right\rceil \leq q < p , \\ (p + 1)[(27q^2 + 6pq + 5p + 42q + 14) + R(p, q)] & q \geq p \end{cases}$$

where $R[p, q] = \left[(6q + 5) \frac{1 - (-1)^p}{2} + 3 \frac{1 - (-1)^q}{2} \right]$.

2. The eccentric connectivity index of $F[p, q]$ is given by

$$\xi(F[p, q]) = \begin{cases} 22pq + 8p^2 + 12p^2q + 18pq^2 & p \leq \left\lceil \frac{q+1}{2} \right\rceil \\ 28pq - 4p^2 + 12p^3 + 21pq^2 + 8p + 3p \frac{1 - (-1)^q}{2} & \left\lceil \frac{q+1}{2} \right\rceil < p \leq q + 1 . \\ 8pq + 16p^2 + 24p^2q + 9pq^2 + 3p + 3p \frac{1 - (-1)^q}{2} & p > q + 1 \end{cases}$$

3. The eccentric connectivity index of $G[p, q]$ is given by

$$\xi(G[p, q]) = \begin{cases} 12p(q+1)(p+q+1) & p \leq \left\lceil \frac{q+1}{2} \right\rceil \\ \frac{4p+q}{2} + \frac{1-(-1)^q}{4} & p > \left\lceil \frac{q+1}{2} \right\rceil \end{cases}.$$

6.5 Conclusions

We have presented here a review of topological-based methods for evaluating the symmetry constraints and topological indices for carbon nanostructures such as nanotubes and nanotori. The first task, has been fulfilled by considering the *topological symmetry* of the graph of a given chemical system; such a symmetry just reflects the symmetry properties of the automorphism group of the graph providing *the upper limit—fully rooted in topology—on the geometrical symmetry* of the nanostructure. The second goal considers the application of topological indices in characterizing nanostructures. The reported theorems are very useful because they allow a fast computation of the topological indices for complex graphs (nanostructures) starting from their structural building elements, to derive exact algorithms easy to programme on the computer.

While the primary application concerns the description of carbon-networks in chemical compounds, other applications exist to rank for example proteins according to their degree of folding and topological invariants are useful in social-networks description.

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References

- Arezoomand M, Taeri B (2009) The full symmetry and irreducible representations of nanotori. *Acta Cryst A* 65:249–252
- Asadpour J, Mojarad R, Safikhani L (2011) Computing some topological indices of nanostructures. *Dig J Nanomat Biostruct* 6:937–941
- Ashrafi AR, Loghman A (2006a) PI index of armchair polyhex nanotubes. *Ars Combin* 80:193–199
- Ashrafi AR, Loghman A (2006b) PI index of zig-zag polyhex nanotubes. *MATCH Commun Math Comput Chem* 55:447–452
- Ashrafi AR, Loghman A (2006c) Padmakar-Ivan index of $TUC_4C_8(S)$ nanotubes. *J Comput Theor Nanosci* 3:378–381
- Ashrafi AR, Loghman A (2008) Computing Padmakar-Ivan index of a $TC_4C_8(R)$ Nanotorus. *J Comput Theor Nanosci* 5:1431–1434
- Ashrafi AR, Rezaei F (2007) PI index of polyhex nanotori. *MATCH Commun Math Comput Chem* 57:243–250

- Ashrafi AR, Yousefi S (2007a) A new algorithm for computing distance matrix and Wiener index of zig-zag polyhex nanotubes. *Nanoscale Res Lett* 2:202–206
- Ashrafi AR, Yousefi S (2007b) Computing the Wiener index of a $TUC_4C_8(S)$ nanotorus. *MATCH Commun Math Comput Chem* 57:403–410
- Ashrafi AR, Rezaei F, Loghman A (2009) PI index of the $C_4C_8(S)$ nanotorus. *Revue Roum Chim* 54:823–826
- Ashrafi AR, Doššlić T, Saheli M (2011a) The eccentric connectivity index of $TUC_4C_8(R)$ nanotubes. *MATCH Commun Math Comput Chem* 65:221–230
- Ashrafi AR, Saheli M, Ghorbani M (2011b) The eccentric connectivity index of nanotubes and nanotori. *J Comput Appl Math* 16:4561–4566
- Balaban AT (1982) Distance connectivity index. *Chem Phys Lett* 89:399–404
- Balaban AT (1983) Topological indices based on topological distances in molecular graphs. *Pure Appl Chem* 55:199–206
- Bosma W, Cannon J, Playoust C (1997) The Magma algebra system I: the user language. *J Symb Comput* 24:235–265
- Das KC (2010) Atom-bond connectivity index of graphs. *Discrete Appl Math* 158:1181–1188
- Das KC, Trinajstić N (2010) Comparison between first geometric-arithmetic index and atom-bond connectivity index. *Chem Phys Lett* 497:149–151
- Diudea MV, Ursu O, Nagy LCs (2002) TOPOCLUJ. Babes-Bolyai University, Cluj
- Diudea MV, Stefu M, Pârv B, John PE (2004) Wiener index of armchair polyhex nanotubes. *Croat Chem Acta* 77:111–115
- Dobrynin A, Gutman I (1994) On a graph invariant related to the sum of all distances in a graph. *Publ Inst Math (Beograd) (N.S.)* 56:18–22
- Dobrynin A, Gutman I (1995) Solving a problem connected with distances in graphs. *Graph Theor Notes NY* 28:21–23
- Dobrynin A, Gutman I, Domotor GA (1995) Wiener-type graph invariant for some bipartite graphs. *Appl Math Lett* 8(5):57–62
- Estrada E (2008) Atom-bond connectivity and the energetic of branched alkanes. *Chem Phys Lett* 463:422–425
- Estrada E, Torres L, Rodriguez L, Gutman I (1998) An atom-bond connectivity index: modelling the enthalpy of formation of alkanes. *Indian J Chem* 37A:849–855
- Farahani MR (2012) Some connectivity indices and Zagreb index of polyhex nanotubes. *Acta Chim Slov* 59:779–783
- Fath-Tabar GH, Vaez-Zadeh B, Ashrafi AR, Graovac A (2011) Some inequalities for the atom-bond connectivity index of graph operations. *Discret Appl Math* 159:1323–1330
- Furtula B, Graovac A, Vukičević D (2009) Atom-bond connectivity index of trees. *Discret Appl Math* 157:2828–2835
- Gutman I (1994) A formula for the Wiener number of trees and its extension to graphs containing cycles. *Graph Theor Notes NY* 27:9–15
- Gutman I, Das KC (2004) The first Zagreb index 30 years after. *Commun Math Comput Chem* 50:83–92
- Gutman I, Trinajstić N (1972) Graph theory and molecular orbitals. Total ϕ -electron energy of alternant hydrocarbons. *Chem Phys Lett* 17:535–538
- Heydari A, Taeri B (2009) Szeged index of $TUC_4C_8(S)$ nanotubes. *Eur J Combin* 30:1134–1141
- HyperChem package Release 7.5 for Windows (2002) Hypercube Inc., Florida, USA
- Iranmanesh A, Ashrafi AR (2007) Balaban index of an armchair polyhex, $TUC_4C_8(R)$ and $TUC_4C_8(S)$ nanotorus. *J Comput Theor Nanosci* 4:514–517
- John PE, Diudea MV (2004) Wiener index of zig-zag polyhex nanotubes. *Croat Chem Acta* 77:127–132
- Khadikar PV, Deshpande NV, Kale PP, Dobrynin A, Gutman I, Domotor G (1995) The Szeged index and an analogy with the wiener index. *J Chem Inf Compute Sci* 35:545–550
- Khadikar PV, Karmarkar S, Agrawal VK (2001) A novel PI index and its applications to QSPR/QSAR studies. *J Chem Inf Comput Sci* 41:934–949

- Khalifeh MH, Yousefi-Azari H, Ashrafi AR (2009) The first and second Zagreb indices of some graph operations. *Discret Appl Math* 157:804–811
- Khodashenas H, Nadjafi-Arani MJ, Ashrafi AR, Gutman I (2011) A new proof of the Szeged-Wiener theorem. *Kragujev J Math* 35:165–172
- Klarner DA (1997) Polyominoes. In: Goodman JE, O'Rourke J (eds) *Handbook of discrete and computational geometry*, CRC Press, Boca Raton, pp 225–242 (Chapter 12)
- Klavžar S (2007) On the PI index: PI-partitions and Cartesian product graphs. *MATCH Commun Math Comput Chem* 57:573–586
- Klavžar S, Rajapakse A, Gutman I (1996) The Szeged and the Wiener index of graphs. *Appl Math Lett* 9:45–49
- Manoochehrian B, Yousefi-Azari H, Ashrafi AR (2008) Szeged index of a zig-zag polyhex nanotube. *Ars Combin* 86:371–379
- Randić M (1974) On the recognition of identical graphs representing molecular topology. *J Chem Phys* 60:3920–3928
- Randić M (1975) On characterization of molecular branching. *J Am Chem Soc* 97:6609–6615
- Randić M (1976) On discerning symmetry properties of graphs. *Chem Phys Lett* 42:283–287
- Saheli M, Ashrafi AR (2010a) The eccentric connectivity index of zig-zag polyhex nanotubes and nanotori. *J Comput Theor Nanosci* 7:1900–1903
- Saheli M, Ashrafi AR (2010b) The eccentric connectivity index of armchair polyhex nanotubes. *Maced J Chem Chem Eng* 29:71–75
- Sardana S, Madan AK (2001) Application of graph theory: relationship of molecular connectivity index, Wiener's index and eccentric connectivity index with diuretic activity. *MATCH Commun Math Comput Chem* 43:85–98
- Sharma V, Goswami R, Madan AK (1997) Eccentric connectivity index: a novel highly discriminating topological descriptor for structure-property and structure-activity studies. *J Chem Inf Comput Sci* 37:273–282
- Staic MD, Petrescu-Nita A (2013) Symmetry group of two special types of carbon nanotori. *Acta Cryst A* 69:1–5
- The GAP Team (1995) *GAP, groups, algorithms and programming*. Lehrstuhl De für Mathematik, RWTH, Aachen
- Trinajstić N (1992) *Chemical graph theory*. CRC Press, Boca Raton
- Wiener H (1947) Structural determination of paraffin boiling points. *J Am Chem Soc* 69:17–20
- Yavari M, Ashrafi AR (2009) On the symmetry of a zig-zag and an armchair polyhex carbon nanotorus. *Symmetry* 1:145–152
- Yousefi S, Ashrafi AR (2006) An exact expression for the Wiener index a polyhex nanotoruse. *MATCH Commun Math Comput Chem* 56:169–178
- Yousefi S, Ashrafi AR (2007) An exact expression for the Wiener index of a $TUC_4C_8(R)$ nanotorus. *J Math Chem* 42:1031–1039
- Yousefi S, Ashrafi, AR (2008a) Distance matrix and wiener index of armchair polyhex nanotubes. *Stud Univ Babes-Bolyai Chem* 53:111–116
- Yousefi S, Ashrafi AR (2008b) An algorithm for constructing Wiener matrix of $TUC_4C_8(R)$ nanotubes. *Curr Nanosci* 4:161–165
- Yousefi S, Ashrafi AR (2011) 3-dimensional distance matrix of a $TC_4C_8(R)$ nanotoruse. *MATCH Commun Math Comput Chem* 65:249–254
- Yousefi S, Yousefi-Azari H, Khalifeh MH, Ashrafi AR (2008c) Computing distance matrix and related topological indices of an achiral polyhex nanotube. *Int J Chem Mod* 1:149–156
- Yousefi S, Yousefi-Azari H, Ashrafi AR, Khalifeh MH (2008d) Computing Wiener and Szeged indices of a polyhex Nanotorus. *J Sci Univ Tehran* 33:7–11
- Yousefi-Azari H, Ashrafi AR, Khalifeh MH (2008e) Computing vertex-PI index of single and multiwalled nanotubes. *Dig J Nanomat Bios* 3:315–318
- Zhou B (2004) Zagreb indices. *MATCH Commun Math Comput Chem* 52:113–118
- Zhou B, Gutman I (2005) Further properties of Zagreb indices. *MATCH Commun Math Comput Chem* 54:233–239