Digest Journal of Nanomaterials and Biostructures Vol. 4, No. 3, September 2009, p. 593 - 596

THE SYMMETRY GROUP OF NANOTUBES

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Euclidean graph associated with a molecule is defined by a weighted graph with adjacency matrix $M = [d_{ij}]$, where for $i \neq j$, d_{ij} is the Euclidean distance between the nuclei i and j. In this matrix d_{ii} can be taken as zero if all the nuclei are equivalent. The symmetry group of a molecule is defined as the set of all permutation matrix P such that $P^tMP = M$. In this paper, the symmetry of a V-phenylenic nanotube is computed for the first time. A permutation representation of this group is also presented.

(Received September 1, 2009; accepted September 30, 2009)

Keywords: Nanotube, Symmetry, Euclidean graph.

1. Introduction

An object is called symmetrical if some movement or operation leaves the object in a position indistinguishable from its original position. The symmetry of molecules and solids is a very powerful tool for developing and understanding of bonding and physical properties used to predict the nature of molecular orbitals. Chemists and physicists classify molecules in terms of their symmetry. It is of some value to recognise that all molecules that have the same basic ”shape” share a number of common properties. The process of doing the rotation, reflection etc. is referred to as a symmetry operation if it does not change the appearance of the molecule. It is easy to see that all symmetry operations of a molecule forms a group named symmetry group of molecule under consideration.[1-3]

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-shapes of which are represented by V(G) and E(G), respectively. The graph G is said to be connected if for every vertices x and y in V(G) there exists a path between x and y. A weighted graph G = (V, E, w) is a combinatorial object consisting of an arbitrary set V = V(G) of vertices, a set E = E(G) of unordered pairs {x, y} = xy of distinct vertices of G called edges, and a weighting function w: V(G) $\longrightarrow$ R assigns positive real numbers (weights) to edges. An automorphism of a weighted graph G is a permutation g of the vertex set of G with the property that: (i) for any vertices u and v, g(u) and g(v) are adjacent if and only if u is adjacent to v; (ii) for every edge e = uv, w(uv) = w(g(u)g(v)). The set of all automorphisms of a graph G, with the operation of composition of permutations, is a permutation group on V(G), denoted Aut(G). Here two groups G and H are said to be isomorphic if there exists a one-to-one correspondence a $\leftrightarrow$ a' such that (ab)' = a'b'.

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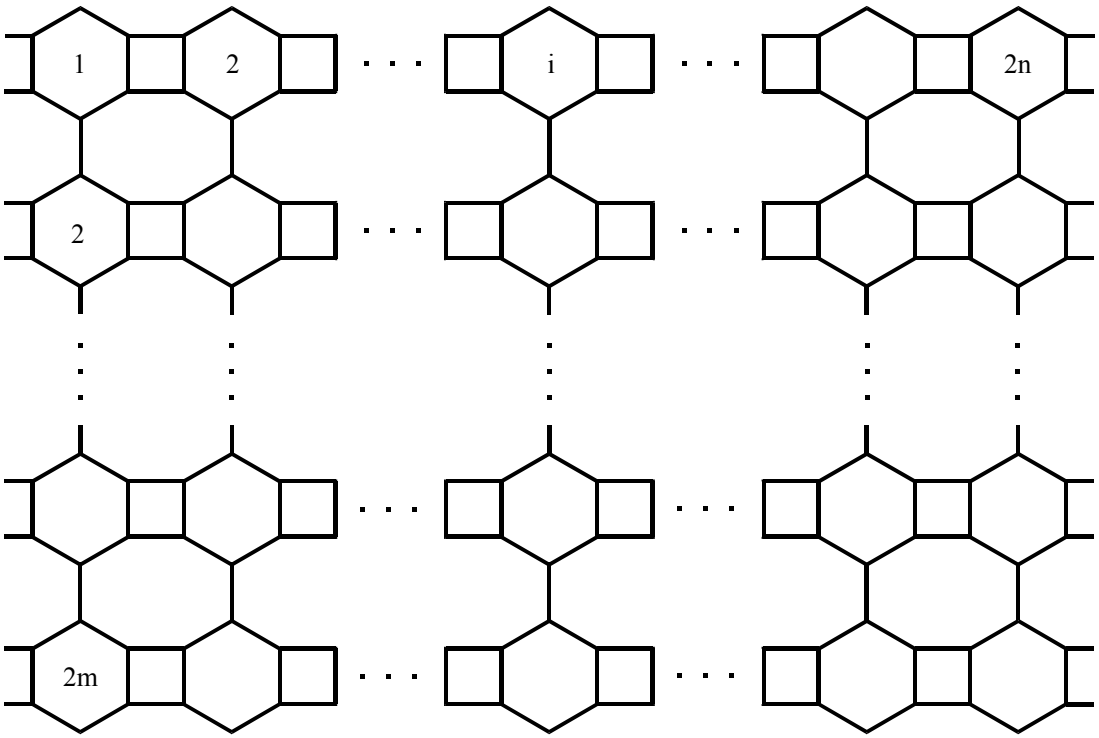

Fig. 1. The 2-dimensional lattice of a V- Phenylenic nanotube.

An Euclidean graph is a weighted graph related to a molecule with the adjacency matrix D = [d_{ij}], where for $i \neq j$, d_{ij} is the Euclidean distance between the nuclei i and j. In this matrix d_{ii} can be taken as zero if all the nuclei are equivalent. Otherwise, one may introduce different weights for different nuclei.

In this paper, symmetry means the automorphism group symmetry of a graph. The symmetry of a graph, also called a topological symmetry, accounts only for the bond relations between atoms, and does not fully determine molecular geometry. The symmetry of a graph does not need to be the same as (i.e. isomorphic to) the molecular point group symmetry. However, it does represent the maximal symmetry which the geometrical realization of a given topological structure may posses.

2. Computational Details

We now recall some algebraic definitions that will be used in the paper. The adjacency matrix or Hamiltonian operator A = [A_{ij}] of a graph G with n vertices is the square n × n symmetric matrix which contains information about the internal connectivity of vertices in the graph. It is defined as

$$A_{ij} = \begin{cases} 1 & \text{if vertices i and j are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

It is well known that the symmetry operators in the point group of a molecule always commute with its Hamiltonian operator. So the symmetry group H of molecular graph must contain the point group H_p of the graph.

A permutations σ on a set A is a one-to-one and onto functions from A into A. The set of all permutations on A = {1,2, …, n} is denoted by S_n, the symmetric group on n letters. A permutation matrix is a matrix that has exactly one 1 in each row or column and 0s elsewhere.

Permutation matrices are the matrix representation of permutations. Suppose Π(n) denotes the set of all permutation matrices on n symbols.

In general, for a permutation σ on *n* objects, the corresponding permutation matrix is an n-by-n matrix P_σ is given by $P_\sigma = [x_{ij}]$, $x_{ij} = 1$ if $i = \sigma(j)$ and 0 otherwise. We can see that $P_\sigma P_\pi = P_{\sigma\pi}$, for any two permutations σ and π on *n* objects, $P_{(1)(2)\ldots(n)}$ is the identity matrix, and, permutation matrices are orthogonal matrices, a square matrix whose transpose is its inverse. Thus, $(P_\sigma)^{-1} = P_\sigma$. Then Π(n) is a group under product of matrices and the function f from S_n into Π(n) defined as $f(\sigma) = P_\sigma$ is an isomorphism between S_n and Π(n).

It is a well-known fact that a permutation of the vertices of a graph belongs to its automorphism group if it satisfies $(P_\sigma)^t A P_\sigma = A$, where $(P_\sigma)^t$ is the transpose of permutation matrix P_σ, $\sigma \in S_n$ and *A* is the adjacency matrix of the graph under consideration.[3-7] One of us (ARA)[8-12], presented an algorithm for computing symmetry of molecules. In the mentioned papers, some GAP and MATLAB programs also presented which are useful for computing symmetry of molecules.[13,14]

3. Main results

Carbon nanotubes are basically sheets of graphite rolled up into a tube. It is constructed from the hexagonal two dimensional lattice of graphite mapped on a given one-dimensional cylinder of radius R. A V−phenylenic nanotube is constructed in a similar way by a sheet covered by squares, hexagons and octagons, see Figure 1.

A subgroup N of a group G is called normal, if $g^{-1}Ng = N$, for all $g \in G$. The dihedral group D_n of degree n, $n \geq 3$, is the subgroup of S_n generated by the permutations a = (1,2,…,n) and b such that:

b = (2,n)(3,n-1)(4,n-2)…(n/2,n/2+2) ; n is even
(2,n)(3,n-1)(4,n-2)…((n+1)/2,(n+3)/2) ; n is odd.

It is easy to see that D_n is non-abelian and <a> is a normal subgroup of D_n. It is possible to prove that D_n is actually isomorphic to the group of symmetries of a regular polygon with n-sides.

Suppose G is a group and H and K are subgroups of G such that (i) G = HK = {xy | x ∈ H & y ∈ K}, (ii) H is normal in G, and, (iii) H ∩ K = 1. Then G is called a semidirect product of H by K. It is a well-known fact that if G is a semidirect product of H by K and K is normal subgroups of G then G is isomorphic to the direct product of H and K.

Suppose L is the 2-dimensional lattice of a V- phenylenic nanotube containing 2n hexagons in each row and 2m hexagons in each column, Fig. 1. Put a = (1,2,…,2n) and b = (2,2n)(3,2n-1)(4,2n-2)…(n,n+2). Then the group H generated by a and b is a subgroup of the symmetry group G of a V- phenylenic nanotube. This shows that the symmetry group of V-phenylenic nanotube contains a subgroup isomorphic to D_{2n}. But a vertical plane determines a symmetry element c of G such that $c \notin H$. Since |H| = 1/2|G|, H is a normal subgroup of G. This implies that G is a semidirect product of H by a cyclic group of order 2. On the other hand, the symmetry element c commutes with a and b. Therefore, <c> is also normal in G. Now <c> ∩ H is the trivial subgroup and so by the mentioned theorem, G is isomorphic to the direct product of H by a cyclic group of order 2. Thus $G = Z_2 \times D_{2n}$ and we proved the following theorem:

Theorem: The group G of the symmetry of a V- phenylenic nanotube is a direct product of D_{2n} by the cyclic group Z_2.

4. Conclusions

Our method presented here can be expanded to other topologies as the V-phenylenic nanotorus. Our main assumption is that the nanotube is achiral. For chiral nanotubes the subgroup <c> is not normal and so the group is not expressed as a direct product of two subgroups.

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