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The enumeration of an infinite class of nanohorns

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Enumeration of chemical compounds has been accomplished by various methods. The Polya-Redfield theorem has been a standard method for combinatorial enumerations of graphs, polyhedra, chemical compounds, and so forth. In this paper by using the computer algebra system GAP we compute the number of isomers of an infinite class of nanohorns with C_2 point group symmetry.

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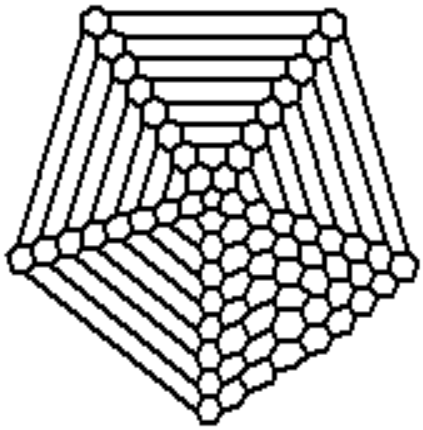
1. Introduction

Carbon exists in several forms in nature. One is the so-called nanotube which was discovered for the first time in 1991. Unlike carbon nanotubes, carbon nanohorns can be made simply without the use of a catalyst [1,2]. The tips of these short nanotubes are capped with pentagonal faces; see Fig. 1. Let *p, h, n* and *m* be the number of pentagons, hexagons, carbon atoms and bonds between them, in a given nanohorn *H*. Then one can see that $n = r^2 + 22r + 41$, $m = \frac{3r^2 + 65r + 112}{2}$ (r = 0,1,…) and the number of faces is $f = p + h$. By the Euler's formula $n - m + f = 2$, one can deduce that $p = 5$ and $h = \frac{r2 + 21r + 24}{2}$, r = 1, 2, ….



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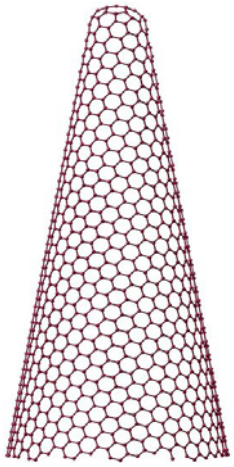

b

Fig. 1. 2-D and 3- D graph of nanohorn H.

Detecting symmetry of molecules is a well-studied problem with applications in a large number of areas. Randic [3,4] and then Balasubramanian [5,6] considered the Euclidean matrix of a chemical graph to find its symmetry. Here the Euclidean matrix of a molecular graph G is a matrix $D(G) = [d_{ij}]$, 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.

Suppose σ is a permutation on n atoms of the molecule under consideration. Then the permutation matrix P_σ is defines as $P_\sigma = [x_{ij}]$, where $x_{ij} = 1$ if $i = \sigma(j)$ and 0 otherwise. It is easy to see that $P_\sigma P_\tau = P_{\sigma\tau}$, for any two permutations σ and τ on n objects, and so the set of all $n \times n$ permutation matrices is a group isomorphic to the symmetric group S_n on n symbols. It is a well-known fact that a permutation σ of the vertices of a graph G belongs

to its automorphism group if it satisfies $P_\sigma^t A P_\sigma = A$, where A is the adjacency matrix of G. So, for computing the symmetry of a molecule, it is sufficient to solve the matrix equation $P^t E P = E$, where E is the Euclidean matrix of the molecule under consideration and P varies on the set of all permutation matrices with the same dimension as E.

Mathematically the isomer counting of poly-substituted nanohorn is essentially the same as that of hetero-fullerene.[7,8] In this paper by a similar way we compute number of isomers of an infinite families of nanohorns.

2. Main result and discussion

Groups are often used to describe symmetries of objects. This is formalized by the notion of a group action. Let G be a group and X a nonempty set. An action of G on X is denoted by G_X and X is called a G-set. It induces a group homomorphism φ from G into the symmetric group S_X on X, where $\varphi(g)x = gx$ for all $x \in X$. The orbit of x will be denoted by Gx and defines as the set of all $\varphi(g)x$, $g \in G$. The set of all G-orbits will be denoted by $G\backslash\backslash X := \{ Gx \mid x \in X\}$. Suppose g is a permutation of n symbols with exactly λ_1 orbits of size 1, λ_2 orbits of size 2, …, and λ_n orbits of size n. Then the cycle type of g is defined as $1^{\lambda_1} 2^{\lambda_2} \ldots n^{\lambda_n}$.

We now introduce the notion of cycle index. Let G be a permutation group. The cycle index of G acting on X is the polynomial $Z(G, X)$ over Q in terms of indeterminates $x_1, x_2, \ldots, x_t$, $t = |X|$, defined by $Z(G, X) = \frac{1}{|G|}\sum_{p\in G}\prod_{i=1}^{t} x_i^{c_i(p)}$, in which $(c_1(p), \cdots, c_t(p))$ is the cycle type of the permutation $p \in G$. The generalized character cycle index is defined as $P_G^{\chi}(x_1, x_2, \ldots, x_t) = \frac{1}{|G|}\sum_{p\in G}\prod_{i=1}^{t}\chi(p)x_i^{c_i(p)}$, where $\chi(g)$ is the linear character of the irreducible representation of G.

Enumeration of chemical compounds has been accomplished by various methods. The Polya-Redfield theorem has been a standard method for combinatorial enumerations of graphs, polyhedra, chemical compounds, and so forth. Combinatorial enumerations have found a wide-ranging application in chemistry, since chemical structural formulas can be regarded as graphs or three-dimensional objects.

Denote by $C_{m,n}$ the set of all functions f: $\{1, 2, \ldots, m\} \rightarrow \{x_1, x_2, \ldots, x_n\}$. The action of $p \in S_m$ induced on $C_{m,n}$ is defined by $\hat{p}(f) = fop^{-1}$, $f \in C_{m,n}$. Treating the colors $x_1, x_2, \ldots, x_n$ that comprise the range of $f \in C_{m,n}$ as, independent variables the weight of f is $W(f) = \prod_{i=1}^{m} f(i)$. Evidently, $W(f)$ is a monomial of (total) degree m. Suppose G is a permutation group of degree m, $\hat{G} = \{\hat{p} : p \in G\}$, $\hat{p}$ is as defined above. Let $p_1, p_2, \ldots, p_t$ be representatives of the distinct orbits of $\hat{G}$. The weight of p_i is the common value of $W(f), f \in p_i$. The sum of the weights of the orbits is the pattern inventory $W_G(x_1,x_2,\ldots,x_n) = \sum_{i=1}^{t} W(p_i)$.

Theorem.1 (Pólya's Theorem[9]**)** If G is a subgroup of S_m, the symmetry group on m symbols, then the pattern inventory for the orbits of $C_{m,n}$ modula $\hat{G}$ is

$$W_G(x_1,x_2,\ldots,x_n) = \frac{1}{|G|}\sum_{p\in G} M_1^{C_1(p)} M_2^{C_2(p)} \ldots M_m^{C_m(p)},$$

where $M_k = x_1^k + x_2^k + \ldots + x_n^k$ is the k^{th} power sum of the x's.

To enumerate all possibilities of the hetero-nanohorns structures, we have to consider the symmetry group to enumerate the number of chiral isomers, see [10] for more details.

From the above discussion our problem is reduced to the coloring of the corresponding nanohorn graph with $n = r^2 + 22r + 41$ vertices. Consider the molecular graph of the nanohorn H, see Fig. 1 for the case of r = 8. By using GAP software [11], one can see that the symmetry group H of these fullerenes is isomorphic to the group C_2 of order 2. Thus the cycle index of H is computed as

$$Z(\mathrm{H}, \mathrm{X}) = (x_1^{r^2+22r+41} + x_1^{1+r} x_2^{(r^2+21r+40)/2}) / 2.$$

But from the cycle indices one can compute the number of possible positional isomers, the number of chiral isomers under the symmetry group C_2, see [12-15].

In what follows we prepare a GAP program to compute the number of possible positional isomers for H. We mention here that our computations of symmetry properties and cycle indices of molecules were carried out with the use of GAP. This software was constructed by the GAP team in Aachen. In Table 1, we apply this program to compute the number of possible positional isomers for the case of $r = 4$, Fig. 2.

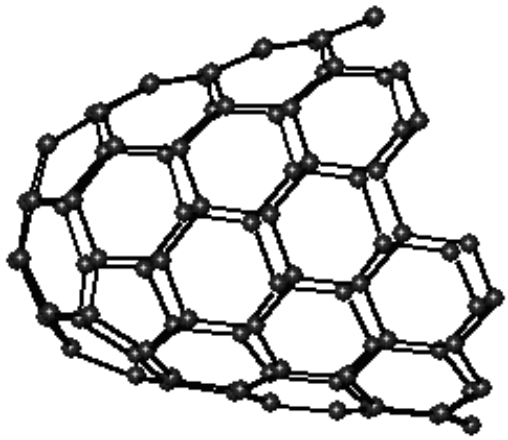

Fig. 2. Nanohorn H for the case of r = 4.

A Gap Program for counting the number of nanohorn *H*.

```
f:=function(n)
        local s,i,f,x,t;
                x:=Indeterminate(Rationals,"x");
                f:=((1+x)^(89)+(1+x)^5*(1+x^2)^(42))/2;
                t := CoefficientsOfLaurentPolynomial(f);
Print("**************************************************","\n");
Print("\n");
Print("Number of Molecules for Symmetry Group =","\n");
        for i in t[1] do
                Print(i,"\n");
        od;
Print("**************************************************","\n");
        return;
end;
```

Table 1. The number of $H_{89-k}B_k$ molecules.

k,89 -k	Number of $H_{89-k}B_k$ molecules for symmetry group
0,89	1
1,88	47
2,87	1984
3,86	56892
4,85	1221456
5,84	20756184
6,83	290563644
7,82	3445167312
8,81	35312741949
9,80	317813975539
10,79	2542510116752
11,78	18259840795912
12,77	118688954831096
13,76	703003784422072
14,75	3816306205549832
15,74	19081530912625424
16,73	88252080242700895
17,72	378964814703449873
18,71	1515859257963982160
19,70	5664526699240696204
20,69	19825843444588399064
21,68	65142057027473837360
22,67	201348176258905833868
23,66	586535991698093381120
24,65	1612973977150092969259
25,64	4193723240560438311493
26,63	10323033453643439331136
27,62	24087078058438832974432
28,61	5333567284359922361417 6
29,60	112188829084695301825888
30,59	224377658169237491264096
31,58	427041349418676753435712
32,57	774012445821111101559914
33,56	1336930588236176461627382
34,55	2202003321800426034874816
35,54	3460290934257434856293432
36,53	5190436401385740907480896
37,52	7434949439822385325514640
38,51	10174141338703878921425976
39,50	13304646365996955576915552
40,49	16630807957495803542747490
41,48	19875843656519036615151870
42,47	22715249893164345209272800
43,46	24828296394853866796169520
44,45	25956855321892585506612240

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