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Cycle Index of the Symmetry Group of Fullerenes C_{24} and C_{150}

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The three-dimensional polya cycle indices for the natural actions of the symmetry group of the small fullerene C_{24} and big fullerene C_{150} over the set of vertices, edges and faces are computed.

Key Words: Symmetry group of fullerene, Cycle index.

INTRODUCTION

In this section we describe some notations which will be kept throughout. Each molecule has a set of symmetry operations that describes the molecule's overall symmetry. This set of operations define the point group of the molecule. A chemical graph is a simple graph (V, E) all whose nodes are labeled by means of chemical elements[1,2].

It is easy to see that all unitary matrices commuting with the adjacency matrix A of a molecular graph form a group H which is called the Hamiltonian group of a graph. The elements of H is defined as a generalized symmetry operator. In a real vector space, these matrices are orthogonal. It is well known that the symmetry operators in the point group of a molecule always commute with its Hamiltonian operator. Thus the group H of the molecular graph must contain the point group of the graph[3].

For a permutation σ on n objects, the corresponding permutation matrix is an $n \times n$ matrix P_σ given by $P_\sigma = [x_{ij}]$, $x_{ij} = 1$ if $i = \sigma(j)$ and 0 otherwise. We can 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 belongs to its automorphism group if it satisfies $P_\sigma^t A P_\sigma = A$, where A is the adjacency matrix of graph under consideration. Set $Aut(G) = \{\sigma_1, \sigma_2, \cdots, \sigma_m\}$. The matrix $S_G = [s_{ij}]$, where $s_{ij} = \sigma_i(j)$ is called a solution matrix for G. Clearly, for computing the automorphism group of G, it is enough to calculate a solution matrix for G.

Lemma 1: (Ashrafi[4]) Suppose $A = [a_{ij}]$ and $B = [b_{ij}]$ are two matrices and P_σ is a permutation matrix. If $B = P_\sigma P_\sigma^t$, $\sigma(i) = r$ and $\sigma(j) = s$, then $a_{rs} = b_{ij}$.

Proof: Suppose $P_\sigma = [y_{ij}]$, then $U_i = [y_{il}, \cdots, y_{im}]$ is the i^{th} row of P_σ. Since $\sigma(i) = r$, $y_{ir} = 1$ and for $j \neq r$, $y_{ij} = 0$. This shows that U_iA is the r^{th} row of A. We now assume that T_j is the j^{th} column of $(P_\sigma)^t$. Since $\sigma(j) = s$, $y_{js} = 1$ and for $i \neq s$, $y_{ij} = 0$. Therefore, $b_{ij} = a_{rs}$, proving the lemma.

Corollary: Let $A = [a_{ij}]$ be the adjacency matrix of a weighted graph and σ be a permutation such that $A = P_\sigma A(P_\sigma)^t$ and σ maps $i_1 \rightarrow j_1$, $i_2 \rightarrow j_2$, $\cdots$, $i_t \rightarrow j_t$. Then we have:

$$\begin{bmatrix} a_{i_1i_1} & \cdots & a_{i_1i_t} \\ \vdots & \cdots & \vdots \\ \vdots & \cdots & \vdots \\ \vdots & \cdots & \vdots \\ a_{i_ti_1} & \cdots & a_{i_ti_t} \end{bmatrix} = \begin{bmatrix} a_{j_1j_1} & \cdots & a_{j_1j_t} \\ \vdots & \cdots & \vdots \\ \vdots & \cdots & \vdots \\ \vdots & \cdots & \vdots \\ a_{j_tj_1} & \cdots & a_{j_tj_t} \end{bmatrix}$$

Using Lemma 1 and its corollary, we can write a MATLAB program to compute the automorphism group of weighted graphs[5]. This MATLAB Program will be used in the next section for computing the automorphism group of fullerenes C_{20} and C_{150}. Let G be the Euclidean graph of a molecule and A = Aut(G). Since for every vertex $\upsilon \in V(G)$ and every $\alpha \in A$, deg $\alpha(\upsilon)$ = deg υ, we can improve the MATLAB program[5] of for computing the symmetry of molecules. In what follows, we write this program.

A MATLAB program for computing symmetry of a molecules

```
function s=permutation1(a)
n=length(a);
b=sort(a);
for i=1:n
    t=[],
    for j=1:n
      if min(b(:,i)==b(:,j))==1
         t=[t j];
        end
    end
    p(i,1:length(t))=t;
end
s=p(1,:)';
s(s==0)=[];
    for i=2:n
    m=size(s);
    w=[];
    v=p(i,:);
    v(v==0)=[];
    k=1:n;
```

```
    k(v)=[];
    for j=1:m(1)
      t=1:n;
      t([s(j,:) k])=[];
       for r=t
          if min(min(a([s(j,:) r],[s(j,:) r])==a(a:i,1:i)))==1
             w=[w;s(j,:) r];
          end
       end
    end
    s=w;
end
```

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 φ(g)x = gx for all x ∈ X. The orbit of x will be indicated as x^G, the stabilizer of x by G_x. The set of all G-orbits will be denoted by G\\X := {x^G | x ∈ X}.

Let G be a permutation group. The cycle index of G acting on X is the polynomial Z(G, X) over Q in the indeterminates $x_1, x_2, \cdots x_t$, t = |X|, defined by $Z(G, X) = \frac{1}{|G|}\sum_{p\in G}\Pi_{i=1}^{t} x_i^{ci(p)}$ in which $(c_1(p), \cdots, c_t(p))$ is the cycle type of the permutation p ∈ G. All elements of a conjugacy class have the same cycle type, so the cycle index can be rephrased in the following way:

$$Z(G,X) = \frac{1}{|G|}\sum_{C\in C}|C|\Pi_{i=1}^{t} x_i^{c_i(gc)}$$

where C is the set of all conjugacy classes C of G with representatives $g_C \in C$.

Suppose a group G is acting on sets V, E and F of vertices, edges and faces, respectively. Then G acts in a natural way on the disjoint union $V \dot\cup E \dot\cup F$. Suppose |V| = r, |E| = s and |F| = t. The 3-dimensional cycle index is given by

$$Z_n(G, V\cup E\cup F) = \frac{1}{|G|}\sum_{p\in G}\Pi_{i=1}^{r}\upsilon_i^{a_i(p)}\Pi_{i=1}^{t} f_i^{c_i(p)}$$

where $(a_1(p), \cdots, a_r(p))$, $(b_1(p), \cdots, b_s(p))$ and $(c_1(p), \cdots, c_t(p))$, are the cycle type of the permutation corresponding to p and to action of p on V, E and F, respectively. These cycle indices are the basic tools for applying polya theory[6] to the isomer count.

In this paper, our notation is standard and taken mainly from the work of Cameron[7], Huppert[8] and Robinson[9]. Computations were carried out with the aid of GAP[10] and MTLAB[11]. We encourage reader to consult the work

of Fripertinger[12,13] for discussion and background material about the 3-dimensional cycle index.

3D cycle indices of some fullerenes

The recent discovery of the C_{60} "Buckminsterfullerene" and a host of other cage carbon molecules has ushered in a new branch of chemistry with quite mind-boggling potential. The arrangement of the carbon atoms and their relative positions at vertices in these structures trace out some interesting polyhedra.

Fullerenes consist essentially of hexagonal carbon rings (benzene) linked to each other partly *via* pentagons. The relationship between the number of spices (a, carbon atoms) and hexagon carbon rings (n) (pentagon rings always number 12) is given by a = 2(n + 10). This will indicate the fullerenes theoretically possible. Although each of these possibilities does represent a definite polyhedron, a large number of them have relatively low symmetry. Using these six dimensional cycle indices returning to the fullerene C_{24} the group $Z_2 \times S_4$ acting on the disjoint union of the sets of all vertices, edges and faces. When denoting the families of indeterminates for these actions by the following symbols υ_i, e_i and f_i we computed:

$$f = \upsilon_1^{24}e_1^{14}f_1^{36} + 3\upsilon_1^{8}\upsilon_2^{8}e_1^{4}e_2^{5}f_1^{4}f_2^{16} + 6\upsilon_2^{12}e_1^{6}e_2^{4}f_1^{6}f_2^{15} + 6\upsilon_4^{6}e_1^{2}e_4^{3}f_4^{9}$$
$$+ 6\upsilon_4^{6}e_2e_4^{3}f_4^{9} + 8\upsilon_3^{8}e_1^{2}e_3^{4}f_3^{12} + 8\upsilon_6^{4}e_2e_6^{2}f_6^{6} + 6\upsilon_2^{12}e_2^{7}f_1^{2}f_2^{17}$$
$$+ 3\upsilon_2^{12}e_1^{2}e_2^{6}f_2^{18} + \upsilon_2^{12}e_2^{7}f_2^{18}$$

We now consider, the fullerene C_{150} with dihedral group D_{10} as its point group. This group acts on the disjoint union of the sets of all vertices, edges and faces. We computed:

$$f = \upsilon_1^{150}e_1^{77}f_1^{225} + 2\upsilon_1^{8}\upsilon_2^{71}e_1^{11}e_2^{33}f_1^{11}f_2^{107} + \upsilon_5^{30}e_1^{2}e_5^{15}f_5^{45}$$
$$+ 3\upsilon_1^{8}\upsilon_2^{71}e_1^{2}e_5^{15}f_1^{11}f_2^{107} + 3\upsilon_5^{30}e_1^{11}e_2^{33}f_5^{45} + 5\upsilon_2^{75}e_1e_3^{38}f_1f_2^{112}$$
$$+ 3\upsilon_5^{2}\upsilon_{10}^{14}e_2e_5^{3}e_{10}^{6}f_5^{3}f_{10}^{21} + \upsilon_5^{25}\upsilon_{10}^{14}e_1^{15}e_2^{31}f_5^{3}f_{10}^{21} + \upsilon_1^{10}\upsilon_2^{70}e_2e_5^{3}e_{10}^{6}f_1^{15}\upsilon_2^{105}$$

Using these 3-dimensional cycle indices we can compute the number of different simultaneous colouring of all vertices, edges and faces with k_1, k_2 and k_3 colours by replacing each variable υ_i by k_1, e_i by k_2 and f_i by k_3. For $k_1 = k_2 = k_3 = 2$ the number of different colouring is $\approx 1.2 \times 10^{136}$.

Consider a fullerene graph G which its carbon atoms labeled by integers 1, 2, ..., n. We associate to any bond of G, an ordered pair (i,j), $1 \leq i,j \leq n$. Similarly, we associate to every face of G, a 5- or 6-tuple of these natural numbers. We now write a GAP program to compute the three-dimensional cycle indices for fullerenes with a given point group. In our GAP program, A is a solution matrix for the symmetry of fullerene under

consideration, BB is the set of all ordered pairs related to the bond of G and AA is the set of all 5- or 6-tuples related to the faces of G.

A GAP program for computing the 3-dimensional cycle index of fullerenes

```
Q:=[]; T:=[];
for i in A do
    Add(Q,PermListList(A[1],i));
od;
GG:=Group(Q);
e:=Elements(GG);
F:=[];FF:=[];HH=[];k:=1;
    for t in e do
       for i in AA do
         for j in i do
              AddSet(F, j^t);
         od;
         Add(FF,F);
         F:=[];
       od;
      h:=PermListList(FF,AA);
       Add(HH,h); FF:=[];
    od;
    H:=Elements(Group(HH));
    F1:=[];FF1:=[];H1:=[];
for t in e do
    for i in BB do for
    j in i do
    AddSet(F1, j^t);
  od;
  Add(FF1,F1); F1:=[];
od;
h1:=PermListList(FF1,BB);
Add(H1,h1); FF1:=[]
od;
w:=[];ww:=[];
for i in [1..20] do
    Print("e[",i);Print("]=",e[i],"");
    Print("H[",i);Print("]=",H[i],"");
    Print("H1[",i);Print("]=",H1[i],"");
od;
```

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