ON THE SYMMETRY OF BIS BENZENE CHROMIUM(0) WITH D_{6d} POINT GROUP

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Abstract

An Euclidean graph associated with a molecule is defined by a weighted graph with adjacency matrix M = [d_{ij}], where for i#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 distinct nuclei.In this paper, the automorphism group of the Bis Benzene Chromium(0) with D_{6d} point group symmetry is computed. We also find an euclidean graph with an odd number of automorphisms. This solved a problem posed by the author in an earlier paper.

Resumen

Un gráfico euclidiano asociado a una molécula es definido por un gráfico con matriz adyacente M = [d_{ij}] donde para i#j, d_{ij} es la distancia euclidiana entre los nucleos i y j. En esta matriz d_{ii} puede ser tomada como cero si todos los núcleos son equivalentes.De otra manera, se pueden introducir diferentes pesos para distintos núcleos. En este trabajo se calcula el grupo de automorfismo del Bis Benceno Cromo(0) con simetría D_{6d}. Se encontró también un gráfico euclidiano con un número impar de automorfismos. Este resultado resuelve un problema planteado por el autor en un artículo publicado previamente.

Introduction

An Euclidean graph G = (V,E,ω) is a combinatorial object consisting of a set V = V(G) of vertices which is a subset of R^3, a set E = E(G) containing all possible unordered pairs {x,y} of distinct vertices of G called edges, and a function ω: E(G) $\longrightarrow$ R in which ω(e) is the Euclidean distance between the vertices x and y. An automorphism or symmetry of an euclidean graph G is a permutation g of the vertex set of G with the property that for every edge e, w(g(e)) = w(e). The set of all automorphisms of a weighted graph G, with the operation of composition of permutations, is a permutation group on V(G) denoted Aut(G).

In the literature [1,2], it was shown by Randi that a graph can be depicted in different ways so that its point group symmetry or three dimensional perception may differ, but the underlying connectivity symmetry is still the same as characterized by the automorphism group of the graph.

However, the molecular symmetry depends on the coordinates of the various nuclei which relate directly to their three dimensional geometry. Although the symmetry as perceived in graph theory by the automorphism group of the graph and the molecular group are quite different, it was shown by Balasubramanian [3-9] that the two symmetries are connected.

The present authors earlier computed the full non rigid group of trimethylamine, cis and trans- platinum (II) and some other molecules, [10-13]. In this paper we consider only Euclidean graphs. The motivation for this study is outlined in Refs [3-9] and the reader is encouraged to consult these papers for background material as well as for basic computational techniques. Our notation is standard and taken mainly from Refs. [14-20].

Methods

In this section we first describe some notation, which will be kept throughout the paper. Suppose X is a set. The set of all permutations on X, denoted by S_X, is a group which is called the symmetric group on X. In the case that $X = \{1, 2, \ldots, n\}$, we denote S_X by S_n or Sym(n).

Our computations of the symmetry properties of molecules were carried out with the use of GAP [21] GAP stands for Groups, Algorithms and Programming. The name was chosen to reflect the aim of the system, which is a group theoretical software for solving computational problems in computational group theory. This software was constructed by the GAP's team in Aachen. GAP contains a large library of functions, which are important for the calculations of this paper.

Suppose P_σ is the permutation matrix corresponding to a permutation σ. Such matrices are 0,1 matrices with a unique 1 in every row and column. Consider the equation $(P_\sigma)^t A P_\sigma = A$, where A is the adjacency matrix of the Euclidean graph G. It is a well known fact that for a graph G with adjacency matrix A, the set of all solutions of this equation constitutes the automorphism group of G. Suppose $Aut(G) = \{\sigma_1, \sigma_2, \ldots, \sigma_m\}$. The matrix $S_G = [s_{ij}]$, where $s_{ij} = \sigma_i(j)$ is called a solution matrix for G. Since the rows of this matrix are elements of the automorphism group of G, to compute the automorphism group of G it is enough to calculate a solution matrix for G. The author in [16] proved a result that is useful for computing the symmetry of molecules. Using this result, Lemma 1 and its Corollary, we can write a MATLAB program [22] for computing a solution matrix for the automorphism group of Euclidean graphs.

A MATLAB Program for Computing the Symmetries of Molecules

```
n=length(a);
  for i=1:n-1
        for j=i+1:n
              b(i,j)=norm(a(i,:)-a(j,:));
        end
  end
b(n,n)=0;
b=b+b';

function y=halat(s,a)
```

```
    t=1:length(a);
    m=length(s);
    t(s)=[];
    j=0;
        for i=t
            if min(min(a(1:m+1,1:m+1)==a([s,i],[s,i])))==1
                j=j+1;
                y(j)=i;
            end
        end

function s=hazf(s)
    m=size(s);
        for i=m(1):-1:1
            if min(s(i,:))==0
                s(i,:)=[];
            end
        end
function s=jaigasht(a)
    m=length(a);
        for i=1:m
            s(i,1)=i;
        end
        for j=2:m
            n=size(s);
            k=0;
                for i=1:n(1)
                    y=[halat(s(i,:),a)];
                        for r=1:length(y)
                            b(r+k,1:n(2)+1)=[s(i,:),y(r)];
                        end
                    k=k+length(y);
                end
            s=b;
            s=hazf(s);
        end
    b=0;
    n=size(s);
        for i=1:n(1)
            for j=1:n(2)
                b(i,s(i,j))=j;
            end
        end
    s=b;
```

Our program needs the Cartesian coordinates of the atoms to determine the Euclidean distances in the molecule under consideration. If we calculate these distances by HyperChem [23], Gaussian 03 [24] or another software, then for computing the symmetry of a molecule under consideration, it is enough to delete the first eight lines of the program and load the distance matrix of the molecule.

Results and Discussion

The aim of this section is to apply our program for computing the automorphism group of Euclidean graph of Bis Benzene Chromium(0). The Cartesian coordinates of the atoms of this molecule is computed by HyperChem. It is useful to mention that in our program the accuracy is very important. In fact, our calculations for computing the symmetry of some fullerenes show that, if we change the accuracy, then the automorphism group would be changed.

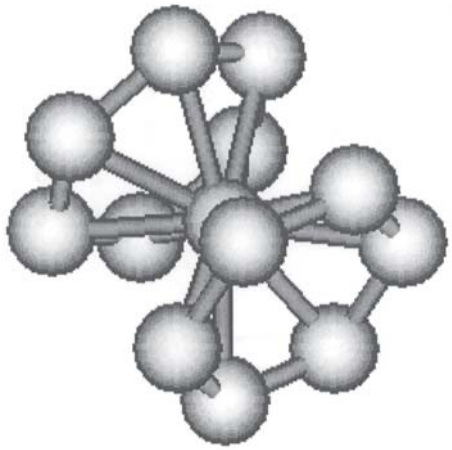

Figure 1. *The Structure of Bis Benzene Chromium(0) With* D_{6d} *Point Group*

We now calculate the symmetry of Bis Benzene Chromium(0). Let Aut(G) be the automorphism group of Euclidean graph G of the mentioned molecule with D_{6d} symmetry point group. Consider this molecule, Figure 1, to illustrate Euclidean graph, Figure 2, and its automorphism group. It is useful to mention here that we do not have to work with exact Euclidean distances since a mapping of weights into a set of integers suffices as long as different weights are identified with different integers. To illustrate this, let us use an euclidean edge weighting for Bis Benzene Chromium(0) obtained from Table 1 and our program. Suppose F is the 13×13 integer matrix obtained from Euclidean distances. From Table 1, the matrix F is as follows:

$$\begin{bmatrix}
0 & 1 & 1 & 2 & 3 & 4 & 3 & 5 & 7 & 8 & 10 & 9 & 6 \\
1 & 0 & 3 & 2 & 1 & 3 & 4 & 6 & 5 & 7 & 8 & 10 & 9 \\
1 & 3 & 0 & 2 & 4 & 3 & 1 & 7 & 8 & 10 & 9 & 6 & 5 \\
2 & 2 & 2 & 0 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 \\
3 & 1 & 4 & 2 & 0 & 1 & 3 & 9 & 6 & 5 & 7 & 8 & 10 \\
4 & 3 & 3 & 2 & 1 & 0 & 1 & 10 & 9 & 6 & 5 & 7 & 8 \\
3 & 4 & 1 & 2 & 3 & 1 & 0 & 8 & 10 & 9 & 6 & 5 & 7 \\
5 & 6 & 7 & 2 & 9 & 10 & 8 & 0 & 1 & 3 & 4 & 3 & 1 \\
7 & 5 & 8 & 2 & 6 & 9 & 10 & 1 & 0 & 1 & 3 & 4 & 3 \\
8 & 7 & 10 & 2 & 5 & 6 & 9 & 3 & 1 & 0 & 1 & 3 & 4 \\
10 & 8 & 9 & 2 & 7 & 5 & 6 & 4 & 3 & 1 & 0 & 1 & 3 \\
9 & 10 & 6 & 2 & 8 & 7 & 5 & 3 & 4 & 3 & 1 & 0 & 1 \\
6 & 9 & 5 & 2 & 10 & 8 & 7 & 1 & 3 & 4 & 3 & 1 & 0
\end{bmatrix}$$

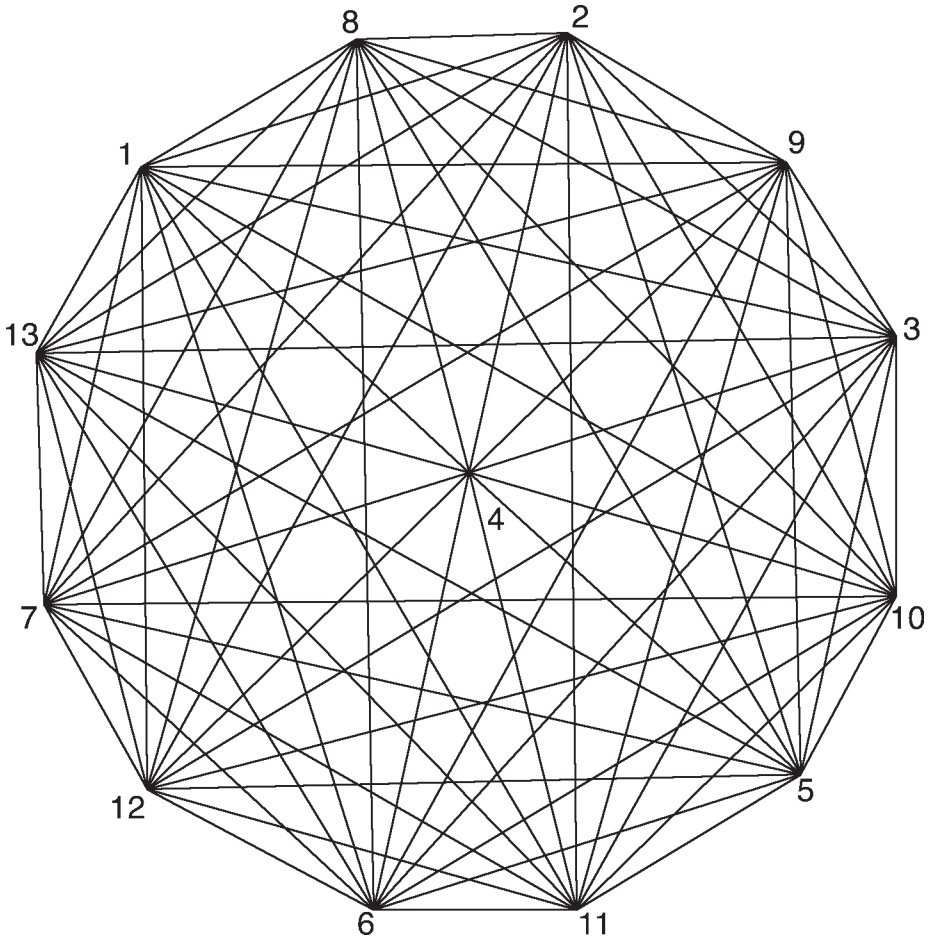

Figure 2. *The Euclidean graph of Bis Benzene Chromium(0).*

Not all 13! permutations of the vertices of the molecule belong to the automorphism group of its weighted graph since the weights of all the edges are not the same. For example, the permutation g = (1,2,3,4,5,6,7) does not belong to the automorphism group since the resulting graph does not preserve connectivity. Let X denote the set of all solutions of matrix equation $P^tFP = F$. Then $Aut(G) = \{\propto \in S_{13} \mid P_{\propto} \in X\}$ is the automorphism group of Euclidean graph of Bis Benzene Chromium(0). We now apply our MATLAB program to find a solution matrix for this group. After running our program, we can see that G is a non-abelian group of order 8. Using the solution matrix and a simple GAP program, we can find the structure of the automorphism group G of the Euclidean graph of Bis Benzen Chromium(0). We mention that this program is very fast and its running time is less than 0.1 s.

G ={ (1)(2)(3)(4)(5)(6)(7)(8)(9)(10),(2,3)(4,7)(5,9)(6,8)(11,12),
(1,4,10,7)(2,5,11,8)(3,6,12,9),(1,4)(2,6)(3,5)(7,10)(8,12)(9,11),
(1,7,10,4)(2,8,11,5)(3,9,12,6),(1,7)(2,9)(3,8)(4,10)(5,12)(6,11),
(1,10)(2,11)(3,12)(4,7)(5,8)(6,9),(1,10)(2,12)(3,11)(5,6)(8,9) }.

Table 1. *Distance Matrix (angstroms) of* $Cr(C_6H_6)_2$

13	12	11	10	9	8	7	6	5	4	3	2	1	d_{ij}
2.56	2.60	3.25	3.75	3.72	3.17	2.52	2.91	2.52	1.91	1.46	1.46	0.00	**1**
2.60	3.25	3.75	3.72	3.17	2.55	2.91	2.52	1.46	1.91	2.52	0.00	1.46	**2**
3.17	2.55	2.60	3.25	3.75	3.72	1.46	2.52	2.91	1.91	0.00	2.52	1.46	**3**
1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	0.00	1.91	1.91	1.91	**4**
3.25	3.75	3.72	3.17	2.56	2.60	2.52	1.46	0.00	1.91	2.91	1.46	2.52	**5**
3.75	3.72	3.17	2.56	2.60	3.25	1.46	0.00	1.46	1.91	2.52	2.52	2.91	**6**
3.72	3.17	2.56	2.60	3.25	3.75	0.00	1.46	2.52	1.91	1.46	2.91	2.52	**7**
1.46	2.52	2.91	2.52	1.46	0.00	3.75	3.25	2.60	1.91	3.72	2.55	3.17	**8**
2.52	2.91	2.52	1.46	0.00	1.46	3.25	2.60	2.56	1.91	3.75	3.17	3.72	**9**
2.91	2.52	1.46	0.00	1.46	2.52	2.60	2.56	3.17	1.91	3.25	3.72	3.75	**10**
2.52	1.46	0.00	1.46	2.52	2.91	2.56	3.17	3.72	1.91	2.60	3.75	3.25	**11**
1.46	0.00	1.46	2.52	2.91	2.52	3.17	3.72	3.75	1.91	2.55	3.25	2.60	**12**
0.00	1.46	2.52	2.91	2.52	1.46	3.72	3.75	3.25	1.91	3.17	2.60	2.56	**13**

Conclusions

This method is usually very useful for calculating symmetries of a molecule, when the number of vertices is at most 100. In the case that the graph under consideration has a large number of vertices, it is better to find a subgroup of the full symmetric group containing automorphism group of our weighted graph. Then apply this subgroup and our GAP program to compute the automorphism group of the graph.

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