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# Computing Orbits of Big Fullerenes

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An 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 elucidean distance between the nuclei i and j. In this matrix $d_{ij}$ can be taken as zero if all the nuclei are equivalent. Otherwise, one may introduce different weights for distinct nuclei. In this paper the symmetry of the big fullerene $C_{320}$ with point group symmetry $I_h$ together with its orbits is computed.

**Key Words: Elucidean graph, Symmetry, Fullerene.**

## INTRODUCTION

Buckminsterfullerene was observed for the first time in 1985 by Kroto during graphite laser evaporation experiments[1]. The name of fullerene goes back to the name of a geodesic designer. Buckminster Fuller, who designed the Fuller Dome at the Montreal International Exposition in 1967[2]. $C_{60}$ has important applications in diverse areas from fuel cells to pharmaceuticals for AIDS and Parkinson's disease[1]. Fullerenes are allotropic form of carbon made up of pentagonal and hexagonal faces consisting of even numbers of of carbon atoms[3] and extensive research works have been carried out since the discovery of the first homologue of these compounds, buckminsterfullerene, $C_{60}$. Fullerenes have various applications in nanotechnology such as for the fabrication of opto-electronic devices[4,5]. These compounds are highly symmetrical cage like molecules of carbon which have been considered as a special class of spherical quasi-aromatic systems[6]. There is a mathematical rule as a consequence of the Euler theorem, which says 12 pentagons are present in each spherical shape of n hexagons with the exception of n = 1.

Symmetry and its mathematical framework-group theory-play an increasingly important role in chemistry and physics. Both classical and quantum systems usually display great complexity, but the analysis of their symmetry properties often gives rise to simplifications and new insights

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which can lead to a deeper understanding. In addition, symmetries themselves can point the way toward the formulation of a correct physical theory by providing constraints and guidelines in an otherwise intractable situation. It is remarkable that, in spite of the wide variety of systems one may consider, all the way from classical ones to molecules, nuclei and elementary particles, group theory applies the same basic principles and extracts the same kind of useful information from all of them. This universality in the applicability of symmetry considerations is one of the most attractive features of group theory. Most workers have an intuitive understanding of symmetry, particularly in its most obvious manifestation in terms of geometric transformations that leave a body or system invariant. This interpretation, however, is not enough to readily grasp its deep connections with physics and it thus becomes necessary to generalize the notion of symmetry transformations to encompass more abstract ideas. The mathematical theory of these transformations is the subject matter of group theory.

Detecting symmetry in 3D models is a well studied problem with applications in a large number of areas. For instance, the implicit redundancy in symmetric models is used to guide reconstruction, axes of symmetry provide a method for defining a coordinate system for models and symmetries are used for shape classification and recognition[7].

We first describe some notations which will be kept throughout. A graph G = (V,E) consists of a finite nonempty set of points with a prescribed set E of pairs of distinct points of V. In a molecular graph, the conventional chemical structure, the set of atoms comprises the point set V and covalent chemical bonds are elements of E. Such a graph retains the full topology of the molecule and represents molecular structure, where the word 'structure' is used to denote a formal system of relations of certain logical types without emphasizing the entities to which they relate. In chemistry, two types of graphs are often employed to model molecular structure, *viz.*, hydrogen-suppressed graph and hydrogen-filled graphs. While in the former only the non-hydrogen atoms are represented by points, in the latter all atoms including hydrogen atoms are represented by vertices.

For real world chemical and spectroscopic applications one needs to utilize graphs which contain weights for edges, for example, to discriminate signals and double bonds. In the context of NMR and multiple NMR spectroscopy, the nuclear spin coupling can be represented by graphs called NMR graphs. In these examples, the vertices are the various nuclei in the molecule while the edges are either isotopic J-coupling constants or dipolar coupling constants. The nuclear coupling constants between the various nuclei in a molecule are often different as they depend on the Euclidean distances between the nuclei. Consequently, it is necessary to

lable the edges of the complete graph of a molecule with the appropriate nuclear spin-spin coupling constants. The same is true for hyperfine structure in the ESR spectra[8-16].

The GAP systems is a useful package for computing the group structure, which merits more attention from the chemical community[17]. One of the present authors (ARA)[18-30] applied this package to solve some problems in mathematical chemistry related to the symmetry of molecules.

Throughout this paper, all groups considered are assumed to be finite. Our notation is standard and taken mainly from the standard books graph theory and group theory. Our computations were carried out with the use of GAP[17]. We encourage the reader to consult the work of Ashrafi[19], for background material as well as basic computational techniques.

## RESULTS AND DISCUSSION

A permutation matrix is a 0-1 matrix that has exactly 1 in each row or column and 0s elsewhere. Permutation matrices are the matrix representation of permutations. In general, for a permutation $\sigma$ on n objects, the corresponding permutation matrix is an n-by-n matrix $P_\sigma$ is given by $P_\sigma = [x_{ij}]$, where $x_{ij} = 1$, if $\sigma(i) = j$ and 0 otherwise. We define a permutation of the vertices of an Euclidean graph G to be an automorphism of G if it satisfies $(P_\sigma)^t A P_\sigma = A$, where $(P_\sigma)^t$ is the transpose of permutation matrix $P_\sigma$ and A is the adjacency matrix of graph under consideration. It is easy to see that the set Aut(G) of all automorphisms of G is a group under composition of automorphisms.

By symmetry we consider the automorphism group symmetry of the graph under consideration. The automorphism group of a graph depends only on the connectivity of the graph and does not depend on how the graph is represented in three dimensions. That is, a graph, in general, can be represented in different ways in three dimensions such that two representations could yield different three-dimensional symmetries and yet their automorphism groups are the same since the latter depends only on which vertices are connected in the graph. For this reason the symmetry of a graph was thought to be quite different from the point group symmetry and it is apparent that the two symmetries need not be related to each other.

In mathematics, groups are often used to describe symmetries of objects. This is formalized by the notion of a group action: every element of the group 'acts' like a bijective map (or 'symmetry') on some set. To clarify this notion, we assume that G is a group and X is a set. G is said to act on X when there is a map $\phi : G \times X \rightarrow X$ such that all elements $x \in X$, (i) $\phi(ex) = x$ where e is the identity element of G and (ii) $\phi(g, \phi(h,x)) = \phi(gh,x)$ for all $g,h \in G$. In this case, G is called a transformation group, X is called a G-set and $\phi$ is called the group action. For simplicity, we defined $gx = \phi(g,x)$.

In a group action, a group permutes the elements of X. The identity does nothing, while a composition of actions corresponds to the action of the composition. For a given X, the set $\{gx \mid g \in G\}$, where the group action moves x, is called the group orbit of x. The subgroup which fixes is the isotropy group of x.

In this section, we investigate the symmetry of the big fullerene $C_{320}$ with point group symmetry $I_h$. Consider the fullerene $C_{320}$ to illustrate the Euclidean graphs and its symmetry group. It suffices to measure the Euclidean distances in terms of the C–C bond lengths and then construct the Euclidean distance matrix D. It should be mentioned that one does not have to work with exact Euclidean distances in that a mapping of weights into a set of integers would suffice as long as diffeent weights are identified with different integers. In fact the automorphism group of the integer-weighted graph is identical to the automorphism group of the original Euclidean graph.

We notice that all permutations of the vertices of $C_{320}$ do not belong to the automorphism group since $Aut(C_{320})$ has order 120 which is different from 320!. For example, the permutation (1, 2, ...., 320) does not belong to the automorphism group since the resulting graph does not preserve connectivity.

We now discuss techniques that are useful in finding symmetry of molecules. We begin with three important results that, in certain situations, are very effective in establishing automorphisms of Euclidean graphs[19].

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

**Lemma 2:** Let $A = [a_{ij}]$ be the adjacency matrix of a weighted graph and $\sigma$ be a permutation such that $A = P_\sigma A(P_\sigma)^t$ and $\sigma$ maps $i_1 \rightarrow j_1$, $i_2 \rightarrow j_2$, ...., $i_t \rightarrow j_t$. Then

$$\begin{bmatrix} a_{i_1i_1} & \cdots & a_{i_1i_1} \\ \vdots & & \vdots \\ a_{i_1i_1} & \cdots & a_{i_1i_1} \end{bmatrix} = \begin{bmatrix} a_{j_1j_1} & \cdots & a_{j_1j_1} \\ \vdots & & \vdots \\ a_{j_1j_1} & \cdots & a_{j_1j_1} \end{bmatrix}$$

**Lemma 3:** Let G be an Euclidean graph, A = Aut(G) and $O_1, O_2 ..., O_t$ are orbits of the action of A on the vertices of G. Then for every $\alpha \in A$ and every positive integer i, $1 \leq i \leq t$, $\alpha(O_i) = O_i$.

Using Lemmas **1-3**, we can write a Matlab program for computing all solution of the equation $(P_\sigma)^t A P_\sigma = A$. To do this we take the Cartesian coordinates of the big fullerene $C_{320}$ from the homepage of Dr. Steffen Weber at "http://jcrystal.com/steffenweber/". Our calculations give the following generating set for the group $Aut(C_{320})$:

$\mathbf{X_{320}}$: = (2,5)(3,4)(6,14)(7,13)(8,12)(9,11)(10,15)(16,29)(17,28)(18,27)(19,26)(20,30)(21,24)(22,23)(32,35)(33,34)(36,56)(37,60)(38,59)(39,58)(40,57)(41,51)(42,55)(43,54)(44,53)(45,52)(47,50)(48,49)(61,66)(62,65)(63,64)(69,73)(70,72)(74,113)(75,114)(76,115)(77,116)(78,117)(79,118)(80,119)(81,120)(82,121)(83,122)(84,123)(85,124)(86,125)(87,105)(88,104)(89,103)(90,102)(91,101)(92,100)(93,106)(94,107)(95,112)(96,111)(97,110)(98,109)(99,108)(126,127)(128,130)(129,131)(133,135)(134,136)(139,170)(140,169)(141,168)(142,167)(143,166)(144,165)(145,171)(146,172)(147,177)(148,176)(149,175)(150,174)(151,173)(152,183)(153,182)(154,181)(155,180)(156,179)(157,178)(158,184)(159,185)(160,190)(161,189)(162,188)(163,187)(164,186)(191,218)(192,217)(193,221)(194,222)(195,219)(196,220)(197,223)(198,226)(199,227)(200,224)(201,225)(202,228)(203,229)(204,248)(205,247)(206,246)(207,245)(208,244)(209,243)(210,249)(211,250)(212,255)(213,254)(214,253)(215,252)(216,251)(230,235)(231,234)(232,233)(238,242)(239,241)(256,261)(257,260)(258,259)(264,268)(265,267)(269,313)(270,312)(271,311)(272,310)(273,309)(274,308)(275,314)(276,315)(277,320)(278,319)(279,318)(280,317)(281,316)(282,300)(283,299)(284,298)(285,297)(286,296)(287,295)(288,301)(289,302)(290,307)(291,306)(292,305)(293,304)(294,303).

$\mathbf{Y_{320}}$: = (1,2)(3,5)(6,19)(7,18)(8,17)(9,16)(10,20)(11,14)(12,13)(21,29)(22,28)(23,27)(24,26)(25,30)(31,35)(32,34)(36,51)(37,55)(38,54)(39,53)(40,52)(41,46)(42,50)(43,49)(44,48)(45,47)(57,60)(58,59)(61,74)(62,75)(63,76)(64,77)(65,78)(66,79)(67,80)(68,81)(69,82)(70,83)(71,84)(72,85)(73,86)(87,113)(88,114)(89,115)(90,116)(91,117)(92,118)(93,119)(94,120)(95,121)(96,122)(97,123)(98,124)(99,125)(100,105)(101,104)(102,103)(108,112)(109,111)(126,166)(127,165)(128,169)(129,170)(130,167)(131,168)(132,171)(133,174)(134,175)(135,172)(136,173)(137,176)(138,177)(139,196)(140,195)(141,194)(142,193)(143,192)(144,191)(145,197)(146,198)(147,203)(148,202)(149,201)(150,200)(151,199)(152,209)(153,208)(154,207)(155,206)(156,205)(157,204)(158,210)(159,211)(160,216)(161,215)(162,214)(163,213)(164,212)(178,183)(179,182)(180,181)(186,190)(187,189)(217,218)(219,221)(220,222)(224,226)(225,227)(230,243)(231,244)(232,245)(233,246)(234,247)(235,248)(236,249)(237,250)(238,251)(239,252)(240,253)(241,254)(242,255)(256,308)(257,309)(258,310)(259,311)(260,312)(261,313)(262,314)(263,315)(264,316)(265,317)(266,318)(267,319)(268,320)(269,300)(270,299)(271,298)(272,297)(273,296)(274,295)(275,301)(276,302)(277,307)(278,306)(279,305)(280,304)(281,303)(282,287)(283,286)(284,285)(290,294)(291.293).

$\mathbf{Z_{320}}$: = (1,6,50,41,18)(2,7,46,42,19)(3,8,47,43,20)(4,9,48,44,16)(5,10,49,45,17)(11,12,13,14,15)(21,30,53,31,40)(22,26,54,32,36)(23,27,55,33,37)(24,28,51,34,38)(25,29,52,35,39)(56,60,59,58,57)(61,126,182,169,76)(62,127,183,170,77)(63,128,179,166,74)(64,129,178,165,75)(65,130,181,168,79)(66,131,180,167,78)(67,132,184,171,80)(68,133,189,176,85)(69,134,188,175,82)(70,135,185,172,83)(71,136,190,177,86)(72,137,187,174,81)(73,138,

186,173,84)(87,114,153,285,209)(88,113,152,284,208)(89,117,156,287,207)(90,118,157,286,206)(91,115,154,282,205)(92,116,155,283,204)(93,119,158,288,210)(94,122,161,291,211)(95,123,162,294,216)(96,120,159,293,215)(97,121,160,290,214)(98,124,163,289,213)(99,125,164,292,212)(100,144,298,273,196)(101,143,297,274,195)(102,142,300,270,194)(103,141,299,269,193)(104,140,295,272,192)(105,139,296,271,191)(106,145,301,275,197)(107,146,304,280,198)(108,151,307,279,203)(109,150,306,276,202)(110,149,303,281,201)(111,148,302,278,200)(112,147,305,277,199)(217,243,309,256,231)(218,244,308,257,230)(219,245,312,258,234)(220,246,313,259,235)(221,247,310,260,232)(222,248,311,261,233)(223,249,314,262,236)(224,250,317,263,239)(225,251,318,264,240)(226,252,315,265,237)(227,253,316,266,238)(228,254,319,267,241)(229,255,320,268,242).

Using the generating set and the following GAP program, one can see that the group Aut($C_{320}$) has exactly five orbits AA, CC, DD, KK, LL under its natural action. AA = {1, 2, ..., 60}; CC = {61,62,63,64,65,66,74,75,76,77,78,79,87,88,89,90,91,92,100,101,102,103,104,105,113,114,115,116,117,118,126,127,128,129,130,131,139,140,141,142,143,144,152,153,154,155,156,157,165,166,167,168,169,170,178,179,180,181,182,183,191,192,193,194,195,196,204,205,206,207,208,209,217,218,219,220,221,222,230,231,232,233,234,235,243,244,245,246,247,248,256,257,258,259,260,261,269,270,271,272,273,274,282,283,284,285,286,287,295,296,297,298,299,300,308,309,310,311,312,313]; DD = {67,80,93,106,119,132,145,158,171,184,197,210,223,236,249,262,275,288,301,314}; KK = {68,70,72,81,83,85,94,96,98,107,109,111,120,122,124,133,135,137,146,148,150,159,161,163,172,174,176,185,187,189,198,200,202,211,213,215,224,226,228,237,239,241,250,252,254,263,265,267,276,278,280,289,291,293,302,304,306,315,317,319} and LL = {69,71,73,82,84,86,95,97,99,108,110,112,121,123,125,134,136,138,147,149,151,160,162,164,173,175,177,186,188,190,199,201,203,212,214,216,225,227,229,238,240,242,251,253,255,264,266,268,277,279,281,290,292,294,303,305,307,316,318,320}.

**A GAP program for computing of orbits of the symmetry group of $C_{320}$**

```
G:=Group(X320,Y320,Z320);
H:=Elements(G);
F:=[1,2..320]:
A:=[];
    for i in H do
            t:=l^i;
            Add(A,t);
    od;
AA:=Set(A);
C:=[]
```

```
    for i in H do
            t:=61^i;
            Add(C,t);
    od;
CC:=Set(C);
D:=[];
    for i in H do
            t:=67^i;
            Add(D,t);
    od;
DD:=Set(D);
K:=[];
    for i in H do
            t:=68^i;
            Add(K,t);
    od;
KK:=Set(K);
L:=[];
    for i in H do
            t:=69^i;
            Add(L,t);
    od;
LL:=Set(L);
```

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