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An Application of Geometrical Isometries in Non–Planar Molecules

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ABSTRACT

In this paper we introduce a novel methodology to transmit the origin to the center of a polygon in a molecule structure such that the special axis be perpendicular to the plane containing the polygon. The mathematical calculations are described completely and the algorithm will be showed as a computer program.

1. INTRODUCTION

An isometry is a distance-preserving injective map between metric spaces. The isometries associated with the Euclidean metric, are called Euclidean motions or rigid motions, which forms a Lie group under composition. This *ancient* group is among the oldest and most studied implicitly, long before the concept of group was invented.

One of the applications of isometries is to transfer or rotate the coordinate system in order to simplify the computations or visions. This usually happens in all branches of sciences which apply the analytic geometry.

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In computational chemistry, sometimes, one needs to calculate some properties in each point on the area of molecule or above and below it, so one must put ghost (Bq) atom in an arbitrary point, exactly. Evaluation of the aromaticity, antiaromaticity and nonaromaticity of compounds by nucleus independent chemical shift criterion (NICS), is an example for it. To NICS calculation at each point above and below of the all polygons, one must put some Bq atoms in various distances on the z axis, straightforwardly. In non-planar molecule, vertically putting Bq atoms in various distances of the rings in different sheets is not very hard, but estimation of components of the nuclear magnetic shielding tensors $\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \ldots$ is very hard and for more complex molecules is impossible. But, using our proposed method and doing calculation separately for each polygon facilitate estimation of nuclear magnetic shielding tensors components. We refer to [3] as a good review published which has collected a large number of works related to NICS criterion.

By mathematical language, in this paper we transfer the origin to the center of a pentagon (or hexagon) in the space, such that the z-axes is perpendicular to the plane containing the polygon (or hexagon). Our motivation is the study of the geometric structure of some molecules such as *Corannulene* and *Sumanene* which are polycyclic aromatic hydrocarbons. This method can be used for other molecules which have polygons in their structure (*Fullerenes*, for example). Thanks to this technique the authors investigated the evaluation of aromaticity of some non-planar molecules in [7]. The content of this article is the mathematical description of the mentioned process. To see the related chemical issues, we refer the reader to [1] and [10].

We begin with a quick review on isometries and frames, and then obtain the desire isometry for our purpose. Finally, as an example we will apply the program for some molecules.

2. ISOMETRIES AND FRAMES

In this section, we shall investigate the isometries of Euclidean space, and see how two frames uniquely determine an isometry.

Definition 2. 1. An isometry, or rigid motion, of Euclidean space is a mapping that preserves the Euclidean distance d between points. More precisely, an isometry is a mapping $F: \mathbb{R}^3 \to \mathbb{R}^3$ for which $d\big(F(p), F(q)\big) = d(p, q)$, for all $p, q \in \mathbb{R}^3$.

The most important examples of isometries are translations and orthogonal transformations.

Definition 2. 2. Translation by a point $a \in \mathbb{R}^3$ is a map $T: \mathbb{R}^3 \to \mathbb{R}^3$, for which $T(u) = u + a$. An orthogonal transformation of $\mathbb{R}^3$ is a linear transformation $C: \mathbb{R}^3 \to \mathbb{R}^3$ which preserves inner product, namely $C(p).C(q) = p.q$.

For instance, rotations around a coordinate axis are orthogonal transformations. By simple computations, one can show that If F and G are isometries of $\mathbb{R}^3$, then the composite mapping $G \circ F$ is also an isometry of $\mathbb{R}^3$. A vital theorem in differential geometry asserts that If F is an isometry of $\mathbb{R}^3$, then there exists a unique translation T and a unique orthogonal transformation C such that $F = T \circ C$ [6].

Definition 2. 3. A set $\{e_1, e_2, e_3\}$ of pair-wise orthogonal unit vectors tangent to $p \in \mathbb{R}^3$ is called a frame at p.

For example, $\{i = (1,0,0), j = (0,1,0), k = (0,0,1)\}$ is a frame at each point of $\mathbb{R}^3$, which is called the standard frame. It is clear that at each point of the Euclidean space, there exist uncountable frames. Depending on the application, certain frames are used. For example in local curve theory, the Frenet frame [5], determines the geometric properties of the curve. Here we use the frames to obtain an important isometry. First we state a vital theorem in differential geometry, see [6] for example.

Theorem 2. 4. For any two frames $\{e_1, e_2, e_3\}$ and $\{f_1, f_2, f_3\}$ at the points $p, q \in \mathbb{R}^3$ respectively, there exists a unique isometry F of $\mathbb{R}^3$ such that F maps the tangent vector e_i to tangent vector f_i, for $i = 1, 2, 3$.

To compute the isometry F in the above theorem, let $e_i = (a_{i1}, a_{i2}, a_{i3})$, $f_i = (b_{i1}, b_{i2}, b_{i3})$, $A = (a_{ij})$, $B = (b_{ij})$, and $C = B^t A$. A and B are the attitude matrices of the $\{e_i\}$ and $\{f_i\}$ frames, respectively. Now C is an orthogonal transformation and $C(e_i) = f_i$. If T be the translation by the point $q - C(p)$, then $F = T \circ C$ is the desired isometry.

3. APPLICATION AND ILLUSTRATION

Here we apply the last theorem in previous section to transfer the origin and the standard frame to the center of an arbitrary pentagon or hexagon in a polycyclic molecule (corannulene, sumanene, or fullerene), such that the z-axis will be perpendicular on this polygon. To do so, we need a frame on the center point of polygon.

Although we don't investigate the chemical aspects of these compounds, a brief introduction may be interesting (for some mathematical facets of Fullerenes, see [2], [8], and [9]).

Corannulene is a polycyclic aromatic hydrocarbon with one central pentagonal ring and five peripheral hexagonal rings, Figure 1(a). Sumanene is a polycyclic aromatic hydrocarbon with one central hexagonal ring and three peripheral hexagonal and three peripheral pentagonal rings, alternately, Figure 1(b). Fullerenes are a family of carbon allotropes which composed entirely of carbon, in the form of a sphere, ellipsoid, cylinder, or tube. The structure of fullerenes is composed of hexagonal, pentagonal or sometimes heptagonal and octagonal rings, Figure 1(c).

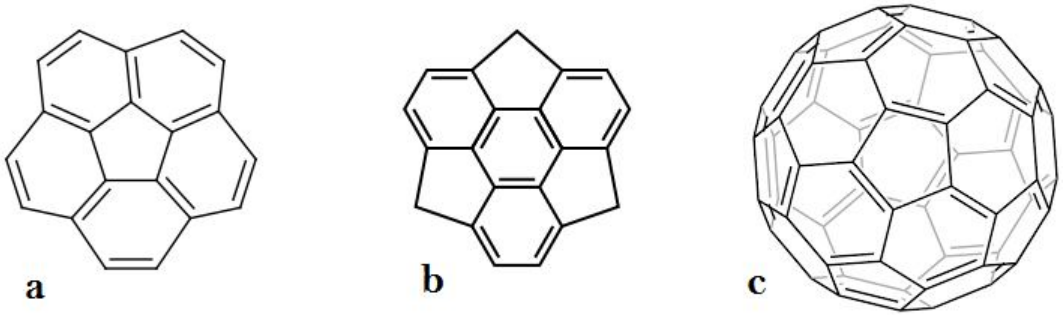

Figure 1. Structure of: (a) corannulene, (b) sumanene, and (c) a fullerene molecules.

We describe the method for a hexagon, the case pentagon is similar. Let p_1, p_2 and p_3 are three consecutive vertices of the hexagon. Then the vector $\overrightarrow{p_1p_2} \times \overrightarrow{p_1p_3}$ is perpendicular to the plane containing the hexagon. Dividing this vector by its own length, we have the unit vector

$$u_3 = \frac{\overrightarrow{p_1p_2} \times \overrightarrow{p_1p_3}}{|\overrightarrow{p_1p_2} \times \overrightarrow{p_1p_3}|}.$$

Multiply u_3 by the unit vector $u_1 = \frac{\overrightarrow{p_1p_2}}{|\overrightarrow{p_1p_2}|}$ to get the unit vector $u_2 = u_3 \times u_1$. Now the set $\{u_1, u_2, u_3\}$ is a frame. To obtain an isometry F which maps the frame $\{u_1, u_2, u_3\}$ to the standard frame $\{i, j, k\}$, let $u_1 = (a_{11}, a_{12}, a_{13})$, $u_2 = (a_{21}, a_{22}, a_{23})$, $u_3 = (a_{31}, a_{32}, a_{33})$, then $A = (a_{ij})$ and B is the identity matrix, so $C = B^tA = A$, namely:

$$C = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix},$$

i.e. if $q = (x, y, z)^t$ be the primary coordinate of the point q, then its new coordinate is given by:

$$F(q) = \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

We did all calculations of coordinate transformation in MATLAB environment. This program has been shown in the following lines.

```
function [B,Fx]=Transfer(A);

%     A: First coordination of the molecule
%     B: New coordination after origin transfer
%     Fx: Final coordination
clc
n1=input('n1=');n2=input('n2=');n3=input('n3=');
n4=input('n4=');n5=input('n5=');n6=input('n6=');
c=mean([A(n1,:);A(n2,:);A(n3,:);A(n4,:);A(n5,:);A(n6,:)])*(-1);
B=[(A(:,1)+c(1,1)),(A(:,2)+c(1,2)),(A(:,3)+c(1,3))];
p1=B(n1,:);p2=B(n2,:);p3=B(n3,:);
p1p2=[p2(1,1)-p1(1,1),p2(1,2)-p1(1,2),p2(1,3)-p1(1,3)];
p1p3=[p3(1,1)-p1(1,1),p3(1,2)-p1(1,2),p3(1,3)-p1(1,3)];
u4=[(p2(1,2)-p1(1,2))*(p3(1,3)-p1(1,3))-(p2(1,3)-p1(1,3))*
(p3(1,2)-p1(1,2)),(p2(1,3)-p1(1,3))*(p3(1,1)-p1(1,1))-(p2(1,1)-p1(1,1))*
(p3(1,3)-p1(1,3)),(p2(1,1)-p1(1,1))*(p3(1,2)-p1(1,2))-(p2(1,2)-p1(1,2))*
(p3(1,1)-p1(1,1))];
Q=norm(p1p2);T=norm(u4);
a11=(p2(1,1)-p1(1,1))/Q;
a12=(p2(1,2)-p1(1,2))/Q;
a13=(p2(1,3)-p1(1,3))/Q;
a31=((p2(1,2)-p1(1,2))*(p3(1,3)-p1(1,3))-(p2(1,3)-p1(1,3))*(p3(1,2)-p1(1,2)))/T;
a32=((p2(1,3)-p1(1,3))*(p3(1,1)-p1(1,1))-(p2(1,1)-p1(1,1))*(p3(1,3)-p1(1,3)))/T;
a33=((p2(1,1)-p1(1,1))*(p3(1,2)-p1(1,2))-(p2(1,2)-p1(1,2))*(p3(1,1)-p1(1,1)))/T;
a21=(a13*a32)-(a12*a33);
a22=(a11*a33)-(a13*a31);
a23=(a12*a31)-(a11*a32);
u1=[a11 a12 a13];
u2=[a21 a22 a23];
u3=[a31 a32 a33];
w=u1*u2';z=u2*u3';v=u3*u2';
H=[a11 a21 a31;a12 a22 a32;a13 a23 a33];
F=B';G=[F(1,:);F(2,:);F(3,:)];
Fx=(H'*G)';
```

As an example we apply the program for corannulene molecule. Figure 2 shows the structure of molecule before and after translating and rotating the coordinate system.

4. CONCLUSION AND REMARK

Proposed methodology in this work helps ones to transmit origin of coordinate to an arbitrary point and changes the axes coordinate direction perpendicular to an arbitrary polygon. It facilitates estimation of components of the nuclear magnetic shielding tensors

in non-planar molecules and can be used for any calculation that needs to such coordinate change. Although our discussion was based on *z*-axis, but it can be used for other axes by a simple rotation.

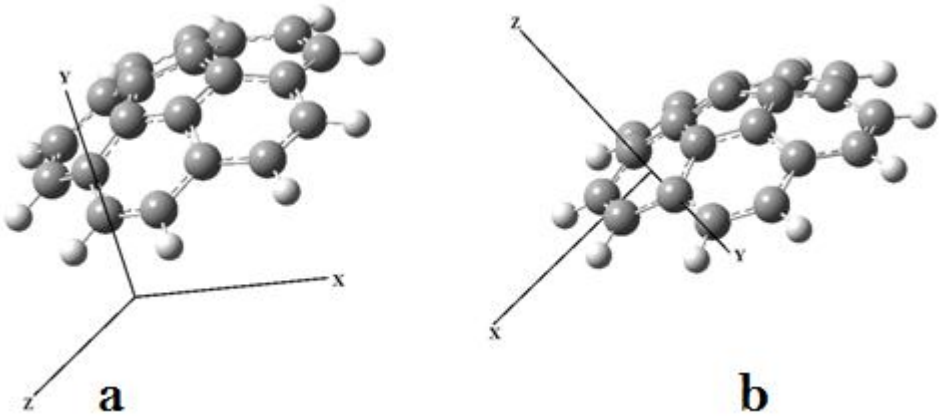

Figure 2. Corannulene molecule: (a) origin coordinate in in arbitrary point, (b) molecule was rotated with uncertain angle such that z-axis is perpendicular to hexagon.

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