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A note on flexible hexagons

by

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1. Introduction

The carbon skeleton of the cyclohexane molecule may be represented by a spatial hexagon with equal sides and equal angles. As has been shown by Sachse [1] this hexagon may assume either a rigid or a flexible form by which it is capable of passing continuously through a sequence of configurations. Accordingly one may expect the existence of two isomeric forms of cyclohexane. The same question has been considered by Oosterhoff and Hazebroek [2] who also observed a similar phenomenon for the cyclohexanedione - 1,4 molecule which corresponds to a hexagon of the type abaaba.

In this note it will be shown that the necessary and sufficient conditions for the existence of a flexible form of a non-degenerate spatial hexagon with fixed sides and angles consist in the equality of opposite elements. Besides there exists a rigid form which is not contained in the sequence of movable forms.

2. Necessary conditions

Consider an arbitrary spatial hexagon $P_1P_2\dots P_6$. Let P_j be given by the Cartesian coordinates (x_{j1}, x_{j2}, x_{j3}) $j=1,2\dots 6$, then we consider the product $M=M_1M_2^T$ of the two 7×7 matrices

$$M_1 = \begin{pmatrix} x_{j1}^2+x_{j2}^2+x_{j3}^2 & -2x_{j1} & -2x_{j2} & -2x_{j3} & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$M_2 = \begin{pmatrix} 1 & x_{j1} & x_{j2} & x_{j3} & x_{j1}^2+x_{j2}^2+x_{j3}^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & & \end{pmatrix}$$

where the first row represents the six rows $j=1,2\dots 6$.
If the square distance between P_j and P_k is denoted by a_{jk} then M takes the form

$$M = \begin{pmatrix} A & 1 \\ 1 & 0 \end{pmatrix}$$

where A is the 6×6 matrix (a_{jk}) and 1 represents either a row or a column of ones. Since M_1 and M_2 are of rank 5 M has also the rank 5.

If the six sides and the six angles of the hexagon are given then out of the 15 different square distances a_{jk} only

$$a_{14} = x , \quad a_{25} = y , \quad a_{36} = z$$

are unknown.
From M various zero determinants may be derived. Let us take A_{33} and A_{66} which are obtained from M by cancelling the third row and column and the sixth row and column respectively. This together with det M=0 ensures the vanishing of all other 6×6 determinants from M. Both $A_{33}=0$ and $A_{66}=0$ are relations between x and y only. In the case of a rigid structure by these relations a single solution (x,y) is determined. If a flexible structure exists these relations are dependent.

Consider the equation $A_{66}=0$. This is a relation of the second degree in each of the variables a_{14} and a_{25}. The geometrical meaning of this relation is obtained as follows. Let the triangle $P_1P_2P_3$ be fixed in space then P_4 and P_5 describe circles C_4 and C_5 around the axes P_3P_2 and P_3P_1 respectively. The condition of P_4P_5 having a fixed length imposes a (2,2) correspondence between vertical chords in C_4 and C_5 respectively, i.e. with respect to $P_1P_2P_3$. This correspondence is degenerate if at least two double elements exist. In that case the curve $A_{66}(x,y)=0$ falls apart into two hyperbolae etc.

If P_4P_5 has a position corresponding to a double element P_4P_5 either passes through P_3 or lies in the plane $P_1P_2P_3$.
If P_4P_5 passes through P_3 in one position then the triangle $P_3P_4P_5$ is degenerate.
If there are two positions of P_4P_5 in the plane $P_3P_4P_5$ the triangle $P_1P_2P_3$ is degenerate. Therefore we may conclude that for non-degenerate hexagons, i.e. for which no three successive points are collinear, the relations $A_{33}=0$ and $A_{66}=0$ are not degenerate.
In the case of a flexible hexagon these relations are consequently identical. A simple calculation shows that

$$A_{66}(x,y) = -x^2y^2 + 2x^2y(a_{23}+a_{53}) + 2xy^2(a_{13}+a_{43}) + \dots \qquad 2.1$$

$$A_{33}(x,y) = -x^2y^2 + 2x^2y(a_{26}+a_{56}) + 2xy^2(a_{16}+a_{46}) + \dots \qquad 2.2$$

Hence we have e.g.

$$a_{23} + a_{53} = a_{26} + a_{56} \; . \qquad 2.3$$

From $A_{55}(x,z)\ A_{22}(x,z)$ we obtain by equating the coefficients of x^2z

$$a_{65} + a_{35} = a_{62} + a_{32} \; . \qquad 2.4$$

From 2.3 and 2.4 we infer the equality of the opposite elements $a_{23}=a_{56}$, $a_{35}=a_{62}$. This is obviously true for the other opposite elements as well so that we may say:

T h e   e x i s t e n c e   o f   a   f l e x i b l e   f o r m   o f   a   n o n - d e g e n e r a t e   h e x a g o n   i m p l i e s   t h e   e q u a l i t y   o f   o p p o s i t e   e l e m e n t s.

In the following section it will be shown that this condition is also sufficient.

3. Sufficient conditions

Consider a non-degenerate hexagon with equal opposite elements. Write for convenience

$$a_{23} = a_{56} = b_1 \qquad a_{35} = a_{62} = c_1$$
$$a_{34} = a_{61} = b_2 \qquad a_{46} = a_{13} = c_2$$
$$a_{45} = a_{12} = b_3 \qquad a_{51} = a_{24} = c_3 \; ,$$

then M takes the form $M = \begin{pmatrix} B & C & 1 \\ C & B & 1 \\ 1 & 1 & 0 \end{pmatrix}$, where

$$B = \begin{pmatrix} 0 & b_3 & c_2 \\ b_3 & 0 & b_1 \\ c_2 & b_1 & 0 \end{pmatrix} \quad \text{and} \quad C = \begin{pmatrix} x & c_3 & b_2 \\ c_3 & y & c_1 \\ b_2 & c_1 & z \end{pmatrix} \; .$$

An equivalent form of M is

$$M' = \begin{pmatrix} C-B & 0 & 0 \\ 0 & C+B & 1 \\ 0 & 1 & 0 \end{pmatrix} \; .$$

Let $D_1=\det(C-B)$, $D_2=\det(C+B)$, and $D_3=\det\begin{pmatrix} C+B & 1 \\ 1 & 0 \end{pmatrix}$.

In order that M and M' have the rank 5 it is sufficient that $D_1=0$ and $D_3=0$. These conditions determine the flexible form of the hexagon. Supposing now $D_1\neq 0$ it follows that the D_3 matrix should have the rank 2. This gives a single solution (x_r,y_r,z_r) with $x_r=b_2+c_2+b_3+c_3-b_1-c_1$, $y_r=b_3+c_3+b_1+c_1-b_2-c_2$, $z=b_1+c_1+b_2+c_2-b_3-c_3$. This corresponds to a rigid position of the hexagon. We have

$$D_1 \equiv xyz - \sum x\ (b_1-c_1)^2 + 2\prod(b_1-c_1) = 0 \quad . \qquad 3.1$$

$$D_3 \equiv - \sum (x-x_r)(y-y_r) = 0 \ . \qquad 3.2$$

Thus in x,y,z space the flexible positions are determined by a curve of the sixth degree lying on a circular cone the vertex of which corresponds to the rigid position.

It may happen that the D_1-surface passes through the vertex of the D_3-cone. In that case for (x_r,y_r,z_r) the matrix M has even the rank 4 so that the hexagon is lying in a plane. In that case no other real positions exist.

4. Examples

In the case of cyclohexane we have

$$b_1=b_2=b_3=1 \qquad\qquad c_1=c_2=c_3=8/3$$

so that

$$D_1 \equiv xyz - \frac{25}{9}\ (x+y+z) - \frac{250}{27} = 0$$

$$D_3 \equiv - \sum (x - \frac{11}{3})(y - \frac{11}{3}) = 0.$$

Putting $x = \frac{11}{3} + \frac{2}{3}\xi$, $y = \frac{11}{3} + \frac{2}{3}\eta$, $z = \frac{11}{3} + \frac{2}{3}\zeta$ we have [3)]

$$\xi\eta\zeta + 24\ (\xi+\eta+\zeta) + 32 = 0$$

and

$$\xi\eta + \eta\zeta + \zeta\xi = 0\ .$$

The projection of the intersection of these surfaces upon the ζ-plane is

$$\xi^2\eta^2 - 24\ (\xi^2+\eta^2+\xi\eta) - 32(\xi+\eta) = 0$$

which is apparently an oval curve within the square

$$-\frac{4}{3} \leq \xi, \eta \leq -2+\sqrt{6} .$$

In the case of cyclohexanedione -1,4 we have

$$b_1 = b_2 = b_3 = 1 \qquad c_1 = c_2 = 8/3, \quad c_3 = 3,$$

so that

$$D_1 \equiv xyz - \frac{25}{9}(x+y) - 4z - \frac{100}{9} = 0$$

$$-D_3 \equiv (x-4)(y-4) + (z - \frac{10}{3})(x+y-8) = 0.$$

The rigid position is $x=y=4$, $z = \frac{10}{3}$.

Putting $x=4+\frac{2}{3}\xi$, $y=4+\frac{2}{3}\eta$, $z = \frac{10}{3} + \frac{2}{3}\zeta$ we have [4]

$$4\xi\eta\zeta - 4\xi\eta + 95(\xi+\eta) + 108\zeta + 90 = 0$$

$$\xi\eta + \eta\zeta + \zeta\xi = 0 .$$

In the case of a plane regular hexagon we have

$$b_1 = b_2 = b_3 = 1 \qquad c_1 = c_2 = c_3 = 3$$

so that

$$D_1 \equiv xyz - 4(x+y+z) - 16 = 0$$

$$D_3 \equiv -\sum(x-4)(y-4) = 0 .$$

Putting $x=4+\xi$, $y=4+\eta$, $z=4+\zeta$ we obtain

$$\xi\eta\zeta + 12(\xi+\eta+\zeta) = 0$$

and

$$\xi\eta + \eta\zeta + \zeta\xi = 0 .$$

The projection of the intersection upon the -plane is

$$\xi^2\eta^2 - 12(\xi^2+\eta^2+\xi\eta) = 0 .$$

In the admissible region there is only the isolated double point $\xi = \eta = 0$ (rigid plane position).

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1) Ber.23 (1890) 1363 and Z.physik.Chem.10 (1892) 203.

2) L.J. Oosterhoff, Restricted free rotation and cyclic molecules. Thesis, Leiden (1949).

3) L.J. Oosterhoff, l.c. ch.V.

4) ib. ch.VI.