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A note on flexible hexagons

by

H.A. Lauwerier

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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

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

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

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

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

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

Hence we have e.g.

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

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

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

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:

The existence of a flexible form of a non-degenerate hexagon implies the equality of opposite elements.

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

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

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 $x_r = b_2 + c_2 + b_3 + c_3 - b_1 - c_1$, $y_r = b_3 + c_3 + b_1 + c_1 - b_2 - c_2$, $z_r = b_1 + c_1 + b_2 + c_2 - b_3 - c_3$. This corresponds to a rigid position of the hexagon. We have

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

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

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

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

so that

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

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

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

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

The projection of the intersection of these surfaces upon the ξ -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

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

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

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

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 $\xi\eta$ -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).

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.