# On the regular heptagon

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The geometry of rings with 5, 6, 7, 8 and 9 links, particularly those with seven links such as occur in cyclo-heptane and analogous molecules<sup>\*</sup> is re-considered with the aid of distance geometry, now more practicable with modern mathematical software. Use is made of a quadric surface which may be fitted to nine points.

# 1. Distance geometry

In considering the geometry of molecules it is convenient to use internal coordinates which do not depend on a particular choice of an axial system. The most immediately intelligible measures are bond lengths  $d_{ij}$ , bond angles  $\theta_{ijk}$  and torsion angles  $\phi_{ijkl}$ . We will consider here only structures in three dimensions, although reference to more dimensions will be necessary. The main problem was propounded by L.N.M. Carnot [2,3] in 1803 as: "In any system whatever of straight lines, in the same plane or not, being given certain of their lengths, or of the angles between them, or of the angles between planes containing them, in number sufficient to determine the figure, find the remainder of these parameters." For uniformity we may use only distances, the bond angles being given by

$$d_{ik}^{2} = d_{ij}^{2} + d_{jk}^{2} - 2d_{ij}d_{jk}\cos\theta_{ijk}.$$

 $A_{ijk} = (1/2)d_{ij}d_{jk}\cos\theta_{ijk}$  is the area of the triangle i, j, k and  $V_{ijkl}$  is the volume of the tetrahedron i, j, k, l. Instead of the torsion angle  $\phi_{ijkl}$  (for which there are well known but much more complicated expressions in terms of the distances), we will use the corresponding distance  $d_{il}$  and call it a 'torsion distance'. In most expressions knowledge of the chirality of tetrahedra is lost. This is a serious loss, the chief disadvantage of systematic distance geometry, and the power of chirality considerations has been discussed elsewhere [14]. However, when necessary, the distance matrix can

<sup>\*</sup> In admiration for the author I have ventured to appropriate the title of Archimedes' work "On the regular heptagon", which came to light only in 1926 [16]. "Regular", as applied to rings in space admits of various definitions.

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be factorised back (using, for example, the Cholesky decomposition) to give x, y, z coordinates [4–6,12,13].

In particular, modern computing facilities, especially the appearance of the Mathematica system [19], enable us to use expeditiously the Cayley–Menger determinant, both numerically and in algebra. The geometry of rings of 5, 6, 7, 8 and 9 links is of some relevance in considering hypothetical carbon networks.

# 2. Determinantal relationships

 $V_{(N-1)}$ , the content of an (N-1)-dimensional simplex defined by N points in N-1 dimensions, is given by

$$V_{N-1}^{2} = \frac{(-1)^{N}}{2^{N-1}((N-1)!)^{2}} \begin{vmatrix} 0 & d_{12}^{2} & d_{13}^{2} & . & d_{1,N}^{2} & 1 \\ d_{21}^{2} & 0 & d_{23}^{2} & . & d_{2,N}^{2} & 1 \\ d_{31}^{2} & d_{32}^{2} & 0 & . & d_{3,N}^{2} & 1 \\ . & . & . & . & . \\ d_{N,1}^{2} & d_{N,2}^{2} & d_{N,3}^{2} & . & 0 & 1 \\ 1 & 1 & 1 & . & 1 & 0 \end{vmatrix} .$$
(1)

The coefficients are, for N = 3, 4, 5, 6 respectively, -1/16, 1/288, -1/9216, 1/460800.

The general form was stated by Blumenthal [1] but must have been known much earlier, since Lagrange gave the relationship of the 10 distances between 5 points in three-dimensional space. The relation states that the four-dimensional content of the simplex formed by five points should be zero. It is thus

For N points in three dimensions (N > 4) the rank of the Cayley–Menger determinant is 5.

The Cayley–Menger determinant for N points can be reduced to the metric matrix for N-1 dimensions by subtracting the first row and column from each other row and column. Thus, the reduced Cayley–Menger determinant for four points becomes

$$\begin{array}{cccc} -2d_{12}^2 & d_{23}^2 - d_{12}^2 - d_{13}^2 & d_{24}^2 - d_{12}^2 - d_{14}^2 \\ d_{23}^2 - d_{12}^2 - d_{13}^2 & -2d_{13}^2 & d_{34}^2 - d_{13}^2 - d_{14}^2 \\ d_{24}^2 - d_{12}^2 - d_{14}^2 & d_{34}^2 - d_{13}^2 - d_{14}^2 & -2d_{14}^2 \end{array} \right|$$

From the cosine rule  $d_{23}^2 - d_{12}^2 - d_{13}^2 = -2d_{12}d_{13}\cos\theta_{213}$ , etc., so that the determinant becomes

$$(-2)^{3} \begin{vmatrix} d_{12}^{2} & d_{12}d_{13}\cos\theta_{213} & d_{12}d_{14}\cos\theta_{214} \\ d_{12}d_{13}\cos\theta_{213} & d_{13}^{2} & d_{13}d_{14}\cos\theta_{314} \\ d_{12}d_{14} & d_{13}d_{14}\cos\theta_{314} & d_{14}^{2} \end{vmatrix},$$

which is seen to be the metric matrix for the parallelepiped with origin at (1) and axes (12), (13), (14) the determinant of which is the square of the volume. The volume of the corresponding simplex (here a tetrahedron), is found by dividing by (N - 1)!. Thus, for N points in three dimensions the rank of the reduced matrix is three.

#### 2.1. "Ptolemaicity"

Ptolemy's theorem, relating distances between four points (1234) on a circle, has been generalised by Blumenthal, following Cayley and others. In a cyclic quadrilateral

$$d_{12}d_{34} + d_{14}d_{23} = d_{13}d_{24}.$$
(3)

This is just the particular case for two dimensions of a more general theorem. For 4 points on a circle the determinant

$$\begin{vmatrix} 0 & d_{12}^2 & d_{13}^2 & d_{14}^2 \\ d_{21}^2 & 0 & d_{23}^2 & d_{24}^2 \\ d_{31}^2 & d_{32}^2 & 0 & d_{34}^2 \\ d_{41}^2 & d_{42}^2 & d_{43}^2 & 0 \end{vmatrix} = 0.$$
(4)

This quantity has been named by Blumenthal as the "Ptolemaicity"  $P_4$ . This determinant  $P_4$  can be factorised as

$$\begin{aligned} (d_{12}d_{34} + d_{23}d_{14} + d_{13}d_{24})(-d_{12}d_{34} + d_{23}d_{14} + d_{13}d_{24}) \\ \times (d_{12}d_{34} - d_{23}d_{14} + d_{13}d_{24})(d_{12}d_{34} + d_{23}d_{14} - d_{13}d_{24}) &= 0. \end{aligned}$$

The four terms are thus seen to be different expressions of Ptolemy's theorem covering the various permutations of the points. One at least is zero.

The condition that 5 points should lie on a sphere is known as Feuerbach's theorem (and was proved also by Cayley). It is

The theorem extends to N dimensions, but  $P_n$  does not factorise for n > 4.

Thus, for any 3 points in  $E^1$ ,  $V_3 = 0$ . If also  $P_3 = 0$  then the 3 points lie on  $S^0$ (a line), that is, two must be coincident.

For any 4 points in  $E^2$ ,  $V_4 = 0$ . If also  $P_4 = 0$  then the four points lie on  $S^1$  (a circle).

For any 5 points in  $E^3$ ,  $V_5 = 0$ . If also  $P_5 = 0$  then the five points lie on  $S^2$  (a sphere). Thus for N points (N > 4) in 3-dimensions the determinant  $P_n$  is of rank 4.

#### 2.2. The generalised spherometer

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For the sphere of radius R circumscribing the tetrahedron (1234) we have

$$-2R^{2} \begin{vmatrix} 0 & d_{12}^{2} & d_{13}^{2} & d_{14}^{2} & 1 \\ d_{21}^{2} & 0 & d_{23}^{2} & d_{24}^{2} & 1 \\ d_{31}^{2} & d_{32}^{2} & 0 & d_{34}^{2} & 1 \\ d_{41}^{2} & d_{42}^{2} & d_{43}^{2} & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{vmatrix} = \begin{vmatrix} 0 & d_{12}^{2} & d_{13}^{2} & d_{14}^{2} \\ d_{21}^{2} & 0 & d_{23}^{2} & d_{24}^{2} \\ d_{31}^{2} & d_{32}^{2} & 0 & d_{34}^{2} \\ d_{31}^{2} & d_{32}^{2} & 0 & d_{34}^{2} \\ d_{41}^{2} & d_{42}^{2} & d_{43}^{2} & 0 \end{vmatrix}$$
(6)

or

$$-2R^2 \times 288 \times V_4^2 = P_4.$$

We can write the factors of  $P_4$  (above) so that

$$36V^2R^2 = \sigma(\sigma - aa')(\sigma - bb')(\sigma - cc'),$$

where

$$aa' + bb' + cc' = 2\sigma$$

and a, a', etc., are pairs of opposite edges of the tetrahedron, giving a solid analogy with Heron's formula  $(A^2 = s(s - a)(s - b)(s - c))$  for the area of a triangle in terms of its sides a, b, c (2s = a + b + c).

A spherometer measures the curvature of a spherical surface, such as that of a lens, by fitting four points to it (3 fixed points at the vertices of an equilateral triangle of side d, and one point at its centre), the displacement x of the latter from the plane of the triangle being measured. The radius is found from  $x(2R - x) = (d/\sqrt{3})^2$ .

Consequently, the expression above might be regarded as a generalised spherometer covering any disposition of four points. This expression generalises to Ndimensions. In two dimensions the expression reduces to  $R = d_{12}d_{23}d_{31}/(4A)$ , the standard expression for the radius of the circumcircle of the triangle (123).

#### 3. **Pseudo-rotation**

For ring molecules which are nearly symmetrical it is convenient to express atomic positions as displacements above and below a circle in a median plane [10]. If atoms move up and down in this plane with phases which increase from one atom to

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its neighbour, then a wave is seen to be propagated round the ring. If the atoms are equivalent to each other then this movement is equivalent to a rotation of the ring and is called pseudo-rotation. For the heptagon, as in a Möbius strip the wave goes round twice before restoring the initial conformation [9].

For chemical purposes it is useful to express the conformation of a distorted ring in normal coordinates corresponding to possible normal modes of vibration, but we choose not to follow this procedure here.

# 4. The pentagon

We may approach the geometry of the heptagon by way of the pentagon and hexagon. In a pentagonal ring 3N - 6 = 9, but there are 10 distances so that there must be one relationship between them. This is that the 4-dimensional content of the simplex defined by 5 points is zero.

# 4.1. The equilateral, equiangular pentagon is planar

The regular equiangular pentagon is planar [8,18]. The sides are of unit length and the bond angles correspond to distances  $\sqrt{x}$ .

For any four points of the pentagon the square of the volume of the tetrahedron (1234) is

$$\begin{vmatrix} 0 & 1 & x & x & 1 \\ 1 & 0 & 1 & x & 1 \\ x & 1 & 0 & 1 & 1 \\ x & x & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{vmatrix} = 288V^2.$$

This multiplies out to  $-2x^3 + 4x^2 + 4x - 2 = 0$ , the roots of which are  $x = \tau^2$  and  $x = 1/\tau^2$ . In these cases V = 0, all five overlapping tetrahedra are planar, and so the regular pentagon as a whole is planar.

There are two flat conformations, the convex pentagon and the pentagram with bond angles  $108^{\circ}$  and  $36^{\circ}$  respectively.

#### 4.2. The sum of torsion angles round a general five-membered ring

For a tetrahedron (1234)

$$6V_{1234} = 4A_{123}A_{234}\sin\phi_{1234}/d_{23}.$$

Define the sign of the volume (1234) (a tetrahedron with vertices at 000, 001, 010, 100) as positive if

$$V = (1/6) \begin{vmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{vmatrix}.$$

Points (123) are numbered clockwise looking out from the origin (a fourth index). The figure, five points in space, can be regarded either as two tetrahedra, (1234) and (2345) sharing the face (234), or as three tetrahedra (1235), (1245) and (1345) sharing the edge (15). Using the convention above for the volumes numbered cyclically round the ring (12345): -(1234), -(2345), +(3451), +(4512), +(5123). Thus, the volumes taken with these signs sum to zero, so that, summing round the ring,

$$\sum \frac{|A_{ijk}||A_{jkl}|}{d_{jk}} \sin \phi_{ijkl} = 0.$$
(7)

This is a slightly more general result than that of Dunitz and Waser [7] who found that

$$\sum \sin \phi_{ijkl} \sin \theta_{ijk} \sin \theta_{jkl} = 0 \tag{8}$$

for five-membered rings with equal bond lengths. This result does not hold for sixmembered rings, but the quantity is a useful parameter of chirality and a parametrisation of the heptagon which treats all seven torsion angles equally.

# 5. The hexagon

If the six interatomic distances round a hexagonal molecule and the six bond angles are specified, then the molecule usually has no further degrees of freedom and the six torsion angles are also fixed. For six atoms 3N - 6 = 12. It is well known that cyclohexane has two conformations, the "boat" shape and the "chair" shape. The former is flexible and has the symmetry 2 (maximum symmetry mm2), while the latter has the symmetry  $\overline{3}$ m. Cauchy's theorem states that for a convex polyhedron, if every face is rigid, the polyhedron as a whole is rigid. Thus the "chair" form of cyclohexane is kinematically similar to an octahedron and is thus rigid.

Configurations of hexagons with irregular bond lengths and angles presumably follow these two patterns, the criterion of convexity separating them.

Figure 1 shows the relationship between the three torsion distances. It was plotted by using the knowledge that the Cayley–Menger determinant for six points is of rank five and that the six determinants obtained by stroking out one row and the corresponding column are also zero. The determinant contains three unknowns, the three diagonals of the hexagon, and two can be solved for directly with Mathematica if one is fixed (thus fixing the shape).

Since physically the conformation of a ring depends on every member, it must also be so mathematically and the constraints give rise to simultaneous non-linear equations. These are best solved by successive approximations involving simultaneous linear equations.

#### 6. The heptagon

Seven points require 3N-6 = 15 suitably chosen internal coordinates to define a conformation. In a heptagon, 7 distances (round the ring) and 7 bond angles leave one quantity lacking. The heptagon, defined in this way, thus has one degree of freedom. Thus, it is not surprising, therefore, that [7] circulene, (a heptagon surrounded by seven hexagons) should be floppy [17]. There are seven torsion angles all of which become fixed when one distance is set. To find the possible combinations of distances (given unit bond distances and fixed bond angles - here tetrahedral, 109.47°, which fix the corresponding torsion distances at  $\sqrt{8/3}$  – 15 distances have been set and the 21 x,  $y_{1,2}$  coordinates of the 7 vertices are found by repeatedly solving 15 linear equations for 21 unknowns using the generalised inverse of a matrix with the SVD (singular value decomposition) programme recommended by 'Numerical Recipes' [15]. The centre of gravity of the molecule is fixed to prevent it from drifting away. When a set of coordinates matching the 15 set distances has been found then the remaining six distances corresponding to the torsion angles can be calculated. The sets of seven distances can then be plotted against the sum of the volumes of the corresponding tetrahedra added round the ring (figures 2a and 2b). This sum resembles the sum of the torsion angles.

There are two conformations, corresponding to the boat and chair forms of cyclohexane.

It is also illuminating to plot the torsion distances against one distance. This shows how the shape changes as one distance is increased from minimum to maximum (figures 3a-3c).

It is quite possible to repeat the same calculations for irregular distances but



Figure 1. In the boat form of the hexagon (with six unit bond distances and tetrahedral bond angles) there is one parameter (here simply the length of one of the three diagonals) against which the lengths of the three different diagonals are plotted. The maximum length is 1.99156, the minimum 5/3 and the cross-over points are at  $\sqrt{11/3} = 1.91485$  and 1.751384. The chair form (with symmetry  $\bar{3}$ m) has three diagonals of  $\sqrt{11/3} = 1.91485$  and all six vertices lie on a sphere.



Figure 2. (a) In the heptagon (with seven unit bond distances and seven tetrahedral bond angles and with seven torsion distances which are fixed when one torsion distance is fixed) the sum round the ring of the volumes of successive tetrahedra gives an index against which the seven torsion distances vary as the ring is twisted. This is a parametrisation which treats all seven torsion angles equally. (b) One torsion distance characterises a conformation. The seven torsion distances in the heptagon can be plotted against one torsion distance.



Figure 3. In the heptagon one torsion distance (as 14) may be plotted against the next torsion distance (as 25)'(a), the next but one (14 against 36) (b), or the third (14 against 47) (c). Like the Möbius strip, two circuits are required in order to return to the starting conformation.

the plot becomes confused and less clearly informative about the process of pseudorotation. We may recall that the flat heptagon with bond angles  $128.57^{\circ}$  has two stellations (with bond angles  $77.14^{\circ}$  and  $25.71^{\circ}$ ) but that these are chemically impossible. The full plot for all bond angles would be difficult to present graphically.

On the basis of numerical tests it is believed that an ellipsoid (or hyperboloid) of revolution can be drawn through any seven points (in three dimensions). Three quantities are needed to specify its centre, two for its proportions and two for the

direction cosines of its axis of symmetry.

This hypothesis was tested with a computer programme which went as follows:

It is known that a quadric surface can be drawn through nine points. The equation of the quadric is

 $a_{11}x^2 + 2a_{12}xy + 2a_{13}xz + 2a_{14}x + a_{22}y^2 + 2a_{23}yz + 2a_{24}y + a_{33}z^2 + 2a_{34}z + a_{44} = 0$ (9)

( $a_{44}$  may be set to 1 if the surface does not go through the origin). Each of the nine points gives a linear equation connecting the  $a_{ij}$  and the set of nine can be solved, using the generalised inverse to invert the matrix, most rapidly following the SVD programme which covers the degenerate cases where the rank of the  $9 \times 9$  matrix to be inverted may be less than nine.

Seven points are chosen at random and the  $7 \times 9$  matrix of seven equations is solved for the nine coefficients of the equation above. The rank of the array is seven. The full solution of the matrix equation A(7,9)X(9) = H(7), putting in the dimensions of the arrays, is, where  $A^+(9,7)$  is the generalised inverse of A(7,9),

$$X(9) = A^{+}(9,7)H(7) + |I(9,9) - A^{+}(9,7)A(7,9)|Z(9),$$
(10)

and where the second term represents the nullity of A and is (in general) of rank two. Z is an arbitrary vector, which, if given all possible values, scans over all possible solutions.

We take the second term (a  $9 \times 9$  matrix of rank 2) and find its eigenvalues and the corresponding eigenvectors by Jacobi's method. Two eigenvalues have the value one and seven are zero. We take the two non-zero eigenvectors  $V_1(9)$  and  $V_2(9)$  and combine them to make an arbitrary vector Z(9) by  $Z(9) = k_1V_1(9) + k_2V_2(9)$ . This is then substituted into the equation for the quadric surface. For numerical values of  $k_1$ and  $k_2$  the values of the invariants of the quadric equation can be calculated.

The shape of the quadric can be characterised by the invariants of the equation or by the three eigenvalues of D. The invariants of the cubic characteristic equation are T the trace, S the second invariant and D the determinant and the further condition that two eigenvalues should be equal, that is, that the quadric should be a figure of revolution is

$$D^{2}/4 + S^{3}/27 - DST/6 - S^{2}T^{2}/108 + DT^{3}/27 = 0.$$
 (11)

We may call this quantity R and adjust the values of  $k_1$  and  $k_2$  until R is nearly zero. Since the two eigenvectors used are orthogonal, this process is straightforward. Finally, the three eigenvalues of the equation for the adjusted quadric are recalculated and two are found to be the same. Since we find in experimental cases that this can be done, grounds for the belief that an ellipsoid (hyperboloid) of revolution can be drawn through seven points are provided. Since this ellipsoid can be characterised by two parameters, c/a and a, then these could be used for characterising the heptagon, which also has two parameters, bond length and 'shape'.

The general background is to be found under Singular Value Decomposition in reference [15].

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# 7. The octagon

For an octagonal ring 3N-6 = 18 so that, after 8 bond lengths and 8 bond angles are fixed, two degrees of freedom remain. Thus, we may fix two further distances and examine how the remaining six torsion angles change. Conditions on the rigidity of the octagon are more complicated. For a ring there are 8 bond lengths, 8 bond angles, 8 torsion angles and 4 cross distances. Examining the case of the tetragonal antiprism we see that fixing a diagonal in each of the quadrilatgeral faces allows Cauchy's theorem to be invoked and this particular case is rigid. Suppose that the eight points are numbered 1 to 8 round the ring.

W.K. Clifford and A. Sylvester (1852) generalised the above determinantal expressions for volume as follows:

$$V_{1357}V_{2468} = (1/288) \begin{vmatrix} d_{12}^2 & d_{14}^2 & d_{16}^2 & d_{18}^2 & 1 \\ d_{32}^2 & d_{34}^2 & d_{36}^2 & d_{38}^2 & 1 \\ d_{52}^2 & d_{54}^2 & d_{56}^2 & d_{58}^2 & 1 \\ d_{72}^2 & d_{74}^2 & d_{76}^2 & d_{78}^2 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{vmatrix} .$$
(12)

Their result follows from the vector identity:

$$[a.b \times c][d.e \times f] = \begin{vmatrix} a.d & b.d & c.d \\ a.e & b.e & c.e \\ a.f & b.f & c.f \end{vmatrix}.$$
(13)

When the bond lengths and bond angle distances are inserted in the above equation it is found that only the torsion 'distances' enter as unknowns. It thus elegantly connects the 4 cross distances and the 8 torsion angles.

Thus, the signed volumes of the two tetrahedra making up the square faces appear to be parameters suitable for describing a conformation, unless they are flat.

Since every distance is involved in fixing the configuration the various unknown distances cannot be found sequentially but only by solving simultaneous polynomial equations. Thus, the most practicable method of solution is that used in solving the heptagon, namely to find, by iteration, a set of coordinates for the vertices which provide the set of required distances. The programme used for the heptagon was readily extended to do this. In using the generalised inverse the second term includes one arbitrary eigenvector (where the heptagon requires two) which can be adjusted to various criteria.

How should the set of 8 distances (corresponding to the 8 torsion angles) be displayed as a function of the two parameters? Properly we require sheets with 3 - D contours but the picture becomes too complex to appreciate easily.

#### 8. The nonagon

For N = 9, 3N - 6 = 21 so that with 9 fixed bond lengths and 9 fixed angles a cyclo-nonane molecule has 3 degrees of freedom. Displaying this flexibility entails difficulties. If we can develop three parameters, such as three distances, a given conformation could be displayed as a point in three-dimensional space, but all points in a given region would be possible. This region of existence could be delineated.

The most general quadric surface is given by the equation (9 above) which involves nine quantities (and an arbitrary scale). Inserting nine values of x, y and z (9 points) gives nine linear equations which can be solved for these coefficients.

If the quadric is centred at the origin its equation reduces to

 $a_{11}x^{2} + 2a_{12}xy + 2a_{13}xz + a_{22}y^{2} + 2a_{23}yz + a_{33}z^{2} + A/D = 0,$ 

where A is the  $4 \times 4$  determinant of the coefficients above and D is the  $3 \times 3$  determinant of the coefficients remaining.

The three eigenvalues of the quadric thus provide parameters characterising the distribution of points in a relatively general way and corresponding to the principal axes of the quadric.

In general, our methods of calculation do not use considerations of symmetry so that most could be repeated for arbitrary bond lengths and angles. However, representations of the results become much less clear.

Extending the above treatment to rings of ten links takes us to the question of the *flexagons* discussed as a recreation by M. Gardner. Complexity increases remarkably rapidly with the number of vertices. For example, the complete graph of the heptagon (21 distances) is closely connected with the Császár polyhedron [11] which has 7 vertices, 14 faces and 21 edges. It is the simplest polyhedron with toroidal topology and has only a two-fold axis of symmetry.

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