

## Werk

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## The Planarity of the Equilateral, Isogonal Pentagon

In a recent publication, van der Waerden has shown that the equilateral, isogonal pentagon must be planar and has also given some interesting insights into the mental processes that led him to his proof of the theorem [1]. As van der Waerden graciously acknowledged, he was made aware of this remarkable property of the pentagon in the course of a conversation with one of us (J. D. D.) in 1969, but the property was first recognized (by J. W.) more than 25 years earlier, in the course of an electron-diffraction study of gaseous arsenomethane,  $(\text{AsCH}_3)_n$ . It must be very rare that a mathematical discovery<sup>1)</sup> has been made from the results of an experimental molecular-structure investigation so that a brief account of the earlier developments may be of interest in supplementing van der Waerden's description.

The result of the electron-diffraction study of arsenomethane [2] was a radial-distribution function<sup>2)</sup> consisting of only two peaks, a sharp one at 2.42 Å and a broad one, of approximately the same area, centred at 3.44 Å. Since As...As interactions would have to dominate over all others ( $Z_{\text{As}} = 33$ ,  $Z_{\text{C}} = 6$ ,  $Z_{\text{H}} = 1$ ) it follows that each arsenic atom in the arsenomethane molecule has the same number of

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<sup>1)</sup> We claim no thorough acquaintance with the mathematical literature but, as far as we are aware, this property of the pentagon had not been recognized earlier. At any rate it came as something of a surprise not only to VAN DER WAERDEN (loc. cit.) but also to G. PÓLYA, with whom J. D. D. discussed the problem in February, 1970. PÓLYA disclaimed any previous knowledge of the theorem and added "if VAN DER WAERDEN didn't know about it then it wasn't known to mathematics"!

<sup>2)</sup> In the electron-diffraction method a beam of monochromatic electrons ( $\lambda \sim 0.06$  Å) impinges on a stream of gas emerging from a nozzle into an evacuated chamber. The electrons are scattered by the molecules, and the scattered intensity recorded on photographic film. The intensity pattern, which is radially symmetric, depends on the structure of the molecules, specifically on the atomic numbers of the constituent atoms and on the interatomic distances. The FOURIER-transform of the experimental intensity distribution is known as the radial distribution function,  $r D(r)$ . It consists of a set of nearly Gaussian peaks at various distances  $r$  from the origin, corresponding to the various interatomic distances occurring in the molecule. The height of each peak is roughly proportional to the product of the atomic numbers of the two atoms involved in that particular distance. For further details see any book on modern structural chemistry.

unbonded neighbours (at approximately 3.44 Å) as bonded neighbours (at 2.42 Å). This is possible only if the arsenic atoms form a five-membered ring, in which the average As-As-As angle would have to be about 90°, a value close to the expected valency angle at arsenic [3]. In a four-membered ring, which is at first sight suggested by the 90° angle, each arsenic atom would have twice as many bonded neighbours as unbonded.

The breadth of the peak at 3.44 Å then had to be explained. It implies that the cross-ring As...As distances are unequal. Since the bonded As-As distances are equal, as shown by the sharpness of the 2.42 Å peak, this would mean that the As-As angles are unequal. Why should they be unequal? Thinking about this question led J. W. to the recognition of a unique property of the pentagon [4].

“Of all  $n$ -gons ( $n \geq 4$ ) the pentagon is the only one for which the following is true: The construction of an equilateral, equiangular pentagon is possible for only two values of the angle. For all other  $n$ -gons (excepting the trivial case of the triangle) there is a whole range of angles for which an analogous construction is possible. The pentagon under consideration is planar, the possible angles are 108° and 36°.”

In an equilateral pentagon with average angle of 90° the angles must then be unequal; the equilateral pentagon with all angles equal to 90° cannot be constructed! The proof provided by J. W. (not published at the time) was simple and straightforward. Slightly condensed, it runs as follows:

*A pentagon (in space) with all angles and all distances equal must be planar*

Since  $\sphericalangle 2 = \sphericalangle 3$ , the grouping 1234 must possess at least a dyad axis; it may also possess a mirrorplane (Fig. 1).

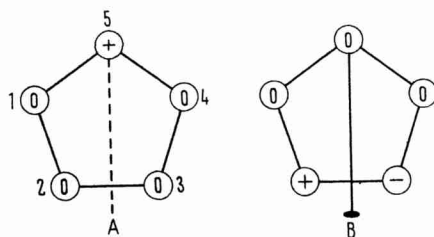


Figure 1  
Equilateral, isogonal pentagon, showing heights of vertices from a reference plane. In A, the grouping 1234 has  $C_{2v}$  symmetry, in B only  $C_2$  symmetry.

Case a) Suppose 1234 possesses  $C_{2v}$  symmetry. Then since  $2-5 = 3-5$ , the pentagon itself has a mirrorplane perpendicular to 2-3, passing through 5 (Fig. 1A).

Case b) Suppose 1234 possesses only  $C_2$  symmetry. Again, since  $2-5 = 3-5$ , 5 lies on the plane that is the perpendicular bisector of 23 and, since  $1-5 = 4-5$ , also on the plane that is the perpendicular bisector of 14. These planes do not coincide by assumption; the line they share is the dyad axis of 1234, and thus a dyad axis of the pentagon itself (Fig. 1B).

Passing round the pentagon, an exactly analogous argument can be applied for every grouping of four vertices. In every case, the remaining vertex must lie on a mirrorplane or dyad axis of the pentagon. The resulting system of intersecting mirrorplanes and/or dyad axes must possess at least  $D_5$  symmetry and hence the pentagon must be planar.

The spark in the genesis of this proof was the idea of considering just four of the five points. It was quickly realized that the four points had to be related by a dyad axis, with two additional mirror planes when the points were coplanar. It was then straightforward to demonstrate that the fifth point had to be on the dyad axis in the non-planar case, and on the mirror plane perpendicular to the plane of the four points in the second case. The fact that the combination of the symmetry elements obtained by cyclic permutation would lead to  $D_5$  or  $D_{5h}$  was prior knowledge; the mind was, so to speak, programmed by relationships of this kind, and this may well have contributed to the genesis of the proof.

Several years later, the structure of crystalline arsenomethane was determined by X-ray diffraction analysis and the puckered pentagonal structure of the molecule confirmed [5]<sup>3</sup>). The structures of several rings containing arsenic and phosphorus atoms were later discussed by Donohue to whom it was known that "the only equilateral, isogonal pentagon is planar" [6]. Nevertheless, the theorem did not become generally known to structural chemists.

If J. D. D. had ever known of it, he had forgotten it by 1966 when he came across a paper on the conformations<sup>4</sup>) of five- and six-membered rings [7]. This paper contains the statement: for a regular five-membered ring which is in the "envelope" conformation and has side  $l$  and internal angle  $2\alpha$ , the angle  $\phi$  between the planes BCD and ABDE (Fig. 2) is given by

$$\cos\phi = \frac{7/4 - 2\cos 2\alpha - \sin^2 2\alpha - \cos^2\alpha}{2\sin 2\alpha \cos\alpha}.$$

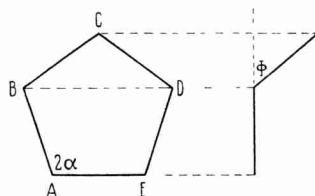


Figure 2  
Dihedral angle  $\phi$  between the planes BCD and ABDE.

A few minutes consideration showed that the regular five-membered ring as described must be planar since, if all angles are set equal to  $2\alpha$ , then

$$BD = l(1 - 2\cos 2\alpha) = 2l\sin\alpha$$

which is satisfied only for  $2\alpha = 108^\circ$  (or  $36^\circ$ ). The formula given for the dihedral angle was obviously incorrect!

J. D. D. was sufficiently impressed and excited by this result that he told it almost immediately to J. Donohue, on sabbatical leave from the University of Pennsylvania, who was spending the academic year 1966–1967 in Zurich. It came as no surprise to Donohue, who already knew of the result in the more general formu-

<sup>3</sup>) In crystalline arsenomethane, the individual As-As-As angles in the puckered five-membered ring are:  $100.4^\circ$ ,  $100.0^\circ$ ,  $105.6^\circ$ ,  $105.4^\circ$ ,  $97.5^\circ$ , mean value  $101.8^\circ$ . The conformation is about midway between one of mirror symmetry and one with a dyad axis (see<sup>4</sup>)).

<sup>4</sup>) In chemistry, the different possible shapes of a molecule with given bond distances and angles are called *conformations*.

lation. According to him, it had been well known among the members of the structural chemistry group at the California Institute of Technology around 1944–1945, but he could not recall any general proof.

J. D. D. was soon able to provide trigonometric proofs for the special cases of the equilateral, isogonal pentagons with  $C_s$  and  $C_2$  symmetry. He was convinced that the theorem *must* be true in the general case but the proof eluded him until he suddenly realized the importance of a property of the pentagon that he had known all along but without connecting it with the problem. If all sides are equal and all angles are equal, then all 1,3-diagonals are equal. Since each 1,3-diagonal of a pentagon is also a 1,4-diagonal, the torsion angles<sup>5)</sup> must also be equal at least in magnitude, if not in sign.

Referring back to Figure 1, suppose that the torsion angles  $\omega(3451)$  and  $\omega(4512)$  have opposite signs; then points 2 and 3 lie on the same side of the plane 451 and are displaced from this plane by the same amount, so that the points 1, 2, 3, 4 are coplanar. In this case the torsion angle  $\omega(1234)$  is zero, hence all torsion angles are zero and the pentagon is planar. Suppose alternatively that  $\omega(3451)$  and  $\omega(4512)$  have the same sign; then points 2 and 3 are equally displaced from the plane 451 but lie on opposite sides of it. In this case the pentagon has a dyad axis passing through 5. Again, the argument can be applied to each vertex in turn. Either some torsion angle (and hence all torsion angles) must be zero or we have a dyad axis through each vertex, leading to  $D_5$  symmetry and planarity, as in J. W.'s proof.

In the meantime we have learned of three other proofs in addition to that given by van der Waerden [1]. One of these, by Ruch [8], is geometrical, like the proofs already discussed, but it introduces some new aspects.

Because of the equality of the sides and angles of the pentagon, the five diagonals are equal in length. By omitting each vertex in turn we obtain five tetrahedra. Each tetrahedron has as its six edges three connected sides and three connected diagonals of the pentagon. The five tetrahedra are thus identical or mirror images.

Let  $AM = MD$  and  $BN = NC$  (Fig. 3). Since  $\triangle ABD = \triangle DCA$  and  $\triangle ABC = \triangle DBC$  it follows that  $BM = CM$  and  $AN = DN$ , so that the line  $MN$  is perpendicular to  $BC$  and  $AD$  and hence a dyad axis of the tetrahedron  $ABCD$ . The point  $E$  must also

<sup>5)</sup> In chemistry, the torsion angle  $\omega(ABCD)$  is defined as the angle between the bonds  $BA$  and  $CD$  in projection down the bond  $BC$ , and is given by

$$\cos \omega = \frac{(\mathbf{AB} \times \mathbf{BC}) \cdot (\mathbf{BC} \times \mathbf{CD})}{AB(BC)^2 CD \sin \theta_1 \sin \theta_2},$$

$$(\mathbf{BC}/BC) \sin \omega = \frac{(\mathbf{AB} \times \mathbf{BC}) \times (\mathbf{BC} \times \mathbf{CD})}{AB(BC)^2 CD \sin \theta_1 \sin \theta_2} = \frac{[\mathbf{AB} \times \mathbf{BC} \cdot \mathbf{CD}] \mathbf{BC}}{AB(BC)^2 (CD) \sin \theta_1 \sin \theta_2}$$

where  $\theta_1$  and  $\theta_2$  are the angles  $ABC$  and  $BCD$ , respectively. If  $\mathbf{AB}$ ,  $\mathbf{BC}$ ,  $\mathbf{CD}$  are unit vectors  $\mathbf{n}_1$ ,  $\mathbf{n}_2$ ,  $\mathbf{n}_3$ , respectively, then

$$\sin \omega = \frac{[\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3]}{\sin \theta_1 \sin \theta_2}.$$

The distance  $AD$  depends on the torsion angle  $\omega$  as well as on the bond distances and bond angles. For all bond distances equal to unity and all bond angles equal to  $\theta$

$$(AD)^2 = 3 - 4 \cos \theta + 2 \cos^2 \theta - 2 \sin^2 \theta \cos \omega$$

lie on this axis; this follows from  $CE = BE$  and  $DE = AE$  in case that the tetrahedron is non-planar, or from one of these equalities in case that the tetrahedron is planar – in the latter case all five tetrahedra must be planar and must lie in a common plane since any two such tetrahedra share three points in common. In either case the line  $MN$  is a dyad axis of the pentagon which thus possesses five such dyad axes and must be planar.

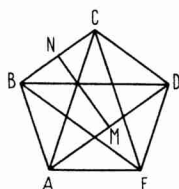


Figure 3

Another proof (by J. W.) is based on vector algebra. Let the directed edges of the equilateral, isogonal pentagon with angle  $\theta$  be represented by unit vectors  $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3, \mathbf{n}_4, \mathbf{n}_5$ . All possible triple scalar products formed by the five unit vectors involve either consecutive vectors, such as  $[\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3]$  or non-consecutive vectors, such as  $[\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_4]$ . The sign of a triple scalar product is, of course, reversed by changing the order of any two vectors in the product. The torsion angle about any edge is given<sup>5)</sup> by

$$\sin \omega_i = \frac{[\mathbf{n}_{i-1}, \mathbf{n}_i, \mathbf{n}_{i+1}]}{\sin^2 \theta}$$

and the sum of the torsion angles by

$$\sum_{i=1}^5 \sin \omega_i = \frac{1}{\sin^2 \theta} \sum_{i=1}^5 [\mathbf{n}_{i-1}, \mathbf{n}_i, \mathbf{n}_{i+1}]$$

where the indices are understood to be modulo 5.

For brevity, we shall write products such as  $[\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3]$  and  $[\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_4]$  simply as  $[123]$  and  $[124]$  with  $\Sigma[123], \Sigma[124]$  for the corresponding sums over the cyclic permutations (modulo 5). For the pentagon

$$[1 + 2 + 3 + 4 + 5, 2, 3] = 0 = [123] + [423] + [523] .$$

Rearrangement and cyclic permutation gives

$$\begin{aligned} [123] + [234] + [235] &= 0 \\ [234] + [345] + [341] &= 0 \\ \dots\dots\dots & \\ [512] + [123] + [124] &= 0 . \end{aligned}$$

Summing,

$$2 \Sigma [123] + \Sigma [124] = 0 .$$

Similarly,

$$[\mathbf{1}, \mathbf{1} + \mathbf{2} + \mathbf{3} + \mathbf{4} + \mathbf{5}, \mathbf{3}] = 0 = [\mathbf{123}] + [\mathbf{143}] + [\mathbf{153}]$$

leading to

$$\Sigma[\mathbf{123}] - 2\Sigma[\mathbf{124}] = 0.$$

Hence  $\Sigma[\mathbf{123}] = \Sigma[\mathbf{124}] = 0$  so that the sum of the torsion angles is zero. But the individual torsion angles are equal in magnitude (from the equality of the 1,3-diagonals, which are simultaneously 1,4-diagonals in the pentagon). Hence every torsion angle must be zero and the pentagon is planar.

It is of interest that for a general, spatial pentagon, quantities of the form  $[\mathbf{123}]$  etc., but defined in terms of vectors representing the pentagonal sides rather than unit vectors, still have the property that  $\Sigma[\mathbf{123}]$  and  $\Sigma[\mathbf{124}]$  are zero;  $[\mathbf{123}]$ ,  $[\mathbf{234}]$ , etc., are again related to the corresponding torsion angles, but not as simply as in the equilateral, isogonal case. For other spatial polygens similar relationships exist, e.g.  $2\Sigma[\mathbf{123}] + \Sigma[\mathbf{124}] + \Sigma[\mathbf{125}] = 0$  and  $3\Sigma[\mathbf{123}] = 2\Sigma[\mathbf{135}]$  for the hexagon.

Finally, at a still more refined level of abstraction, is a proof by Oosterhoff [9] based on matrix algebra, given here in slightly modified form.

Again let the directed edges of the equilateral, isogonal pentagon with angle  $\vartheta$  be represented by unit vectors  $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3, \mathbf{n}_4, \mathbf{n}_5$ . From the ring-closure condition we have

$$\mathbf{n}_1 + \mathbf{n}_2 + \dots + \mathbf{n}_5 = 0$$

from which we obtain five equations by successive scalar multiplication with  $\mathbf{n}_1, \dots, \mathbf{n}_5$  ( $s_{kl} = (\mathbf{n}_k, \mathbf{n}_l) = s_{lk}$ )

$$\begin{aligned} (\alpha) \quad & s_{11} + s_{12} + \dots + s_{15} = 0 \\ (\beta) \quad & s_{21} + s_{22} + \dots + s_{25} = 0 \\ (\gamma) \quad & s_{31} + \dots + s_{35} = 0 \\ (\delta) \quad & s_{41} + \dots + s_{45} = 0 \\ (\epsilon) \quad & s_{51} + s_{52} + \dots + s_{55} = 0. \end{aligned}$$

The Matrix  $\mathbf{S}$

$$\mathbf{S} = \begin{bmatrix} s_{11} & s_{12} & \cdot & \cdot & s_{15} \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ s_{51} & \cdot & \cdot & \cdot & s_{55} \end{bmatrix}$$

determines the linear dependence of the vectors  $\mathbf{n}_1, \dots, \mathbf{n}_5$  and the planarity of the pentagon follows if  $\mathbf{S}$  can be shown to be of rank 2.

From the conditions imposed on the pentagon we have

$$\begin{aligned} s_{k,k} &= 1 \\ s_{k,k+1} &= -\cos\vartheta = a \end{aligned}$$

noting again that the cyclic structure implies that when  $k = 5$ ,  $k + 1 = 1$  (modulo 5). By appropriate adding and subtracting the five equations above we obtain also

$$s_{k,k+2} = -1/2 - a = b$$

For example,  $s_{13}$  is obtained from  $(\alpha) + (\beta) + (\gamma) - (\delta) - (\epsilon)$ . (At this stage a geometric proof can be based on the equality

$$s_{k,k} + s_{k,k+1} + s_{k,k+2} = 1/2$$

from which it follows that the vector sum of any three consecutive sides projected on the first of these sides bisects that side. The subsequent steps follow the lines of the proofs discussed earlier. Oosterhoff prefers a more abstract approach).

We can now rewrite  $\mathbf{S}$  explicitly in terms of its elements as

$$\mathbf{S} = \begin{bmatrix} 1 & a & b & b & a \\ a & 1 & a & b & b \\ b & a & 1 & a & b \\ b & b & a & 1 & a \\ a & b & b & a & 1 \end{bmatrix} = \begin{bmatrix} \sigma_1 & \sigma_2 & \sigma_3 & \sigma_4 & \sigma_5 \\ \sigma_5 & \sigma_1 & \sigma_2 & \sigma_3 & \sigma_4 \\ \sigma_4 & \sigma_5 & \sigma_1 & \sigma_2 & \sigma_3 \\ \sigma_3 & \sigma_4 & \sigma_5 & \sigma_1 & \sigma_2 \\ \sigma_2 & \sigma_3 & \sigma_4 & \sigma_5 & \sigma_1 \end{bmatrix}.$$

$\mathbf{S}$  is seen to be a circulant matrix of order 5. It is a property of any circulant  $\mathbf{C}$  of order  $n$  that its determinant  $|\mathbf{C}|$  can be expressed as a product of  $n$  factors of the form [10]

$$\sigma_1 + \sigma_2 \omega_j + \sigma_3 \omega_j^2 + \dots + \sigma_n \omega_j^{n-1}$$

where  $\omega_j (j = 1, 2, \dots, n)$  is one of the  $n$ th roots of unity,  $\exp(2\pi i j/n)$ . Thus in our case

$$|\mathbf{S}| = \prod_{j=1}^5 \sum_{k=1}^5 \sigma_k \omega_j^{k-1}.$$

The factor with  $j = 5$  is zero because it is identical with the left side of  $(\alpha)$ . Of the remaining four factors those with  $j = 1$  and  $j = 4$  are complex conjugate, and similarly those with  $j = 2$  and  $j = 3$ . Therefore the rank of  $\mathbf{S}$  is either 0, 2 or 4. It is certainly not 0 (e.g.  $s_{11} \neq 0$ ) and it cannot be 4 since the vectors are three-dimensional. Hence the rank of  $\mathbf{S}$  is 2, which proves the theorem.

We remark that the  $3 \times 3$  subdeterminants of  $|\mathbf{S}|$  are identical with products (and squares) of the quantities [123] etc. referred to earlier. For example, the  $3 \times 3$  determinant of scalar products obtained by retaining rows 1, 3, 5 and columns 2, 3, 4 of  $|\mathbf{S}|$  is equal to [135] [234], being a generalization of Gram's determinant [11].

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