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Regular spatial hexagons

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1 Introduction

Regular spatial n-gons are understood to be nonplanar n-gons in E^3 that are equilateral and equiangular, i.e., they have sides of equal length and equal angles between consecutive sides. Evidently, the second property implies equal length of the diagonals between a vertex and the next but one. As n increases, it rapidly becomes more difficult to maintain an overview of these n-gons.

The simplest case is that of $n=4$. In Figure 1, it is easy to see that for each angle $\alpha < 90°$ there exists a regular spatial quadrangle: by rotating one subtriangle of the rhombus (left) around the diagonal of length q, we can obtain q for the length of the other diagonal and thus the four equal angles α (right).

Ein n-Eck heisst hier regulär, wenn es lauter gleich lange Seiten und gleiche Winkel zwischen allen Nachbarseiten hat. Während sich die Klassifikation von regulären n-Ecken in der Ebene noch sehr einfach darstellt, ist die Situation in drei Dimensionen ungleich komplexer. Die vorliegende Arbeit gibt einen Überblick über alle regulären räumlichen Hexagone, d.h. die nicht-planaren regulären Sechsecke im dreidimensionalen euklidischen Raum. Basierend auf Symmetrien ergeben sich sechs Klassen solcher Hexagone, welche elementargeometrisch auf viele Eigenschaften hin untersucht werden. Eine Koordinatendarstellung ermöglicht die Berechnung der Diagonalen, die dann ihrerseits erlauben, die Mannigfaltigkeit in spezieller Form darzustellen. Zum Schluss werden ohne Beweis noch weitere Eigenschaften von Hexagonen genannt. Ergänzend finden sich unter [8] Animationen und zusätzliche Figuren zu verschiedenen Aspekten dieser Arbeit.

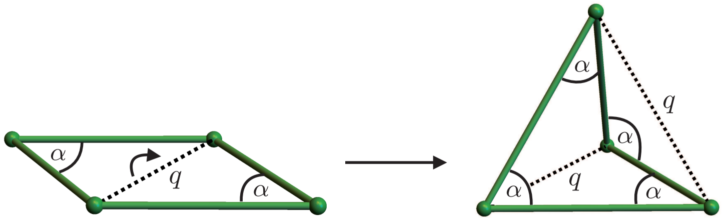


Figure 1: Generation of a regular spatial quadrangle ($\alpha < 90°$).

The next case, $n = 5$, yields the astonishing result that no regular spatial pentagon exists. This has been reported or proved by various authors, independent of each other [1, 2, 10, 12]. For a short and elegant proof, see [11], and for more historical details, the reader is referred to the introduction in [9].

With $n = 6$, we arrive at the subject of this article: What do regular spatial hexagons look like? The six-membered ring of cyclohexane, which has an angle $\alpha = \arccos(-\frac{1}{3})$ approximately equal to 109.5°, has been examined for a long time in stereochemistry. Detailed mathematical studies of cyclohexane, based on distance geometry, can be found in [3, 13].

Concerning regular spatial hexagons of any possible angle α, coordinates are given in [6]; they have been generated from the hexagon's net (see Figure 3 below) and consist of trigonometric terms. Moreover, aspects of symmetry are addressed in [14] and in some chemically motivated approaches (see [4]).

In this article, we show that the set of all regular spatial hexagons can be subdivided into six classes, the characteristic of each class being a common symmetry group of the hexagons contained therein. Regarding this classification, and by using elementary geometry, we examine various structural properties and calculate different determining parameters. The hexagons are also described by coordinates, which enables the computation of the diagonals. Finally, we summarize by means of a specific representation and mention some further properties, but without underlying proofs.

It should be added that, based on different definitions of regularity, also n-gons in higher-dimensional Euclidean spaces have been the subject of investigations, with particular regard to their existence; see [5, 7, 9] and the references therein. The general results of these studies, however, have no impact on this article.

The reader is also referred to a series of animations and figures that, in addition, graphically illustrate results of this paper [8].

2 Preliminaries

In the following, regular spatial hexagons are called *hexagons* for short. Since the problems we discuss are independent of similarity, we restrict ourselves to hexagons with side length 1. Intersecting sides are permitted; however, unless stated otherwise, coinciding vertices are not.

In a hexagon with angle α, we use concepts and notations, which are shown in Figure 2. The consecutive vertices are denoted by $v_1, v_2, \dots, v_6$. The common length q of the six diagonals connecting a vertex with the next but one is given by α as follows:

$$q = 2\sin\frac{\alpha}{2}. \tag{1}$$

Apart from the (secondary) diagonals q, there are the three (main) diagonals x, y, and z between opposite vertices. In general, they differ in length and we write $x = \overline{v_1v_4}$, $y = \overline{v_2v_5}$, and $z = \overline{v_3v_6}$. In the following, when referring to q, x, y, or z, we always mean either the corresponding line segment or its length depending on the context.

Of course, the diagonals x, y, and z are interchangeable. For a given q, one, three, or even six different triples (x, y, z) determine congruent hexagons depending on whether all three, exactly two, or none of its elements are equal, respectively. Thus, a result about diagonals x, y, and z remains true when these are accordingly permuted.

Further concepts are useful: The triangle $v_1v_3v_5$ of a hexagon is equilateral with side q and we call it a *q-triangle*. Each of the attached isosceles triangles $v_1v_2v_3$, $v_3v_4v_5$, and $v_5v_6v_1$ is rotated outwards around its base q into the plane of the q-triangle. The resulting planar figure with the new vertices $\widehat{v}_2$, $\widehat{v}_4$, and $\widehat{v}_6$ and angles α and $\widehat{\alpha}$, as shown in Figure 3 (in the plane of the paper), is said to be the *net* of the hexagon. Clearly, there is a second q-triangle $v_2v_4v_6$ with a congruent net.

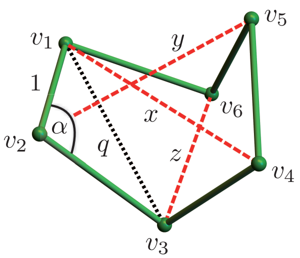


Figure 2: Notations for a hexagon.

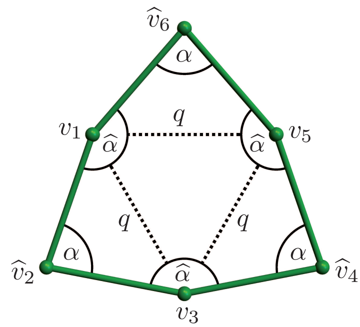


Figure 3: Net of a hexagon.

By means of the net, we prove the following:

Theorem 1. *A hexagon with angle α exists if and only if* $0° < \alpha < 120°$.

Proof. Evidently, we have $0° < \alpha$. The angle α of the hexagon at vertices v_1, v_3, and v_5 is compared with the corresponding angle $\widehat{\alpha}$ of the net. By applying twice the inequality for spherical triangles, it follows that $\alpha < \widehat{\alpha}$ (for $\widehat{\alpha}$ at v_1, for instance, consider the central projections of the triangles $v_2v_3v_5$ and $v_2v_5v_6$ from v_1 onto the unit sphere with center v_1). The angle sum of the net hexagon is now $3\alpha + 3\widehat{\alpha} = 720°$, and therefore that of the hexagon becomes smaller than $720°$, which implies $\alpha < 120°$.

Conversely, if $0° < \alpha < 120°$, then the side p of the equilateral triangle $\widehat{v}_2\widehat{v}_4\widehat{v}_6$ of the net is larger than q. Consider a rotation of each of the outer isosceles triangles $v_1\widehat{v}_2v_3$,

$v_3\widehat{v_4}v_5$, and $v_5\widehat{v_6}v_1$ around its base q with the same angle into the same half-space. With an increasing rotation angle, p becomes smaller and at 90° it is $\frac{1}{2}q$. Hence, in between there exists a q-triangle $v_2v_4v_6$ of a hexagon with angle α. □

From (1) and Theorem 1 it follows that a hexagon exists if and only if

$$0 < q < \sqrt{3}. \tag{2}$$

This range of q is in the sequel always tacitly presumed. Hexagons, as generated in the proof of Theorem 1, have a relatively high symmetry. In general, then, what are the symmetry properties of hexagons? We answer this question in the next two sections. (In a modified version, the method used can be applied to any finite set of points in E^3; see [13].)

3 Structure of symmetry groups

Let π be a permutation of the vertices $v_1, v_2, \ldots, v_6$ of a hexagon that is *length-preserving*, i.e., $\overline{v_i v_j} = \overline{\pi(v_i)\pi(v_j)}$ $(1 \le i < j \le 6)$, and *ring-preserving*, i.e., if $v_i v_j$ is a side, then $\pi(v_i)\pi(v_j)$ is a side as well. We refer to such a vertex permutation π as a *vertometry* of the hexagon.

A vertometry π is associated with a symmetry: As is well known, an isometry in space (length-preserving mapping of E^3 onto itself) is already uniquely determined by four points in general position and their images. By definition, a hexagon is nonplanar, so general position is valid for at least four of its vertices. Since π is length-preserving, it determines such an isometry, which is the same independently of the four vertices it is based on. This isometry is denoted by $s(\pi)$, and since π is ring-preserving, $s(\pi)$ will be a symmetry of the hexagon. Clearly, $s(\pi)$ maps q onto q and permutes x, y, and z.

The vertometries of a hexagon form a group $\mathcal{V}$, called the *vertometry group*, which is isomorphic to the symmetry group $\mathcal{S}$; the isomorphism is given by $\pi \mapsto s(\pi)$. Note that the vertometry group $\mathcal{V}$ gives the abstract group of a hexagon. However, as will be seen in the next section, $\mathcal{V}$ can be isomorphic to different symmetry groups $\mathcal{S}$ (concrete groups).

The following vertex permutations, all being ring-preserving, will be used to generate vertometry groups (permutations are written in cycle notation):

$$\begin{gathered} \pi_1 = (v_1v_4)(v_2v_5)(v_3v_6), \;\; \pi_2 = (v_1v_4)(v_2v_3)(v_5v_6), \\ \lambda = (v_1v_2v_3v_4v_5v_6). \end{gathered} \tag{3}$$

Since π_1 maps each diagonal x, y, and z onto itself, it is length-preserving and represents a vertometry of any hexagon, and thus $s(\pi_1)$ is always a symmetry.

In other words, every hexagon is symmetric, or more precisely:

Theorem 2. *The symmetry group $\mathcal{S}$ of a hexagon is isomorphic to the dihedral group* D_6 (*order* 12)*, the Klein group* K_4*, or the cyclic group* Z_2*, depending on whether all three, exactly two, or none of the diagonals x, y, and z are equal, respectively.*

Proof. Due to the isomorphism $\mathcal{S} \cong \mathcal{V}$, it suffices to examine the vertometry group $\mathcal{V}$.

A maximal number of vertometries is obtained if x, y, and z are arbitrarily permutable, i.e., if $x = y = z$. In this case, the vertometry group is generated by λ and π_2 from (3), and it follows that $\mathcal{V} \cong \mathrm{D}_6$ (compare with a regular planar hexagon and its symmetries in E^2, whose restrictions to the vertex set also lead to D_6).

Next, let $x \neq y = z$. Each vertometry must then preserve the diagonal x, i.e., it must contain subcycles $(v_1)(v_4)$ or $(v_1 v_4)$. The resulting vertometry group is generated by π_1 and π_2 from (3), and we have $\mathcal{V} = \{\varepsilon, \pi_1, \pi_2, \pi_3\}$ with $\pi_3 = \pi_1\pi_2$ (ε is the identity). Since all vertometries are involutions, it follows that $\mathcal{V} \cong \mathrm{K}_4$.

The last case, where x, y, z are pairwise distinct, evidently yields $\mathcal{V} = \{\varepsilon, \pi_1\} \cong \mathrm{Z}_2$. □

Remarks.

a. The group structure of $\mathcal{V}$ (and thus of $\mathcal{S}$) also results from the group homomorphism that assigns to each vertometry π the induced permutation of the diagonals x, y, and z. The resulting group is the symmetric permutation group S_3, S_2, or S_1, depending again on whether all three, exactly two, or none of the diagonals x, y, and z are equal, respectively. In each case, the homomorphism has kernel $\{\varepsilon, \pi_1\}$, which implies a direct product: $\mathrm{D}_6 \cong \mathrm{Z}_2 \times S_3$, $\mathrm{K}_4 \cong \mathrm{Z}_2 \times S_2$, and $\mathrm{Z}_2 \cong \mathrm{Z}_2 \times S_1$.

b. We emphasize that $\mathrm{Z}_2 \subset \mathrm{K}_4 \subset \mathrm{D}_6$.

4 Symmetry groups

Having established the possible structures of the symmetry groups, we examine the particular types of contained symmetries. If a symmetry is involutional, it must be one of three types, which we denote by names that are used in chemistry: *inversion* (point reflection), 180°-*rotation* (line reflection), or *reflection* (plane reflection). In the following, by a *rotation* (without specified angle) we will always mean a 180°-rotation.

Consider $s(\pi_1)$ with π_1 from (3), the symmetry of every hexagon, which is involutional and thus one of the three types. We call $s(\pi_1)$ the *prime symmetry*, and it holds the following:

Theorem 3. *The prime symmetry $s(\pi_1)$ of a hexagon is an inversion or reflection if all three diagonals x, y, and z are equal; otherwise it is a rotation.*

Proof. First, we show that if $x = y = z$, then $s(\pi_1)$ is an inversion or reflection. Assume that $s(\pi_1)$ is a rotation. Since the cycle λ from (3) of the corresponding vertometry group $\mathcal{V}$ satisfies $\pi_1 = \lambda^3$, the symmetry $s(\lambda)$ must be a 60°-rotation. But this would imply a planar hexagon.

Conversely, we show that if $s(\pi_1)$ is an inversion or reflection, then $x = y = z$. Consider the quadrangles $R_1 = v_1 v_2 v_4 v_5$, $R_2 = v_2 v_3 v_5 v_6$, and $R_3 = v_3 v_4 v_6 v_1$. If the prime symmetry $s(\pi_1)$ is an inversion, then these quadrangles are parallelograms with sides 1 and q. If $s(\pi_1)$ is a reflection, they are isosceles trapezoids with lateral side $q < 1$ and diagonal 1 (lateral side 1 and diagonal q would lead to contradictions). In both cases, it follows from a congruence theorem that R_1 and R_2 with common y, R_2 and R_3 with common z, and

R_3 and R_1 with common x are congruent and thus $x = y = z$. Furthermore, R_1, R_2, and R_3 are rectangles.

Hence, if at least two of the diagonals x, y, and z are distinct, $s(\pi_1)$ must be a rotation. □

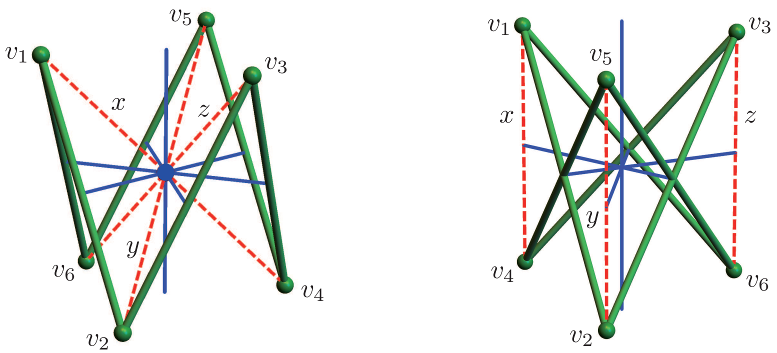
To obtain a general view of all symmetry groups $\mathcal{S}$, we distinguish the three cases according to Theorem 2. The resulting hexagons are shown in Figures 4–7 below together with their symmetry elements, i.e., inversion points, rotation axes, and (except in Figure 4) reflection planes. The ranges of q for which corresponding hexagons are defined (indicated in parentheses in the captions of the figures) could be determined geometrically, but they are also part of computations below.

Case 1. $x = y = z$. By Theorem 3, the prime symmetry $s(\pi_1)$ is an inversion or reflection and it immediately follows:

1.1. If $s(\pi_1)$ is an inversion, we obtain a hexagon, as shown in Figure 4a. Its convex hull forms a triangular antiprism. The symmetry group $\mathcal{S}$ is generated by the roto-reflection $s(\lambda)$ with angle 60° and the rotation $s(\pi_2)$. We call this hexagon a *crown*.

A crown already appeared in the proof of Theorem 1. For the appropriate structure of cyclohexane in chemistry, the concept of a chair is used instead of a crown.

1.2. If $s(\pi_1)$ is a reflection, we get a hexagon, as shown in Figure 4b. Its convex hull forms a triangular prism. The symmetry group $\mathcal{S}$ is here generated by the roto-reflection $s(\lambda)$ with angle 120° and the rotation $s(\pi_2)$. This hexagon is said to be a *star*.

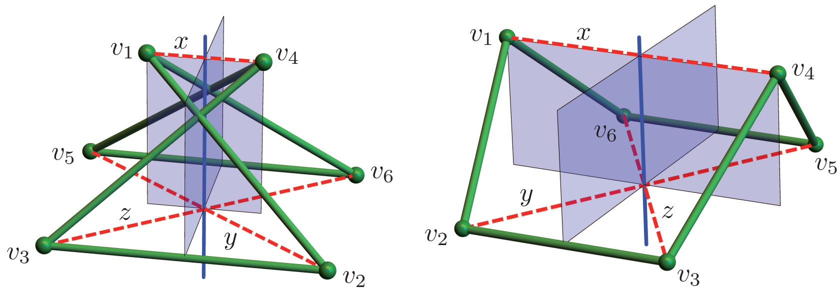


a. crown (any q). b. star ($q < 1$).

Figure 4: Hexagons with $x = y = z$.

Case 2. $x \neq y = z$. By Theorem 3, the prime symmetry $s(\pi_1)$ is a rotation. Consider the corresponding vertometry group $\mathcal{V} = \{\varepsilon, \pi_1, \pi_2, \pi_3\}$ with π_1 and π_2 from (3), and $\pi_3 = (v_1)(v_4)(v_2 v_6)(v_3 v_5)$. The corresponding symmetries are involutional and we have $s(\pi_3) = s(\pi_1)s(\pi_2)$.

2.1. If $s(\pi_2)$ is a reflection, then $s(\pi_3)$ is also a reflection. Indeed, $s(\pi_3)$ is orientation-reversing and an inversion can be excluded because it has only one fixed point. The so-defined symmetry group $\mathcal{S}$ leads to a hexagon (with or without intersecting sides), as shown in Figure 5. The rotation axis is the intersection line of two perpendicular reflection planes. Such a hexagon is called a *boat*.



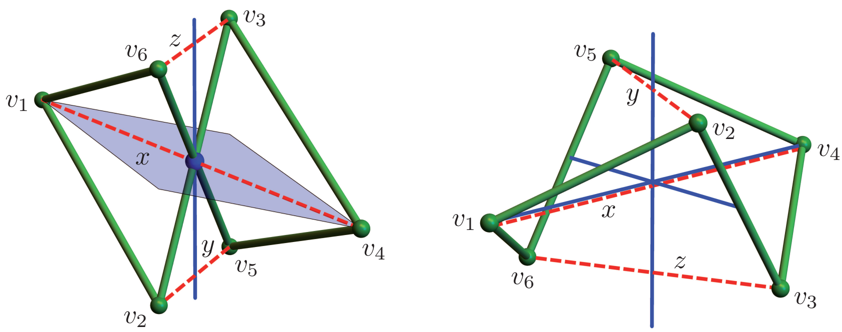
a. boat ($q < 1$). b. boat ($q > 1$).

Figure 5: Hexagons with $x \neq y = z$.

2.2. If $s(\pi_2)$ is an inversion, then $s(\pi_3)$ is a reflection. Again, $s(\pi_3)$ is orientation-reversing and no second inversion exists. The symmetry group $\mathcal{S}$ yields a hexagon, as shown in Figure 6a. The rotation axis perpendicularly pierces the reflection plane in the inversion point. This hexagon is called a *cross*.

2.3. If $s(\pi_2)$ is a rotation, then $s(\pi_3)$ is also a rotation. This follows because $s(\pi_3)$ is orientation-preserving. Here, $\mathcal{S}$ determines a hexagon, as shown in Figure 6b. The three pairwise perpendicular rotation axes intersect each other at a common point. This hexagon is said to be a *twist*.

Note that the names boat and twist are used for the appropriate structures of cyclohexane in chemistry.

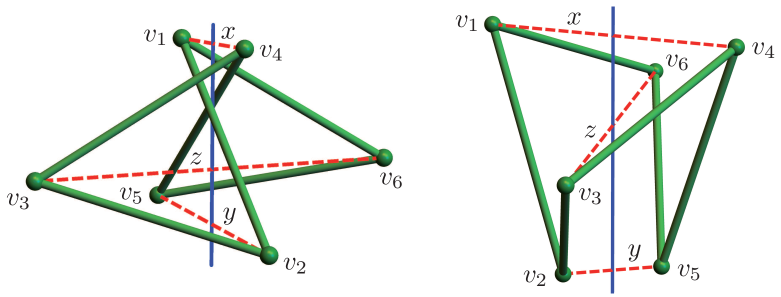


a. cross ($q < 1$). b. twist ($q > 1$).

Figure 6: Other hexagons with $x \neq y = z$.

Case 3. x, y, and z are pairwise distinct. Again by Theorem 3, the prime symmetry $s(\pi_1)$ is a rotation. Evidently, $\mathcal{S}$ defines a hexagon with one rotation axis, as shown in Figure 7. Because of the lowest symmetry, we call this hexagon a *low*.

Summarizing, we have six *symmetry classes*:



a. low ($q < 1$). b. low ($q > 1$).

Figure 7: Hexagons with pairwise distinct x, y, and z.

Theorem 4. *A hexagon where all three diagonals x, y, and z are equal is a crown or star; if exactly two of them are equal, the hexagon is a boat, cross, or twist; and if they are pairwise distinct, it is a low.*

Remarks.

a. The characterizing symmetry group $\mathcal{S}$ of each class can be indicated by using Schoenflies symbols, which are common in chemistry: crown D_{3d}, star D_{3h}, boat C_{2v}, cross C_{2h}, twist D_2, and low C_2.

b. The lows and twists are chiral, i.e., each of them cannot be brought to coincide with its mirror image by a motion (no corresponding orientation-preserving isometry exists). All the other hexagons are achiral.

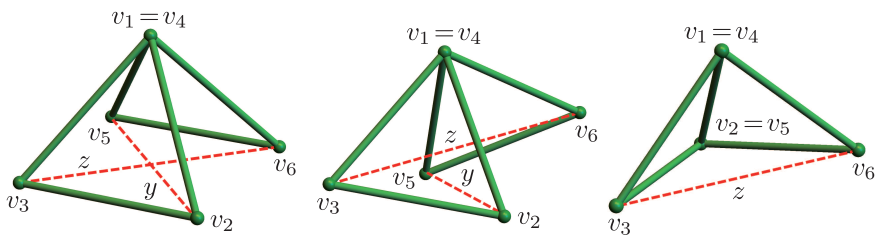
The crowns and stars are uniquely determined (up to congruence) by the parameter q. Indeed, for a fixed q (fixed angle α), the convex hull of a crown or star is a convex polyhedron with rigid boundary polygons, and Cauchy's rigidity theorem implies that it is not continuously deformable. For that reason, crowns and stars are said to be *rigid* hexagons.

The set of the boats, crosses, twists, and lows is determined by two parameters, as for instance q and x. This follows because the prime symmetry is a rotation with an axis being perpendicular to the diagonals x, y, and z: Initially, we have 7 degrees of freedom, namely 1 for $x = \overline{v_1 v_4}$, 3 for the vertex v_2, and 3 for v_3. Again taking into account the prime symmetry, there are the 5 constraints $\overline{v_1 v_2} = \overline{v_2 v_3} = \overline{v_3 v_4} = 1$ and $\overline{v_1 v_3} = \overline{v_2 v_4} = \overline{v_3 v_5}$. This leaves the parameters q and x, and for a fixed q, as can be seen below, x is continuously variable. Therefore, boats, crosses, twists, and lows are called *flexible* hexagons.

At this point, we make a short excursion to hexagons with coinciding vertices: Since $q > 0$, coinciding vertices can only occur if at least one of the diagonals x, y, or z equals 0. This requires that every triangle of consecutive vertices be equilateral or, equivalently, that $q = 1$. Furthermore, it follows that coinciding vertices are always double vertices.

Consider the Figures 4–7: The symmetry class of crowns obviously contains a hexagon with $q = 1$. As regards the other classes, $q = 1$ stands for limiting cases with at least one double vertex. For $q \to 1$ one obtains two planar figures, from the stars an equilateral triangle with side 1 (three double vertices) and from the crosses and twists a rhombus with side 1 and a diagonal 1 (two double vertices). The boats result in what we call the *penta-boat* (Figure 8a). From the lows we generally get *penta-lows* (Figure 8b) and by special limiting processes again the penta-boat or rhombus. Note that all these limiting cases also follow from the formulas for the diagonals x, y, and z in Theorems 8, 12, and 14 below. Additionally, there exist *tetras* (Figure 8c); however, these are not limiting cases of other hexagons.

It is easily seen that, apart from the hexagons in Figure 8, further (regular spatial) hexagons with double vertices do not exist. Of course, the penta-boat and the boats have the same symmetry group, as well as the penta-lows and lows. The symmetry group of tetras is the same as that of boats, but $s(\pi_1)$ is a reflection whereas in boats it is a rotation.



a. the penta-boat ($y = z$). b. penta-low. c. tetra.

Figure 8: Hexagons with double vertices ($q = 1$).

5 Some properties

We return to hexagons without double vertices. In the following, *contained* tetrahedra of a hexagon are understood to be those with hexagon vertices. The first theorem expresses that the lows are in some way general hexagons:

Theorem 5. *A hexagon is a low if and only if none of the contained tetrahedra are degenerate.*

Proof. We show that a contained degenerate tetrahedron would lead to symmetries in addition to those of a low. Without loss of generality, it suffices to examine a tetrahedron with four, with three, and with two consecutive vertices: $T_1 = v_1v_2v_3v_4$, $T_2 = v_1v_3v_4v_5$, and $T_3 = v_2v_3v_5v_6$.

Assume that T_1 is degenerate. Then, from the prime symmetry (a rotation) it follows that T_1 and $T_1' = v_4v_5v_6v_1$ are congruent quadrangles, either isosceles trapezoids with the common base x or parallelograms with the common diagonal x. Both imply a symmetry plane containing x.

Assume that T_2 is degenerate. Again, as a consequence of the prime symmetry, we have congruent quadrangles T_2 and $T_2' = v_4v_6v_1v_2$, which here are kites with the common diagonal x. This implies a further symmetry axis containing x.

A degenerate T_3 is a parallelogram with diagonals y and z or an isosceles trapezoid with bases y and z. Consider the mid-perpendicular planes of v_2v_6 and v_3v_5. The vertices v_1 and v_4 must lie on both planes. In the case of the parallelogram, the planes are parallel and must therefore coincide and we would have a symmetry plane. In the case of the isosceles trapezoid, the planes must coincide again; otherwise it is $\overline{v_1v_2} = \overline{v_1v_5}$ and thus $q = 1$. Once more, we would have a symmetry plane, provided that the lateral sides are q (in a trapezoid with diagonals q coinciding planes are impossible).

Conversely, it is seen from Figures 4–6 that the symmetry properties of hexagons different from lows lead to contained degenerate tetrahedra. □

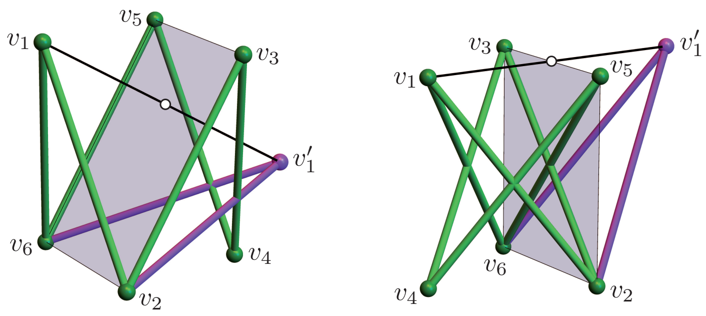
The next theorem confirms what is to be expected:

Theorem 6. *A hexagon has intersecting sides if and only if it is a star, a boat with $q < 1$, or a cross.*

Proof. Intersecting sides result in a degenerate contained tetrahedron. Hence, by Theorem 5, lows with intersecting sides can be excluded. This also applies to twists, which can be seen as follows: For intersecting sides it is necessary that three consecutive sides or two opposite sides lie in a plane. It is easy to check that both are impossible; just take into account that the triangles $v_1v_2v_6$ and $v_4v_5v_3$ in Figure 6b lie in two different planes, which intersect in the symmetry axis containing x. The rest of the proof follows by inspecting the remaining hexagons in Figures 4, 5, and 6a. □

The hexagons different from lows and twists contain rectangles, which are involved in the following:

Theorem 7. *In a crown (with $q \neq 1$) and boat or in a star and cross, consider one of the two vertices that do not belong to a contained rectangle. If this vertex and its adjacent sides are reflected across the rectangle plane, the crown becomes a boat and the star a cross, and conversely.*



a. crown and boat. b. star and cross.

Figure 9: Related hexagons.

Proof. We consider the tinted rectangles in Figure 9. Let v_1' be the point obtained by reflecting v_1 at the rectangle plane. Since a reflection is length-preserving, it is clear by inspection that the vertices $v_1, v_2, \ldots, v_6$ form a crown exactly if $v_1', v_2, \ldots, v_6$ form a boat, and analogously for a star and a cross. □

Remark. For $q = 1$, we have a corresponding relation between the crown and the penta-boat. The sides of both hexagons are edges of the same octahedron.

Next, we look at the diagonals of the hexagons just discussed:

Theorem 8. *The diagonals of hexagons different from twists and lows with $y = z$ are given by*

$$\text{crowns:}\quad \text{any } q\,,\ x = y = z = \sqrt{1+q^2}; \tag{4}$$

$$\text{stars:}\quad q < 1,\ x = y = z = \sqrt{1-q^2}; \tag{5}$$

$$\text{boats:}\quad q \neq 1,\ x = |1-q^2|,\ y = z = \sqrt{1+q^2}; \tag{6}$$

$$\text{crosses:}\quad q < 1,\ x = \sqrt{1+2q^2},\ y = z = \sqrt{1-q^2}. \tag{7}$$

Proof. The ranges of q are evident for crowns (already used in the proof of Theorem 1) and for stars. Theorem 7 implies that these ranges accordingly apply to boats (for $q \neq 1$) and to crosses. The diagonals x, y, and z are directly given by the Pythagorean theorem with the exception of x for boats and crosses. For these, we must examine the quadrangle $v_1v_2v_3v_4$, which is a trapezoid in boats (Figure 5) and a parallelogram in crosses (Figure 6a), so that x can be calculated by using Ptolemy's theorem and the parallelogram law, respectively. □

From now on, we primarily focus on flexible hexagons. Further, in the following the concept of tetrahedron will also include degenerate cases.

Theorem 9. *In a flexible hexagon, let T and T' be the two contained congruent tetrahedra determined by consecutive hexagon's vertices and a common edge d, which is a diagonal x, y, or z. Then T is mapped onto T' by a rotation with axis containing d and angle φ where*

$$\cos\varphi = \frac{(d^2-1)^2 + (q^2-1)^2 - 1}{\big((d+q)^2-1\big)\big((d-q)^2-1\big)}. \tag{8}$$

Proof. Without loss of generality, we can consider $d = x$ and thus $T = v_1v_2v_3v_4$ and $T' = v_1v_6v_5v_4$, as shown in Figure 10. The composition of the rotational symmetry of T (axis through the midpoints of x and v_2v_3) and the prime symmetry (also a rotation) leaves v_1 and v_4 fixed and maps $v_2 \mapsto v_6$ and $v_3 \mapsto v_5$. Thus, this composition must be the stated rotation. Formula (8) is obtained by calculating the dihedral angle φ at edge x of the tetrahedron $T^* = v_1v_2v_4v_6$. □

Remark. The rotation angle φ can be limited to $60° \leq \varphi \leq 180°$. The lower bound follows because $v_2v_4v_6$ is a q-triangle with angle $60°$ at v_4, whereas $180°$ for the upper bound is evident. With $60°$ we obtain the crosses and with $180°$ the twists.

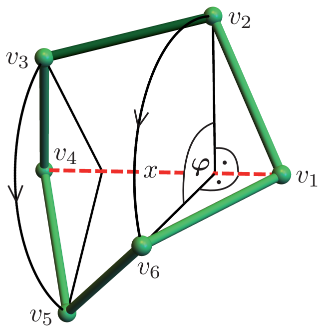


Figure 10: Congruent tetrahedra in a flexible hexagon related by a rotation.

Theorem 9 helps prove the following:

Theorem 10. *A hexagon has a circumscribed sphere if and only if it is a rigid hexagon or a boat.*

Proof. The rigid hexagons obviously have a circumscribed sphere. It remains to show that a flexible hexagon with a circumscribed sphere must be a boat: For at least two diagonals d the tetrahedra T and T', as considered in Theorem 9, are nondegenerate; otherwise the hexagon would be planar. Without loss of generality, we can assume that this is true for $d = y$ and for $d = z$. Let T and T' be the tetrahedra with common $d = y$. Since the circumscribed sphere of the hexagon must coincide with those of T and T', it follows from Theorem 9 that y is a diameter. Analogously, z is a diameter as well. Hence, y and z are equal and bisect each other, so we have the rectangle of a boat (see Figure 5). □

We complete this section with an application:

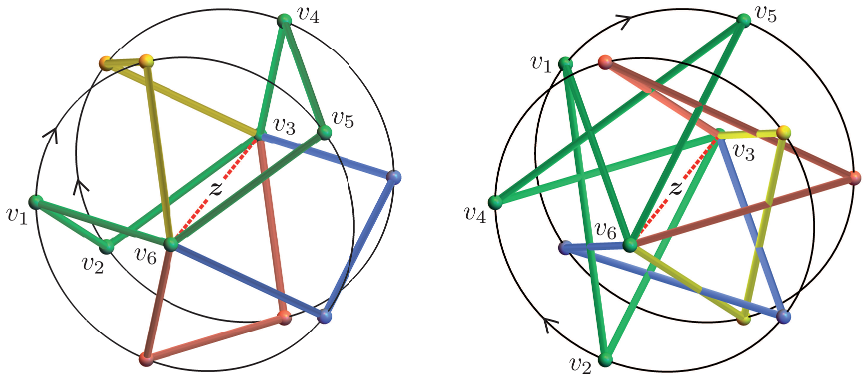
Let us consider the special boat determined by the diagonals from (6) with $q > 1$ and $x = q$. It follows that $q = \Phi$ (golden ratio) and thus $\alpha = 108°$. Further, consider the rotation according to Theorem 9 with $d = z$ and angle $\varphi = 144°$ (resulting from (8)).

Rotating the tetrahedron $T = v_6 v_1 v_2 v_3$ not only with φ, but also with 2φ, 3φ, and 4φ leads to 5 bundled boats, as shown in Figure 11a. It turns out that the 12 vertices form an icosahedron with edge length 1. Simple counting yields 30 such boats with $\alpha = 108°$ in total.

Moreover, by inspection, one finds that the icosahedron additionally contains 5 bundled boats, as shown in Figure 11b, with the (exceptionally) larger side $s = \Phi$, $q = 1$ and thus $\alpha = 36°$, and $\varphi = 72°$. The total number of these boats is again 30.

By Theorem 7, the icosahedron also contains crowns, 10 with $s = 1$ and 10 with $s = \Phi$. It is easily seen that stars or further boats and crowns do not exist. And from Theorem 10 it follows that any other regular spatial hexagon, where the vertices are the corners of the icosahedron, can be excluded as well.

Of course, the mere number of overall 80 regular spatial hexagons can also be found with a computer program that tests all $\binom{12}{6} 5!/2$ $(= 55440)$ six-rings contained in a icosahedron.



a. $s = 1$ and $\alpha = 108°$. b. $s = \Phi$ and $\alpha = 36°$.

Figure 11: Five boats in an icosahedron with edge length 1.

6 Vertex coordinates

We now develop a coordinate representation for the vertices of hexagons. This facilitates determining the diagonals of flexible hexagons and thus, in addition to Theorem 8, those of twists and lows. From calculations we only give results. (To reproduce the computation, it is advisable to use a computer algebra system.)

The existence of flexible hexagons is guaranteed as follows:

Theorem 11. *A flexible hexagon with diagonals q and x exists if and only if*

$$m_1 \le x \le \begin{cases} M_1 & \text{for } q < 1 \\ M_2 & \text{for } q > 1 \end{cases} \quad \text{with} \tag{9}$$

$$m_1 = |1 - q^2|, \; M_1 = \sqrt{1 + 2q^2}, \; M_2 = \tfrac{1}{2}\left(\sqrt{3}\,q + \sqrt{4 - q^2}\right).$$

Proof. As a first step, we consider separately the contained tetrahedron $T = v_1v_2v_3v_4$. For a fixed q, the edge x of T monotonically increases from a lower bound m_1 to an upper bound M_1 by varying the dihedral angle at the opposite edge v_2v_3 from 0° to 180°. Since 0° appears in a boat (see Figure 5) and 180° in a cross (see Figure 6a), we obtain m_1 from (6) and M_1 from (7).

As a second step, we include the vertices v_5 and v_6. Theorem 9 (with $d = x$) implies that it suffices to ensure the existence of the vertex v_6 or, equivalently, of the tetrahedron $T^* = v_1v_2v_4v_6$. For a fixed q, the possible edges x of the separately considered T^* are the result of varying again the dihedral angle at the opposite edge v_2v_6 from 0° to 180°, and with the Pythagorean theorem we get the lower bound $m_2 = \frac{1}{2}|\sqrt{3}q - \sqrt{4 - q^2}|$ and the upper bound M_2.

It is shown that $m_1 > m_2$, $M_1 < M_2$ for $q < 1$, and $M_1 > M_2$ for $q > 1$. Since the existence of the hexagon is guaranteed exactly if both tetrahedra T and T^* exist, we finally obtain the necessary and sufficient condition from (9). □

The upper bound M_2 is involved in the twists:

Theorem 12. *The diagonals of twists with $y = z$ are given by*

$$q > 1,\ x = \tfrac{1}{2}\big(\sqrt{3}\,q + \sqrt{4-q^2}\big),\ y = z = \sqrt{1 + 2q^2 - q\sqrt{3(4-q^2)}}. \qquad (10)$$

Proof. Consider a twist with $x \neq y = z$ (see Figure 6b). Due to the symmetry, the tetrahedron $T^* = v_1v_2v_4v_6$ is degenerate (it is a kite) with 180° for the dihedral angle at v_2v_6. From the proof of Theorem 11 it follows that the latter is true exactly if $q > 1$ and $x = M_2$ from (9). The diagonal y can be determined by a repeated use of the Pythagorean theorem. Nevertheless, this derivation becomes rather cumbersome, and y is also obtained by inserting $x = M_2$ in Theorem 14 below. □

In the following two theorems, we refer to flexible hexagons with any diagonals q, x, y, and z.

Theorem 13. *Let x be from* (9) *and φ defined by* (8) *with $d = x$, then coordinates of the vertices $v_1, v_2, \ldots, v_6$ of flexible hexagons are given by*

$$\begin{gathered} v_{1,4} = (\pm\tfrac{1}{2}x, 0, 0),\ v_{2,3} = (\pm a, \pm b, c), \\ v_{5,6} = (\mp a,\ \mp b\cos\varphi - c\sin\varphi,\ \mp b\sin\varphi + c\cos\varphi) \ \textit{with} \end{gathered} \qquad (11)$$

$$a = \frac{q^2-1}{2x},\ b = \frac{1}{2x}\sqrt{x^2-(q^2-1)^2},\ c = \frac{1}{2}\sqrt{2q^2-x^2+1}.$$

Proof. The tetrahedron $T = v_1v_2v_3v_4$ with x from (9) is placed in a coordinate system such that x lies on the first coordinate axis, and the axis of the rotational symmetry of T on the third coordinate axis. One verifies that $\overline{v_1v_2} = \overline{v_2v_3} = \overline{v_3v_4} = 1$ and $\overline{v_1v_3} = \overline{v_2v_4} = q$. Using Theorem 9 with $d = x$ and an appropriate rotation matrix, we obtain the remaining vertices v_5 and v_6. □

Remarks.

- **a.** After substituting $\cos\varphi$ and $\sin\varphi$ by means of (8), the vertex coordinates are expressed with q and x by rational operations and square roots.
- **b.** It is possible to limit φ to $60° \leq |\varphi| \leq 180°$ (cf. Remark to Theorem 9). A positive φ leads then to diagonals with $y \geq z$ and a negative φ to those with $y \leq z$.
- **c.** For $\varphi = 180°$, one obtains $v_{5,6} = (\mp a, \pm b, -c)$, which implies that the three symmetry axes of a twist are the axes of the chosen coordinate system.
- **d.** Setting $q = 1$ gives the vertices of pentas.
- **e.** Substituting b with $-b$ would change the orientation of chiral hexagons (lows and twists).

Corollary 13.1. *The coordinates $v_{1,4}$ and $v_{2,3}$ from* (11) *can also be used in the case of rigid hexagons. Then, the coordinates of crowns are given with q and x from* (4) *and the remaining vertices $v_{5,6} = (\mp a, \mp b, -c)$, and those of stars with q and x from* (5) *and $v_{5,6} = (\mp a, \pm b, c)$.*

Proof. This follows immediately in both cases by applying the prime symmetry. □

The coordinates of flexible hexagons now allow to calculate their diagonals. It should be added that the diagonals can also be determined without coordinates, by using distance geometry for instance (a tool that is applied in some stereochemical investigations).

Theorem 14. *The diagonals of flexible hexagons are given by*

$$q \neq 1,\ x \text{ from } (9),\ y = \sqrt{\frac{f \pm g}{h}},\ z = \sqrt{\frac{f \mp g}{h}} \text{ with} \tag{12}$$

$$\begin{aligned} f &= -(q^2+1)\,x^4 + 2(q^4+q^2+1)\,x^2 + (q^2-1)^3, \\ g &= 2q\sqrt{\big(x^4-(q^2+2)x^2+(q^2-1)^2\big)\big(x^2-2q^2-1\big)\big(x^2-(q^2-1)^2\big)}, \\ h &= (x+q+1)(x+q-1)(x-q+1)(-x+q+1). \end{aligned}$$

Proof. It remains to determine the diagonals $y = \overline{v_2 v_5}$ and $z = \overline{v_3 v_6}$ using the coordinates from (11). □

Remarks.

a. Of course, pairwise distinct x, y, and z are the diagonals of lows. In the special cases where exactly two diagonals are equal, (12) gives (up to permutations) the diagonals from (6) of boats, from (7) of crosses, or from (10) of twists.

b. For $q = 1$, one obtains the pentas.

Corollary 14.1. *Among the diagonals x, y, and z of all hexagons with a fixed q ($\neq 1$), m_1 from* (9) *of a boat is smallest, M_1 of a cross for $q < 1$ and M_2 of a twist for $q > 1$ are largest.*

Proof. For a fixed $q \neq 1$, the diagonals from (4) and (5) of rigid hexagons are between the extreme values from (9) of flexible hexagons. □

7 Summary and further properties

The derived results are now summarized by using a specific representation. To every hexagon (whether it has double vertices or not) with diagonals x, y, and z, we assign a point (x, y, z) in E^3, called a *diagonal point*. Figure 12 shows the diagonal points with $x \geq y \geq z$ (left) and with any x, y, and z (right) according to Theorem 14. There is a one-to-one correspondence between the diagonal points on the left and the classes of congruent hexagons.

Let us consider in more details the diagonal points on the left of Figure 12: The points of flexible hexagons and the pentas form an area; its interior points represent lows and penta-lows, and the points on the contour curves (without B, C, and D) boats, crosses, twists, and the penta-boat. The rigid hexagons lead to a line segment for both crowns and

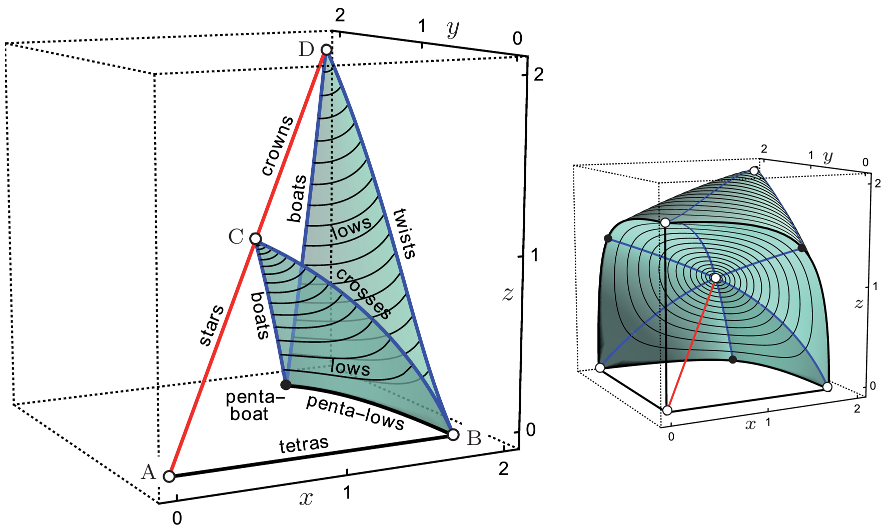


Figure 12: Hexagons represented by diagonal points (x, y, z).

stars. In addition, there are iso-q-curves, i.e., curves representing sets of hexagons with a fixed q, especially pentas and tetras with $q = 1$. These curves show that for each given q the rigid hexagons are isolated from the continuously connected flexible hexagons.

The points A, B, C, and D represent planar figures, which are limiting cases that do not fall under our definition of hexagons. With $q = 1$, we have two planar figures, as already mentioned at the end of Section 4, namely in $A = (0, 0, 0)$ a triangle with three double vertices and in $B = (\sqrt{3}, 0, 0)$ a rhombus with two. Furthermore, with $q = 0$ we have in $C = (1, 1, 1)$ a line segment between two triple vertices, and with $q = \sqrt{3}$ in $D = (2, 2, 2)$ the well-known regular planar hexagon.

Lastly, we consider on the right of Figure 12 a diagonal point $P = (x, y, z)$ that represents a chiral hexagon H (low or twist). Of course, P also represents the mirror image H' of H. Thus, a movement of P along the iso-q-line defines a continuous transformation of H and also one of H'. Moving P around the whole iso-q-line, the two transformations map $H \mapsto H$ and $H' \mapsto H'$ for $q < 1$, and $H \mapsto H'$ and $H' \mapsto H$ for $q > 1$. This can be seen as follows: On the iso-q-line there exist six diagonal points that represent congruent hexagons if H is a low and three if it is a twist (due to permutations of x, y, and z). Two such successive hexagons are in both transformations the mirror image of each other exactly if a boat or cross (both achiral) is passed in between, which occurs six times for $q < 1$ and three times for $q > 1$. Moreover, for a point P representing a chiral hexagon H with $q < 1$ (i.e., a low), the mirror image H' can never be reached with a continuous transformation defined by a closed path from P to P on the area limited to $q < 1$.

Different aspects of this summary appear in the already mentioned animations in [8]. To conclude, we give some further properties of hexagons (without double vertices), whose proofs are left to the reader.

Property 1. *Assuming that q and x determine a hexagon, consider the four congruent triangles with common side x, as shown in Figure* 13. *A hexagon can be generated by rotations of the triangles around x until $\overline{v_2v_3} = \overline{v_5v_6} = 1$ and $\overline{v_2v_6} = q$.*

This leads to a rigid hexagon if q and x satisfy (4) *or* (5) *and the resulting congruent tetrahedra $v_1v_2v_3v_4$ and $v_1v_6v_5v_4$ are differently oriented, and it leads to a flexible hexagon if q and x satisfy* (9) *and the tetrahedra are equally oriented or degenerate.*

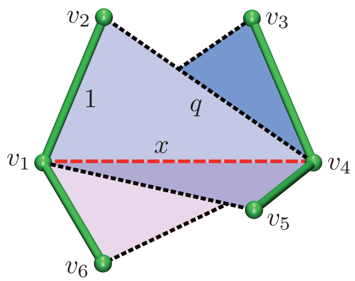


Figure 13

Property 2. *Consider the net of a hexagon. By rotating all three outer triangles into the same half-space, one can generate the hexagons with $q < 1$ and the crowns, i.e., the diagonals x, y, and z are then in one half-space.*

For $q > 1$, the lows and boats are obtained by rotations such that the smallest of the diagonals x, y, and z comes to lie in one and the other two in the other half-space. In the case of the twists, the largest diagonal remains in the net plane and the other two come to lie in different half-spaces.

If d denotes the involved diagonal, then the rotation angle ϱ is given by

$$\cos\varrho = \frac{2d^2 - q^2 - 2}{q\sqrt{3(4-q^2)}}.$$

Property 3. *For any two of the vectors $\overrightarrow{v_1v_4}$, $\overrightarrow{v_3v_6}$, and $\overrightarrow{v_5v_2}$ of a hexagon, the scalar product is $1-q^2$.*

The intermediate angle between two vectors becomes obtuse for $q>1$ and acute for $q<1$. A right angle occurs only in the crown with $q=1$ (and in pentas).

Property 4. *The angle ϑ $(0° \le \vartheta \le 90°)$ between the two different planes containing the q-triangles of a hexagon assumes extreme values as follows:*

$\vartheta = 0°$ in rigid hexagons and crosses;

$\vartheta = 90°$ in the boat with $q = \sqrt{\frac{3}{2}}$, in the twist with $q = 2\sqrt{\frac{3}{7}}$, and in one low for each q in between.

Property 5. *All six vertices of a hexagon are those of its convex hull.*

Property 6. *A hexagon without intersecting sides is unknotted.*

In the last two properties, we refer to regular spatial hexagons with any side length s but diagonals that are still denoted by q, x, y, and z. These hexagons, similar to those with $s = 1$, are named *s-hexagons*.

Property 7. *Given any positive lengths x, y, and z. If at least two of these lengths are distinct, then they are the diagonals of exactly two incongruent s-hexagons similar to flexible hexagons, one with $q < s$ and another with $q > s$. If the three lengths are equal, they are the diagonals of infinitely many incongruent s-hexagons similar to rigid hexagons.*

Finally, we need a special type of planar hexagons, called *p-hexagons*. These are defined as non-regular point-symmetric planar hexagons whose diagonals between opposite vertices are perpendicular to two parallel diagonals.

Property 8. *Consider an s-hexagon that is similar to a flexible hexagon different from a cross. Its orthogonal projection in direction of the axis of the prime symmetry is a p-hexagon (see Figure 14). Conversely, each p-hexagon is the projection of such an s-hexagon. The diagonals x, y, and z appear in the p-hexagon in true length.*

The projected q-triangles are obtuse for $q < s$ and acute for $q > s$, or, equivalently, the prime symmetry axis pierces the q-triangle areas if and only if $q > s$.

In the case of an s-hexagon similar to a cross, one obtains a projection with two double vertices.

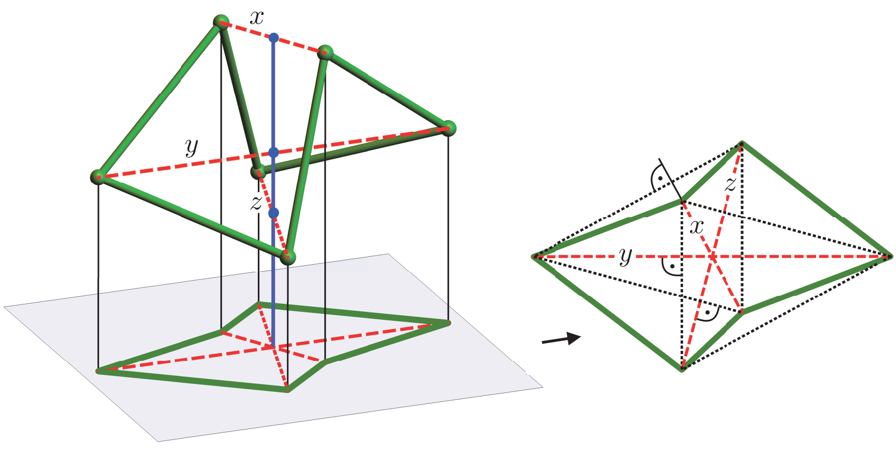


Figure 14

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