

# Calculation the Segmented Helix Formed by Repetitions of Identical Subunits

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## Abstract

Eric Lord has observed:

In nature, helical structures arise when identical structural subunits combine sequentially, the orientational and translational relation between each unit and its predecessor remaining constant.[1]

This paper proves Lord's observation as a consequence of screw theory. Algorithm-like formulae for the segmented helix generated from the intrinsic properties of a stacked object and its conjoining rule are given. Standard results from screw theory[2] and previous work for finding the axis of a helix from points[3] are combined with corollaries of Lord's observation to allow calculations of segmented helices from either transformation matrices or four known points. The construction of these from the intrinsic properties of the rule for conjoining repeated subunits of arbitrary shape is provided. allowin the complete parameters describing the unique segmented helix generated by arbitrary stackings can be easily calculated. Interactive software is provided which performs this computation for arbitray prisms along with 3D visualization. This allows either the deduction of intrinsic properties of a repeated subunit from known properties of a segmented helix, as a chemist might want to do, or the design of a segmented helix from known properties of a repeated subunit, as a mechanical engineer or robotocist might want. As a verification and demonstration, the software and paper compute, render, and catalog a "zoo" of stackings of platonic helices, such as Boerdijk-Coxeter tetrahelix and various species of helices formed from dodecahedra, for example.

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# 1 Introduction

During the Public Invention Mathathon of 2018[4], software was created to view chains of regular tetrahedra joined face-to-face. The participants noticed that whenever the rules for which face to add the next tetrahedron to were periodic, the resulting chain was always a helix.

Although unknown to us at that time, we now call Lord's Observation:

In nature, helical structures arise when identical structural subunits combine sequentially, the orientational and translational relation between each unit and its predecessor remaining constant.[1]

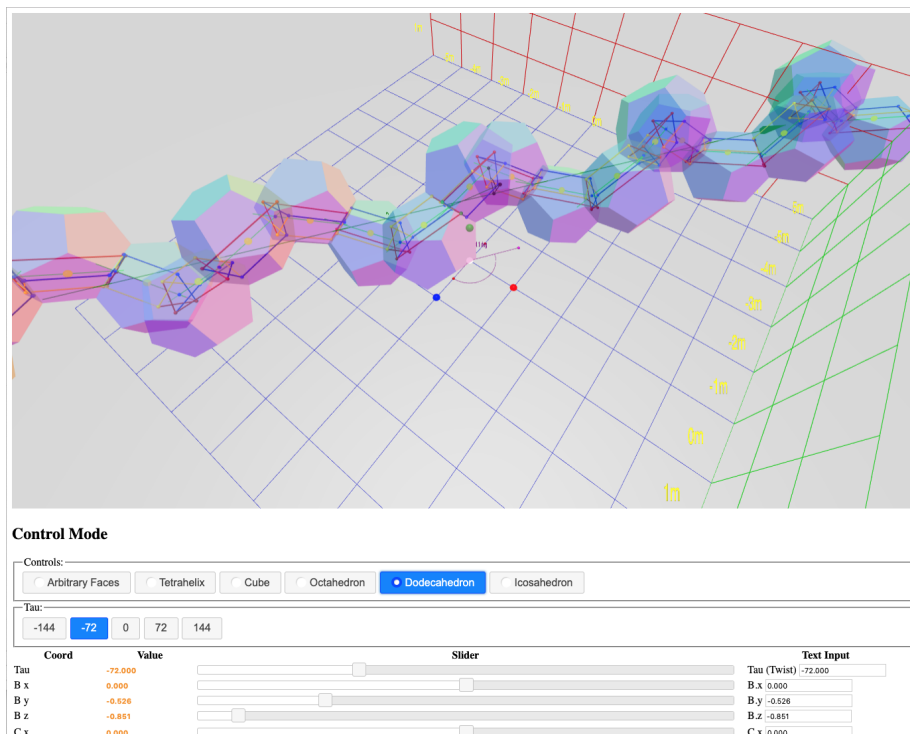


Figure 1: Example Segmented Helix Generated From the Dodecahedron

The purpose of this paper is to prove Lord's Observation and provide mathematical tools and software for studying arbitrary segmented helices generated in this way.

Finding the properties of a segmented helix from four contiguous segments on the helix from screw theory[5, 2, 6], which we call Kahn's method[3], is explained and reformulated and an interactive, 3D rendering website written in JavaScript which allows both calculation and interactive play and study, with an aim to allow a helix to be designed from an object or an object designed to produce a particular helix. Kahn's method is extended to cover some degenerate situations.

We exploit Lord's Observation to discover symmetry which allows us to apply Kahn's method when subunits are joined face-to-face with the same *twist*. Kahn was investigating proteins, which do not have faces, but geometric solids and other macroscopic solid objects do. This symmetry allows us compute the parameters of the segmented helix purely from properties intrinsic to a single object and the joining rule. This paper thus provides a set of tools to either design a subunit and rule to produce a helix as desired, or to investigate possible subunit configurations that produce a particular discerned helix. Finally, as an example, we use these tools to produce an initial table of all possible helices generated by vertex-matched face-to-face joints of the Platonic solids, of which only the tetrahelix[7, 8, 9, 10, 11] has been completely described to date.

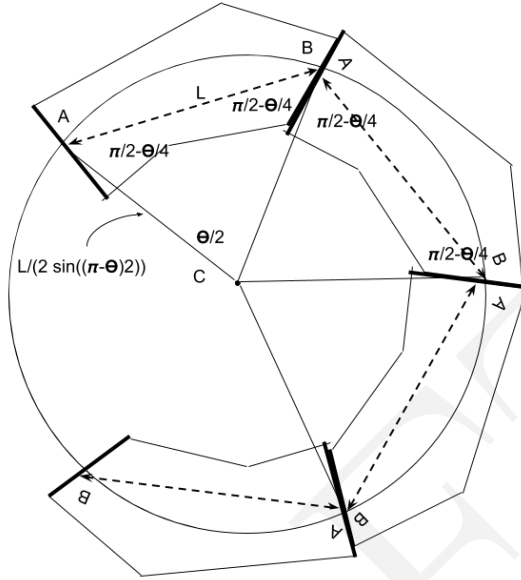


Figure 2: A 2D Analog of a Helix Generated by Repeated Subunits

## 2 A Warm-up: Two Dimensions

Considering the problem in two dimensions may be a valuable introduction. Suppose that we consider a polygon that has two edges, called  $A$  and  $B$ , and that we define the length  $L$  of the polygon as the distance between the midpoints of these edges. Suppose that we are only allowed to join these polygons by aligning  $A$  of one polygon to  $B$  of another polygon, with their midpoints coincident. Let us further assume that we disallow inversions of the polygon. Let us imagine that we have a countable number of polygons  $P_i$  indexed from 0. Then what shapes can we make by chaining these polygons together?

Each joint  $J_i$  between polygons  $P_i$  and  $P_{i+1}$  will place the axes of at the same angle,  $\theta$ , since our polygons do not change shape. Let us define  $\theta$  to be positive if we move anti-clockwise from  $P_i$  to  $P_{i+1}$  and negative if we move clockwise. If  $\theta = 0$ , the joints will be collinear.

If  $\theta \neq 0$ , it seems the polygon joints will always lie on a circle. A proof of this is that each polygon has associated with it an isosceles triangle  $A, B, C$ , where  $\angle CBA = \angle CAB = \theta/2$ , and  $\angle ACB = (\pi - \theta)$ .  $AC$  and  $BC$  are not necessarily aligned with an edge of the polygon. The length  $AB$  is  $L$ , and the lengths  $AC$  and  $BC$  are  $(L/2)/\sin(\pi - \theta)/2$ . In any chain of polygons, these triangles all meet at point  $C$ , and there all joints are on the circle centered at  $C$  with radius  $\frac{L}{2 \sin \frac{\theta}{2}}$ .

### 3 The Segmented Helix

An analogous, though far more complicated, result holds in three dimensions.

In this section we consider segmented helix, or a helix evaluated only at regular points.

Following the Wikipedia article <https://en.wikipedia.org/wiki/Helix>, we set up a helix parametrically.

$$\begin{aligned}P_x(t) &= r \sin t \\P_y(t) &= r \cos t \\P_z(t) &= bt\end{aligned}$$

Such a helix has a radius of  $r$  and slope (if  $r \neq 0$ ) of  $b/r$ . The pitch of helix, the change in  $t$  needed to make one complete revolution, is  $2\pi b$ . Note that a helix may be degenerate in two ways. If  $r = 0$ , these equations become a line. If  $b = 0$ , these equations describe a circle in the  $xy$ -plane. If  $r = 0$  and  $b = 0$ , the figure is a point.

Such helices are continuous, but we are investigating stacks of discrete objects. We in fact wish to derive the parameters for a continuous helix from such discrete objects which constrain discrete points, so we wish to study a helix evaluated at integral points. We call such an object a *segmented helix*. A segmented helix may be thought of as function that given an integer gives back a point in three space.

$$\begin{aligned}P_x(n) &= r \sin n\theta \\P_y(n) &= r \cos n\theta \\P_z(n) &= nd\end{aligned}$$

$d$  is the distance or *travel* along the  $z$ -axis between adjacent joints, and  $\theta$  is the rotation around the  $z$ -axis between adjacent points.  $r$  is the radius of the segmented helix. Note that if  $\theta = \pi$ , we have a third form of degeneracy (to the human eye) of a segmented helix which is a zig-zag contained completely within a single plane.

If we think of the segmented helix as describing a polyline in 3-space, we would like to investigate the properties of that polyline.

Because the segmented helix is a discrete structure, we reframe the concept of *pitch* as *sidedness*  $s$ : how many segments (sides) make a complete rotation?

- $L$  is the distance between any two adjacent points.
- $\theta$  rotation about the axis between two joints.
- $c$  is the length of a chord formed by the projection of the segment between two points projected along the axis of the segmented helix.
- $d$  is the distance along the axis of the helix between any two joints.
- $\phi$  is the angle between any vector between two adjacent joints and the axis of the helix. In physical screws used in mechanical engineering, this is analogous to the *helix angle*. <https://www.linearmotiontips.com/examining-screws-three-different-angles/>
- $p$  is the pitch of the helix, the distance travelled in one complete rotation.
- $s$  is the number of segments in a complete rotation (in general not rational.)

These quantities are related:

$$c = 2r \sin \frac{\theta}{2} \quad (1)$$

$$L^2 = c^2 + d^2 \quad (2)$$

$$\arctan \frac{c}{d} = \phi \quad (3)$$

$$s = \frac{2\pi}{\theta} \quad (4)$$

$$d = L \cos \phi \quad (5)$$

$$p = d \frac{2\pi}{\theta} \quad (6)$$

$$(7)$$

Note: Measuring  $\phi$  requires us to decide on the sign of the direction of the axis, which is arbitrary and not based on the physical shape.

Any point on the segmented helix has a closest point on the axis of the helix. In particular, we will call the points closest to the joints “joint axis points”. Then  $d$  is the distance between consecutive joint axis points.

Now we are attempting to relate these properties to properties intrinsic to the joint or interface between two segments or objects in the segmented helix. If given an object, the length between the joints  $L$  is intrinsic.

## 4 The Intrinsic Properties of Periodic Chains of Solids

If we have chains of repeated 3D units conjoined identically, they generate a segmented helix. Although fairly obvious from Chasles’ Theorem, we have not found this state in writing elsewhere, so we call this Lord’s Observation:

**Observation 1** (Lord’s Observation). *In nature, helical structures arise when identical structural subunits combine sequentially, the orientational and translational relation between each unit and its predecessor remaining constant.[1]*

Lord’s Observation may perhaps be clarified that in fact identical objects conjoined via a rule produce periodic chains of objects that are uniformly intersected by segmented helices and that they may degenerate in one of three ways that we might not strike us as a helix if we are not seeking them:

1. The segments may form a straight line.
2. The segments may be planar about a center, forming a polygon or ring.
3. The segments may form a planar saw-tooth or zig-zag pattern of indefinite extent.

TODO: Add figures for each of these cases, maybe in one figure.

There are two complementary ways of learning about such segmented helices. In one approach, we may have knowledge of the segmented helix, and wish to learn about the subunits and the rule with which the subunits are combined. For example, we may have microscopic objects such as proteins or atoms, and we know from crystallography

something about the positioning of these objects, without knowing ahead of time the angles at which these objects would combine in their natural environment. In this case, we use a method we call Kahn's method[3] for determining the radius, travel, and twist of the segmented helix (these terms will be defined precisely below.)

In the other approach, we may know *a priori* exactly the relevant properties of the objects and the rule which they combine, and we seek to compactly describe the segmented helix they create. For example, a mathematician may consider a chain of dodecahedra, or a woodworker may cut identical blocks of maple wood, which are to be glued together face-to-face. In these cases everything about the objects and the rules for conjoining is known before the first two objects are glued together. We call this the *joint face normal method*, because it can be simulated by joining two flat faces together with a specified twist, even if the objects in question do not actually have a physical face (such as molecules).

In both cases, we would like to understand how a change in a face normal or a twist affects the parameters of the segmented helix, and, conversely, we would like to be able to choose the construction of the subunits to achieve a particular segmented helix.

In engineering, sometimes the term "special helix"[12] is used for helical curves on non-cylindrical surfaces. This paper uses the term "helix" only in the sense of "cylindrical helix".

## 5 Periodic Chains Produce Segmented Helices

A periodic chain is in fact a simple object which demonstrates tremendous symmetry. Before using this symmetry in the construction of the segmented helix, we prove that such a segmented helix indeed exists.

**Theorem 1** (Segmented Helix). *Consider  $N$  identical objects which each have two points,  $A$  and  $B$ , called joints, and a vector  $U$  not collinear with  $A$  and  $B$ . Call  $\overline{AB}$  the axis of this object. Consider the frame of reference for this object to have its axis on the  $z$ -axis with  $B$  in the positive direction, the midpoint of the axis at the origin, and the up-vector pointing in the positive  $y$  direction.*

*Consider any rule that conjoins  $A$  of object  $i + 1$  to  $B$  such that from the frame of reference of  $i$ , the object  $i + 1$  and anything rigidly attached to it is always in the same position in the frame of reference for  $i$ . Informally,  $i + 1$  "looks the same" to  $i$ , no matter what  $i$  we choose,  $i < N$ . Call a chain of  $N$  identical rigid objects conjoined via a rule that conjoins  $A$  to  $B$  in such a way that every vector of  $B$  is always in the same position relative to a frame of reference constructed from  $A$  a periodic chain.*

*Any periodic chain of three or more objects has a unique segmented helix whose segments correspond to the axes of these objects.*

*Proof.* We will proceed by induction.

Base Case ( $k == 3$ ):

Take an object  $AB$ . By Chasles' theorem [https://en.wikipedia.org/wiki/Chasles%27\\_theorem\\_\(kinematics\)](https://en.wikipedia.org/wiki/Chasles%27_theorem_(kinematics)), there is a screw axis  $S$ , a set of rotations, and a transposition  $d$  which moves the first object to position where the second object  $BC$  is. Take one of the rotation angles of smallest value. Construct the points  $A'$ ,  $B'$  and

$C'$  as the closest points to  $A, B$  and  $C$  on this axis. These points are collinear by construction.

Now add the object  $CD$  to object  $BC$  by our rule of periodic chains. Consider the points  $B'$  and  $C'$  from  $A$ 's frame of reference. Let  $d = \|\overline{C'} - \overline{B'}\|$ . Construct the point  $D'$  on our screw axis as the point closest to  $D$  on that line.

Now because  $C'D'$  in  $BC$ 's frame or reference must look like  $B'C'$  in  $A$ 's frame of reference, must look like  $B'C'$ , the distance  $\|\overline{D'} - \overline{C'}\| = d$ . From  $A$ 's frame of reference,  $A'B'C'$  are collinear, the points  $B'C'D'$  must be collinear in  $B$ 's frame of reference.

In any frame of reference, if  $A'B'C'$  are collinear and  $B'C'D'$  are collinear, then  $A'B'C'D'$  are collinear.

Now, looking backward from  $CD$  towards  $A$ , the distance  $A'B'$  must be the same as the distance  $B'C'$  so as to not violate our rule. So  $d = \|A'B'\| = \|B'C'\| = \|C'D'\|$ . Similarly because by construction  $r = \|BB'\| = \|CC'\|$ , and  $AA'$  is a rigid transformation of  $BB'$ , so  $r = \|AA'\|$ . By symmetry,  $r = \|DD'\|$ . Compute  $\theta$  as the rotation about  $S$  that takes  $BB'$  into  $CC'$ . By our rule of attachment,  $\theta$  also takes  $CC'$  into  $DD'$  and  $AA'$  into  $BB'$ .

Now construct a segmented helix, the radius  $r$ , distance, and angle  $\theta$ . This segmented helix can be positioned coincident with  $S$  so that  $H_0 = A$ . Then  $H_1 = B$ ,  $H_2 = C$ , and  $H_3 = D$ .

Therefore, for the base case of three objects, there is a segmented helix whose segments coincide with the axes of the objects.

Inductive Case  $(k+1)$ : Assume there is a segmented helix coinciding with the first  $k$  objects, and consider the frame of reference of the  $k$ th object. The axis and any other rigid property of the  $k+1$ th object stands in relation to object  $k$  as  $k$  stood to  $k-1$ . By induction, the  $k$ th object had a segment of a segmented helix corresponding to its axis. Attach vectors  $V_{Ak}$  and  $V_{Bk}$  from the joints of  $k$  to the axis of the helix perpendicularly. Define these vectors in the frame of reference for  $k$ .

To the  $k-1$ th, the tips of  $V_{Ak}$  and  $V_{Bk}$  define a line segment which lies on the axis of the segmented helix  $H$ , with the tip of  $V_{Ak}$  coincident with the tip of  $V_{B(k-1)}$ .

By our rule and by induction, since this is true of the  $k-1$ th object, it is true of the  $k$ th object. Therefore the  $k+1$ th objects  $V$  vectors point to a line segment which lies on the axis of  $H$ , extending it in the same direction. The axis of the  $k+1$ th object therefore coincides with the  $k+1$ th segment of  $H$ .

Therefore, by induction, identical objects conjoined by the same rule always coincide with some segmented helix, whose parameters are discoverable.  $\square$

This theorem leads to the following corollary.

**Corollary 1** (Segment Similarity). *The angle between the axis of each object in a periodic chain and the axis of the segmented helix coincident to it is the same.*

*Proof.* The axes of each object coincide with a segment of a segmented helix. A segmented helix is completely symmetric no matter in which direction of the axis you look down or which point on the axis you begin at. The angle between each pair of objects is exactly the same.  $\square$



Note that the objects themselves may not be symmetric; for example, The  $B$  face does not have to be the same size as the  $A$  face. In fact, the object itself might be shaped like the letter “C”, and not completely enclose the axis. Taking the idea further, the object might be spiky like a stellated polyhedron or a sea urchin, and still be joined by joints relatively close to the center of the object. In this paper we do not concern ourselves with the issue of self-collision of the objects, which would have to be considered if one attempted to make a period chain of sea urchins.

Corollary 1 will be used in our development of KahnAxis algorithm and in our computation of segmented helix properties and to justify balancing face normals to produce an intrinsic out-vector and to apply the KahnAxis algorithm without actually assigning objects Cartesian coordinates.

## 6 Computing Screws and Segmented Helices from Transformation Matrices

The rule for how objects in a periodic chain are joined may be convenient captured as a transformation matrix. In general, a human engineer will have to compute this transformation matrix from some other information, such as the face-to-face conjoining rule. We discuss how to do this from joint-face normal vectors in Section 7.3. However, a transformation matrix clearly capture the idea of “repetition”. Since by definition the objects in the chain are the same shape, moving one object into a new position and place an identical copy of that object in that position are practically the same.

Using standard screw theory[2], a screw can be computed from such a transformation matrix. This consists of the axis of the screw  $S$ , a point on the screw axis  $P$ , the rotation  $\theta$  around the axis, and the transposition, or travel, along the axis of one transformation.

Neither a transformation matrix or its corresponding screw completely define all of the intrinsic properties of a segmented helix. In particular, a matrix  $M$  maps any point  $p$  to a point  $p'$ . Since this applies to all points no matter how far from the screw axis or the axis of rotation and such transformation preserve distance to this axis (the radius), the radius of a segmented helix is not determined by a transformation matrix or a screw. Since the helix angle  $\phi$  changes with radius for a helix of a given pitch,  $\phi$  is not determined.

However, if we have transformation matrix and one joint position, all of the properties of segmented helix are determined. If we have a screw and one point on the axis of the screw fixing it in space and the location of one joint, all of the properties of the segmented helix are completely determined.

In our software, we have coded the calculation of the screw directly from a transformation matrix, and the additional routines which determine all intrinsic properties from a joint position.

As is common in kinematics[13], there are many ways to represent the same physical or mathematical situation. Four consecutive joint positions also completely determine a segmented helix. We present an approach to doing this in the code below. Because joints can be computed from transformation matrices and transformation matrices from joints, which method of calculation is preferable would be a matter of choice and

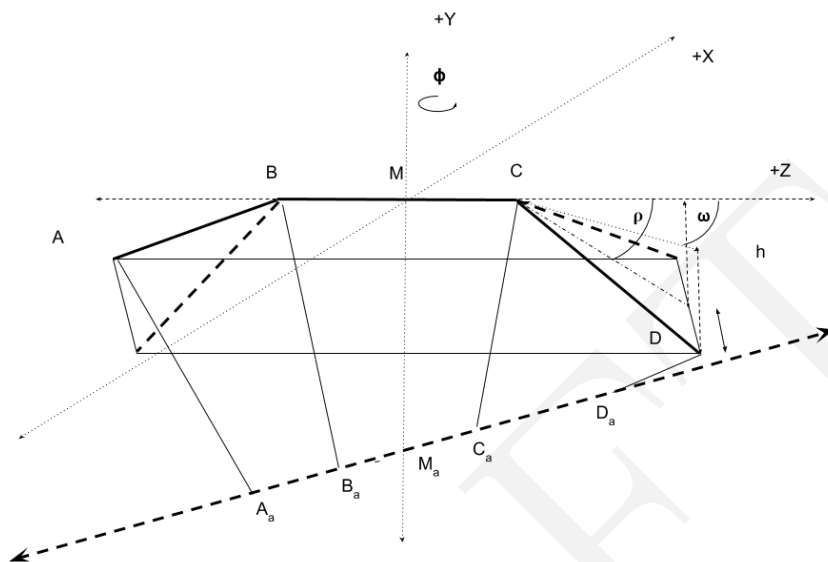


Figure 3: Three Symmetric Members

clarity. We have in fact coded both and used the comparison as automated tests in our software to ensure the correctness of our coding.

A mechanical engineer, robotocist, or computer graphics expert is likely to find the computation from the transformation matrix more natural and convenient. A chemist or crystallographer is more likely to have learned the position of four points and wish to compute from that. At one level, of course, either method can be used.

## 7 KahnAxis: Computing Segmented Helices from Joints

Kahn[3] has given a method for computing the axis of a helix in the context of chemistry. This method uses the observation that the angle bisectors of the segments on a segmented helix are perpendicular and intersect the axis of the helix. Kahn's method was a prelude to some error-tolerant methods applicable to the realm of organic chemistry. In this paper we are concerned with pure geometry. Also, Kahn was writing in 1989, and we now have more convenient computing tools. We give here a modification of Kahn's algorithm, called *KahnAxis*, which relies on our ability, working in the realm of pure geometry, to position the segments on the axes to simplify the derivation and computation.

## 7.1 The 4-Point Method

**Theorem 2** (Segmented Helix Test). *Four arbitrary sequential points  $A, B, C, D$  are consecutive joints of a segmented helix if and only if the segments  $\overline{AB}$ ,  $\overline{BC}$ , and  $\overline{CD}$  are equal length and the scalar projection of  $\overline{CD}$  onto  $\overline{BC}$  is equal to the negation of the scalar projection of  $\overline{AB}$  onto  $\overline{BC}$ .*

*Proof.* (Sketch) By Chasles' Theorem, there is a screw  $S$  that takes  $\overline{AB}$  into  $\overline{BC}$ , and a screw  $R$  that takes  $\overline{CD}$  into  $\overline{BC}$ . If  $R$  is the negation of  $S$ , the projections will be the same.

If the projections are the same, there is a midpoint. Without loss of generality, rotate around  $\overline{BC}$  so that the midpoint points straight down. Now  $A.x = -D.x$ , if the projections have the same length. If this is so, the screw that takes  $\overline{CD}$  into  $\overline{BC}$  ( $R$ ) has the same magnitude of rotation as  $S$ . The direction vector of  $S$  points in the opposite direction to  $R$ . The distance travelled is the same, therefore  $R$  is the negation of  $S$ .  $\square$

Therefore four consecutive points completely determine a segmented helix. We provide a modification of the KahnAxis algorithm which takes four such points (without loss of generality  $B$  and  $C$  are assumed to be centered on the  $z$ -axis, and that a rotation has been performed to balance  $A$  and  $D$ ).

In the derivations below, we rely on certain facts about the segmented helix formed by the stack of objects, the first of which is key:

- Without loss of generality, we may think of any member whose faces and twist generate a non-degenerate helix as being “above” the axis of the helix. We furthermore choose to place the object in this figure so that  $B_y = C_y$ , that is, that the members are symmetric about the  $z$ -axis.  $A$  and  $D$  are “balanced” across the  $YZ$ -plane, and  $A_x = -D_x$  and  $A_y = D_y$ .
- Every joint  $(A, B, C, D)$  is the same distance  $r$  from the axis  $H$  of the helix.
- Every member is in the same angular relation  $\phi$  to the axis of the helix.
- Since every member cuts across a cylinder around the axis, the midpoint of every member is the same distance from the axis which is generally a little less than  $r$ . In particular the midpoint  $M$  whose closest point on the helix axis  $m$  is on the  $y$ -axis and  $\overline{Mm} < \overline{Bb}$ .
- The points  $(A_a, B_a, C_a, D_a)$  on the axis closest to the joints  $(A, B, C, D)$  are equidistant about the axis and centered about the  $y$ -axis. In particular,  $\|\overline{B} - \overline{B_a}\| = \|\overline{C} - \overline{C_a}\|$ .

From the observations that  $\|\overline{B} - \overline{B_a}\| = \|\overline{C} - \overline{C_a}\|$  we concluded that the helix axis is in a plane parallel to the  $XZ$ -plane, it intersects the  $y$ -axis, but in general is not parallel to the  $z$ -axis.

Because the angle bisectors of each joint are in general skew, and intersect the axis perpendicularly, it is clear we can use linear algebra and the algorithm for the closest points on two skew lines to find  $B_a$  and  $C_c$ .

However, we can take advantage of the fact that a segmented helix has tremendous symmetry, and the angle bisectors are very far from being two generally skew lines.

In fact, by taking advantage of the fact that the generating rule for an object chain requires similarity in every joint, we can arrange the objects as in Figure 3.

KahnAxis takes a length and a point  $D$  known to be in a specific relation to  $B$  and  $C$ . From there, he goes on to compute various parameters.

We have modified this method by carefully arranging our axes so that we can compute  $\phi$ , the angle between the helical axis and the  $z$  axis. This, in combination with symmetry and the knowledge that the helical axis is in the  $XZ$  plane, lets us compute the points on the axis corresponding to the joints directly from  $\phi$ .

This algorithm coded below, is simple enough that Mathematica can actually produce symbolic closed-form formula for all computed valued in terms of  $L, x, y, z$ , but they are less comprehensible to the human eye than this algorithm, although their existence opens the possibility that, for example, the derivative representing the change in  $r$  with a change in  $D$  could be calculated.

## 7.2 Degenerate Cases

The fundamental insight that the axis of the helix  $H$  can be computed by a cross product of the angle bisector vectors ( $Bb$  and  $Cb$ ) applies only when the angle-bisectors have a non-zero length and when they are not anti-parallel. When the are of zero length, this is the degenerate case of a straight line coinciding with all segments. This occurs only when  $z = L$ . When  $Bb$  and  $Cb$  are parallel (pointing in opposite directions), the zig-zag degeneracy occurs. This occurs only when  $y = 0$ .

Once  $H$  has been calculated, the signed travel along the axis  $da$  is the scalar projection of a segment  $(C - B)$  onto  $H$ . From this  $\phi$  is directly calculatable.  $\phi$  allows a direct calculation of the  $x, y$  and  $z$  components of the point  $Ba$  on the axis pointed to by  $Bb$ .  $r$  is the distance between  $Ba$  and  $B$ .  $c$  and  $\theta$  are easily computed from these values.

TODO: Move the tests that I have coded in JavaScript into Mathematica, handle special cases as separate math routines to report here.

```
ChordFromLDaxis[L_, Da_] := Sqrt[L^2 - Da^2]
RotationFromRadiusChord[R_, C_] := 2 ArcSin[C/(2R)]
KahnAxis[L_, {x_, y_, z_}] := Block[{A, B, C, D, Cb, Bb, H,
                                     Bax, Bay, Baz, Ba,
                                     r, theta, da, c, phi},
  D = {x, y, z};
  A = {-x, y, -z};
  B = {0, 0, -L/2};
  C = {0, 0, L/2};
  Cb = (B+D)/2 - C;
  Bb = (A+C)/2 - B;
  H = Normalize[Cross[Bb,Cb]]; // Why am I calling Normalize twice?
  da = (C - B) . Normalize[H];
  phi = ArcCos[da/L];
  Bax = Sin[phi] da / 2;
  Baz = -Cos[phi] da / 2;
  Bay = Bb[[2]] (Bax / Bb[[1]]);
```

```

Ba = {Bax, Bay, Baz};
r = Norm[Ba - B];
c = ChordFromLDaxis[L, da];
theta = RotationFromRadiusChord[r, c];
{r, theta, da, c, phi, H}
]

```

Note that in Figure 3 there is great room for confusion in terms of plane  $\omega$  is actually measured against. The three triangles  $\triangle BB_aC$ ,  $\triangle BM_aC$ , and  $\triangle BM_aC$  are all in general not co-planar, that is, they are all at slight angles to each other.

There is one reason one might prefer the transformation matrix method or the point method over the other: with modern computer algebra systems such as Mathematica it might be possible to use these “algorithms” to produce closed-form expressions of closed-form (alebraic) inputs. For example, the Platonic solids all have lengths and face normals which can be specified exactly in closed (though irrational) form. Thus it might be possible to produce an expression for the radius of one of the Platonic Dodecahelices of unit edge length. We have not understaken this work.

### 7.3 The Face Normal Method

KahnAxis takes a point  $A$  known to be in a specific, balanced relation to  $B$  and  $C$ . A chemist might know 4 such points from crystallography, and be able to move them into this symmetric position along the  $z$ -axis.

However, we might instead know something of the subunits and how they are conjoined, without actually knowing where poitns  $A$  and  $D$  are.

We start with these intrinsic properties of an object, and additionally the rule for how objects are laid face-to-face. That is, knowing the length between two joint points and a vector normal to the faces of the two joints, we almost have enough to determine the unique stacking of objects. The final piece is that we must know the *twist*. That is, when face  $A$  of a second objects is placed on face  $B$  of a first object so that they are flush (that is, their normals are in opposite directions), it remains the case that the second object can be rotated about the normals. To define the joining rule, we must attach an *up vector* to each object. Then a joining rule is “place the second object against the first, joint point coincident to joint point, and twist it so that its up vector differs by  $\tau$  degrees from the up vector of the first object.” In this definition, the up vectors are considered to be measured against the plane containing the two axes meeting in a joint.

Define the *joint plane* to be the plane which contians the two axes meeting in a joint. Define the *joint line* to be the line throught the joint perpendicular to the joint plane. Define the *joint angle* to be the angle of the first axis to the second measured about the joint line. The twist  $\tau$  is the change in the a vector attached to the object rotated about the joint line by the joint angle. That is, take any vector attached to the first object, place it at the joint, rotate it about the joint line via the joint angle.  $\tau$  is the difference between the angle of this vector measured against the joint plane and the angle of the up vector of the second object measured against the joint plane.

If the objects are macroscopic objects which have faces, this is the same as the rotation of the axis of the second object relative to the first in the plane of the coincident

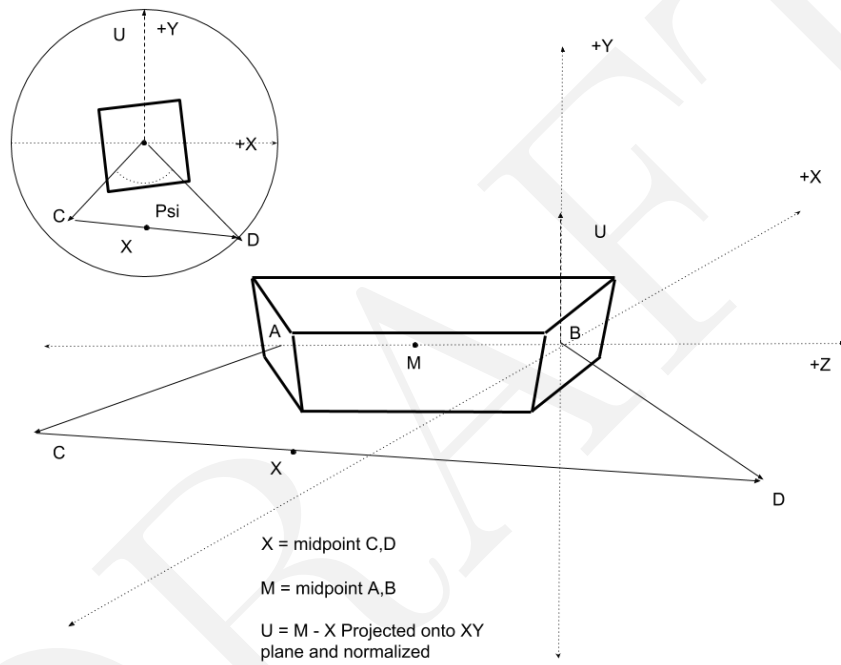


Figure 4: The rotatable prism of three objects

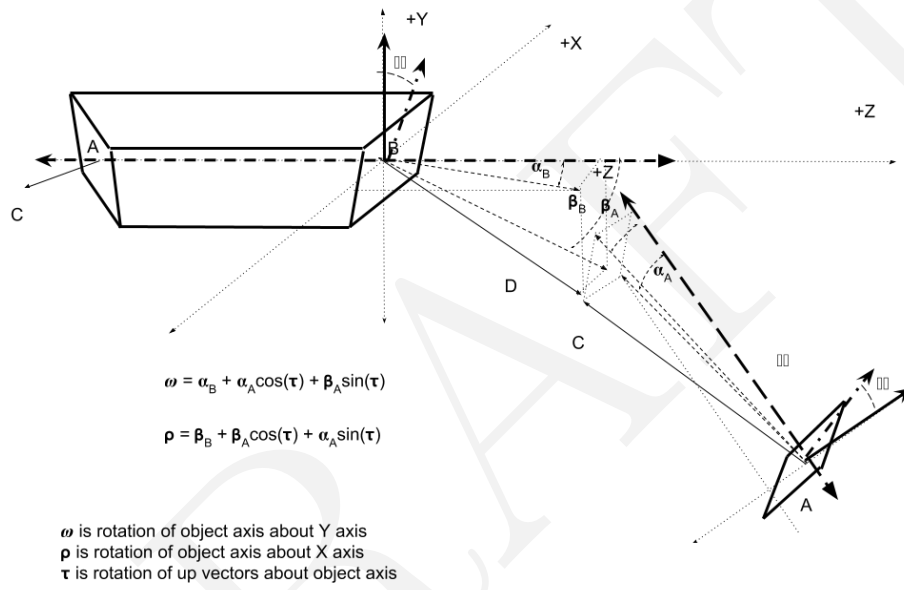


Figure 5: Joint Geometry

faces. We can identify intrinsic properties:

- An object with two identified faces, labeled  $B$  and  $C$ . Assume there normalized vectors  $N_B$  and  $N_C$  from each of these points that is aligned with the axis of the conjoined object attached to that face. This normals might be enforced by the fact that flat faces are joined in the joint plane. However, molecules don't have faces; this conjoining relationship may be enforced some other way.
- The length  $L$  of an object, measured from joint point  $A$  to joint point  $B$ .
- A joint twist  $\tau$  defining the change in computed out-vector between objects, measured at the joint face.

## 7.4 Rotating into balance from face normal vectors

In order to use the KahnAxis algorithm, we need a way to compute points  $A$  and  $D$  in balance around the axis  $BC$ . From Lord's Observation, we know that after placing  $BC$  along the  $z$ -axis, there is always an angle  $\psi$  which will rotate the points  $A$  and  $D$  into balance.

It is relatively easy to work out the math to adjoin objects face-to-face bases on the face normals; we will assume this as a subroutine called "adjoinPrism" which takes  $\tau$  (the rotation inside the plane of the joint).

The key insight to finding  $\psi$  to note that we can consider the projections of the  $B$  and  $C$  face normal vectors projected into the  $XY$  plane, and rotate these so that they are balanced around the negative  $y$  unit vector. Even if the lengths of the projections of the face normals in  $XY$  are different, this mechanism works.

TODO: Properly code in Mathematica and place code here. Figure out how to express this mathematically.

## 7.5 On the Choice of the Screw Axis Direction

Given only a physical segmented helix without position in space, we may arbitrarily choose the direction for the axis. Changing our decision will make the screw axis point in the negative direction, change the sign of the travel  $d$  along the axis, and choose  $\phi$  to be  $\pi - \phi$ .

As can be seen from interactive play with our software, it is entirely possible for the travel along the axis of the helix to be 0—in fact, choosing  $\tau \approx 0$  produces toruses, which have no travel along the axis.

We could represent this by making the length of the vector representing the axis be the length of the travel  $d$ . However, this would have the drawback than when  $d$  is zero we would be unable to determine the axis of revolution of the torus. Although somewhat arbitrary, I have chosen instead to represent the axis as a normalized vector of unit length, and to allow the travel to be negative. This has the value that changing  $\tau$  through zero smoothly changes  $d$ . However, it creates the problem that as  $\tau$  approaches  $\pi$  from different directions the signs of the axes are different. That is,  $\tau = \pi$  and  $\tau = -\pi$  describe exactly the same shape, but in our calculation they will have different signs for the axes. The radius, pitch and absolute value of the travel, which are intrinsic to the shape, will be the same, but the axis vector,  $\phi$ , and the sign of  $d$  will be different.



## 8 Checks and Explorations

Note: It is useful to compute  $\psi$ , the direction angle of the midpoint of the projections of the face normals. We also need to define the differences between these angles as well  $\delta$ . Choosing  $\tau$  so that the  $\delta$  is zero produces a torus-like structure. Choosing  $\tau$  so that  $\delta$  is  $180^\circ$  produces the zig-zag case, which is of maximum length.

### 8.1 Changing $\tau$ Smoothly Changes Tightness

**Theorem 3** (Twist Spectrum). *For any choice of face normals having non-zero  $x$  or  $y$  components, changing  $\tau$  smoothly varies the segmented helix between a torus and zig-zag cases.*

*Proof.* By interactively manipulating the software it is apparent.  $\square$

**Theorem 4** (Torus Corollary). *For any choice of face normals, there is choice of the twist  $\tau$  for which the segmented helix is a planar polygon, thereby resembling a torus.*

*Proof.* By interactively manipulating the software it is apparent.  $\square$

TODO: Can we calculate the  $\tau$  value as a function of the face normals? That would make a nice little constructive theorem.

In this section add graphs. Also, a check against the BC helix. Possibly software should be used to produce a 3D simulation of the issues.

Idea: Define “tightness” to be  $p/r$ , where  $p$  is pitch and  $r$  is radius. Attempt to prove that in some ways tightness increases with increasing  $\tau$ .

### 8.2 Qualitative observations

Varying  $\tau$  smoothly varies the tightness of the coiling of the helix, moving through vary linear cases towards a torus, to a torus, to a very linear case on the other side.

In fact it is possible to that there is always a “tightest coil” which does not self-intersect. If we had many objects, we could pack them into a convenient space by computing the  $\tau$  of the tightest coil and stacking them this way. If we had a means to change  $\tau$ , perhaps via motors in a robot arm, we would have a smoothly telescoping and contracting robot arm.

## 9 Applying to The Boerdijk-Coxeter Tetrahelix

The Boerdijk-Coxeter tetrahelix is a periodic chain of conjoined regular tetrahedra which has been much studied[7, 8, 9, 10] and happens to have irrational measures, making it an ideal test case for our algorithms. Because the face-normals can be calculated and the positions of the elements of the BC helix directly calculated, we can use it to test our algorithms, and in fact these algorithms give the correct result.

However, it should be cautioned that the helix which Coxeter identified[7] goes through every node of every tetrahedron. Constructing the helix that goes through only “rail” nodes allows the tetrahelix to be modified[10]. However, the segmented

helices defined in this paper do neither; rather, it is most natural to imagine them moving through the centroid of face of a tetrahedron. The rotation of a segment thus matches the BC Helix ( $\arctan -3/2$ ), but the radius of the generating segmented helix in the paper would be smaller than those segmented helices that intersect the nodes.

In light of Lord’s observation and the Segmented Helix algorithms, we can now consider the BC Helix, and in fact a variety of segmented helices generated by face-to-face stacking of Platonic solids, examples of called *Platonic segmented helices*.

This complementary view is to think of the BC Helix not as the helix that intersects the vertices of the tetrahedron as Coxeter did[7], nor a single rail as may be valuable to engineers[10], but rather as a helix through the center point of the faces of the tetrahedron. This is a segmented helix of very small radius compared to the other two approaches, but it has the advantage that it is far more general. For example, it is clearly defined if one used truncated tetrahedra.

More generally, the same approach gives the segmented helices created by placing dodecahedra or icosahedra or octahedra face-to-face in a regular pattern.

Note this also makes clear that in these cases we must also specify the *twist*, even if we insist on perfect face-to-face matching. Thinking of it this way, there are actually 3 tetrahedral segmented helices, depending on which twist  $120^\circ$  is chosen (keeping the faces matching). In the case of the tetrahedron, this creates the clockwise BC Helix, the anti-clockwise BC Helix, and the not-quite-closed tetrahedral torus.

In the case of the icosahedron, there are in fact many possibilities, as one need not choose the precisely opposite face as the joining face, and one may choose up to three twists. The “zoo” or Platonic helices can be studied via the calculations described here, and our software makes these interactively selectable.

## 10 Implications

One of the implications of having an easily-calculatable understanding of the math is that it may be possible to design helices of any radius and pitch by designing periodic (possibly scalene) segments. Combined with slight irregularities, this means that you have a basis of design molecular helices out of “atoms” which correspond to our objects.

This would mean that if you wanted to build a brace of length exactly 3 meters with bars of exactly 1/2 meter you would be able to come as close to this as mathematically possible.

A modular robot constructed out of repetitions of the same shape-changing module will always product a helix whose precise shape can be controlled by uniformly changing the shape of all of the modules.

## 11 Future Work

We propose that the math developed in this paper can be used to build an exhaustive table of the properties Platonic segmented helices, that is, segmented helices constructed solely out of regular Platonic solids. Such tetrahelices, icosahelices, octahelices and dodechelices have been mentioned in a number of papers[14, 15, 16], but not exhaustively studied in the purely helical form. Because in some cases Platonic segmented

helices may be found in nature or related to structures found in nature[17, 11], it would be convenient to have a table, and images, of all such Platonic segmented helices for reference.

The algorithms and software described herein allow numerical calculation of the intrinsic properties of these Platonic helices, but it would be even better to describe them in with closed-form expressions, as Coxeter did for the Boerdijk-Coxeter tetrahelix. The math and the algorithms are simple enough that if coded in a symbolic algebra system like Mathematica, or with careful work, closed-form expressions could be produced for all the Platonic helices. These would be interesting if they happen to be short; we have no reason to believe they will be.

## 12 To Do

- Clean up the code. 3 days
- Go through each reference 1 day
- Try to get list of references to the computation of a screw from an arbitrary matrix, and compare and contrast to our code. 1 day
- Need to understand what an “alpha coil” protein structure is. (Done: An alpha coil is one of the most common and studied protein forms, roughly providing distance in the protein, consisting of a helix formed by amino acids, which tend to be cross bonded. 1 hour
- Need to understand possibility of further simplifying specification of object.
- Need to understand if I can redefine things in terms of “pitch”. 2 hours
- Need to define and calculate analogs of curvature and torsion for the segmented helix, and make those part of the interactive software.
- Complete the table of platonic helices, including a count software to identify intrinsically symmetric cases. That is, create software to create the “zoo” of platonic helices. - almost done
- Note further that Equations 7 and 8 of this paper[3] give BETTER equations for radius  $r$  and the distance  $d$  than what I have so far given.
- Need to get this paper, by hook or by crook, and probably cite: Note: An historical review of the theoretical development of rigid body displacements from Rodrigues parameters to the finite twist <https://www.sciencedirect.com/science/article/pii/S0094114X0500087X>
- Add in Unit Edge Length conversions - 2 hours
- Complete LaTeX table of Platonic Helices - 4 hours
- Give mnemonic names to each Helix - 2 hours
- Create a spinner for the number in the helix - 2 hours
- Create screenshot figures of each helix - 8 hours
- Improve qualitative section, talk about toruses - 8 hours
- Talk about 0-face Platonic Degeneracies - 1 hour

- Consider better naming mechanism for faces - 4 hours
- Fix bug with  $\phi$  in  $\tau = 0$  cases - 4 hours
- Write all of the algorithms in mathematical notation
- Explain the face-vertex match issues.
- Consider assigning colors to faces, which would allow for more visibility

## 13 References that need to be studied or reviewed

This is a long, expensive book, but it may be quite relevant[18]: [https://books.google.com/books?hl=en&lr=&id=1LZ1SZ70RrQC&oi=fnd&pg=PP1&ots=0hSEwJv1UB&sig=xNG9UWv\\_H10XHwa0i0BJN7TW6xA#v=onepage&q&f=false](https://books.google.com/books?hl=en&lr=&id=1LZ1SZ70RrQC&oi=fnd&pg=PP1&ots=0hSEwJv1UB&sig=xNG9UWv_H10XHwa0i0BJN7TW6xA#v=onepage&q&f=false)

Note: There is another long, deep book that needs to be obtained and studied[19]. <https://books.google.com/books?hl=en&lr=&id=FHP1DWvz1bEC&oi=fnd&pg=PP1&ots=TsOnodavEZ&sig=H086UUV1qRVWGqY-Tv02nb7x7NA#v=onepage&q&f=false>

[https://www.researchgate.net/publication/236066626\\_Segmented\\_helical\\_structures\\_formed\\_by\\_ABC\\_star\\_copolymers\\_in\\_nanopores](https://www.researchgate.net/publication/236066626_Segmented_helical_structures_formed_by_ABC_star_copolymers_in_nanopores)

This is a discussion of segmented coils in a protein structure:

<https://www.sciencedirect.com/science/article/pii/S0022283688903701>

This talks about tuning the period of a helix inside a nanopore:

<https://aip.scitation.org/doi/abs/10.1063/1.4794785>

A modern helix structure protein paper:

<https://www.sciencedirect.com/science/article/pii/S1476927108000583>

“Local Frustration Determines Molecular and Macroscopic Helix Structures”

<https://pubs.acs.org/doi/abs/10.1021/jp4040503>

“Analyzing Protein Structure Using Almost Delaunay Tetrahedra”

[https://www.researchgate.net/profile/Alexander\\_Tropsha/publication/250901525\\_Analyzing\\_Protein\\_Structure\\_Using\\_Almost-Delaunay\\_Tetrahedra/links/5578584408ae75215870347c/Analyzing-Protein-Structure-Using-Almost-Delaunay-Tetrahedra.pdf](https://www.researchgate.net/profile/Alexander_Tropsha/publication/250901525_Analyzing_Protein_Structure_Using_Almost-Delaunay_Tetrahedra/links/5578584408ae75215870347c/Analyzing-Protein-Structure-Using-Almost-Delaunay-Tetrahedra.pdf)

“Simulation of Suspensions of Helical Rigid Fibers” Y Al-Hassan : British Journal of Mathematics and Computer Science (PDF downloaded)

“HELFIT: Helix fitting by a total least squares method” : This needs to be studied closely! <https://www.sciencedirect.com/science/article/pii/S1476927108000418>

QHELIX: A Computational Tool for the Improved Measurement of Inter-Helical Angles in Proteins <https://link.springer.com/article/10.1007/s10930-007-9097-9>

Note: “On the Screw Axes and Other Special Lines Associated With Spatial Displacements of a Rigid Body” <http://manufacturing-science.asmedigitalcollection.asme.org/article.aspx?articleid=1439697>

Note: An historical review of the theoretical development of rigid body displacements from Rodrigues parameters to the finite twist <https://www.sciencedirect.com/science/article/pii/S0094114X0500087X>

Note: Might need to get this book. [https://link.springer.com/chapter/10.1007/978-3-319-31126-5\\_1](https://link.springer.com/chapter/10.1007/978-3-319-31126-5_1)

## 14 Acknowledgements

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## A Tables for the Platonic Helices

Table 1: The Platonic Helices

Name	Solid	C-Face #	$\tau$	radius	d	$\phi$	$\theta$
Boerdijk-Coxeter Tetrahelix	Tetrahedron	2	-120	0.17	-0.95	-161.57	131.81
Boerdijk-Coxeter Tetratorus	Tetrahedron	2	0	0.87	0	-90	70.53
Boerdijk-Coxeter Tetrahelix	Tetrahedron	2	120	0.17	0.95	-18.43	131.81
Dodecahelix	Dodecahedron	8	-144	0.09	-0.99	-170.31	149.52
Dodecahelix	Dodecahedron	8	-72	0.4	-0.81	-144.11	93.03
Dodecahelix	Dodecahedron	8	0	0.95	0	-90	63.43
Dodecahelix	Dodecahedron	8	72	0.4	0.81	-35.89	93.03
Dodecahelix	Dodecahedron	8	144	0.09	0.99	-9.69	149.52