GRAPHITE AND DIAMOND

Taren Miller
Math 308-101
December, 2005

A pencil and a diamond ring...
what could these two objects possibly have in common?

Graphite, from the Greek word "graphos" which means "to write", makes up pencil lead. Diamond, from the Greek word "adamas" which means "the invincible", is the hardest material found in nature.

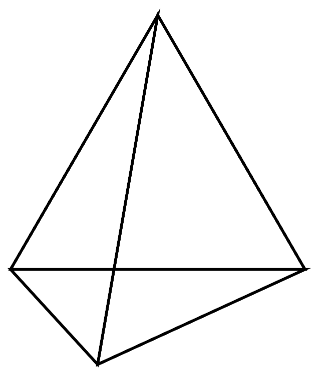
These two are both made of the same element - carbon!

The extreme differences in the two materials are due to the way in which the carbon atoms are arranged.

Let us investigate this...

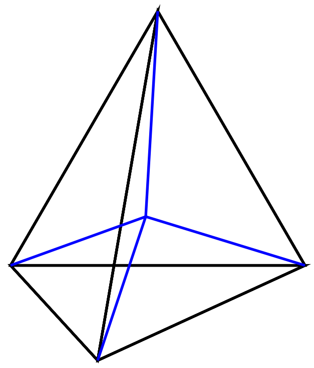
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



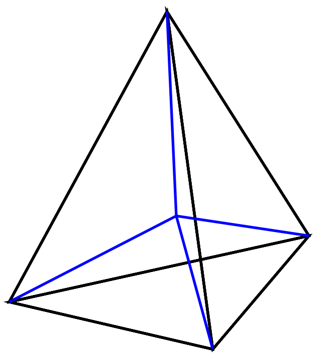
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



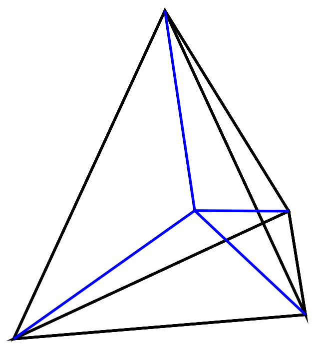
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



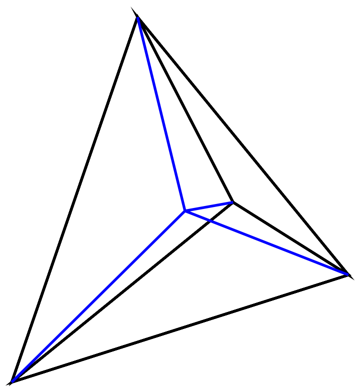
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



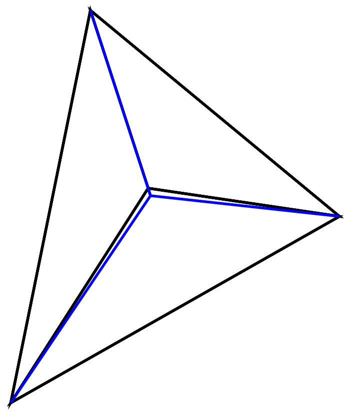
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



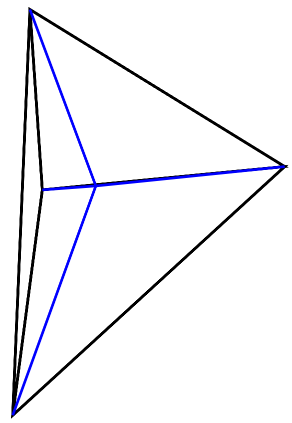
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



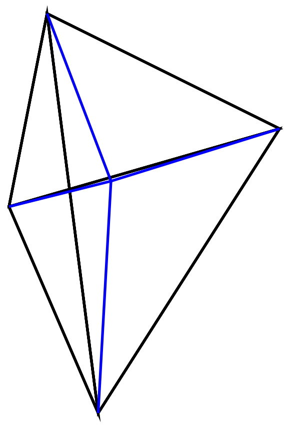
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



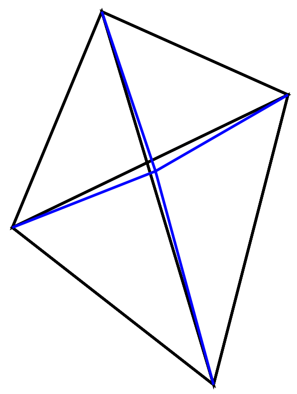
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



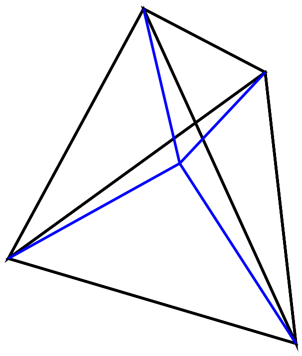
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



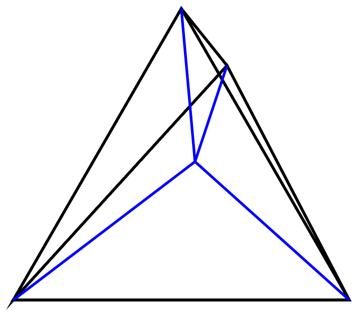
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



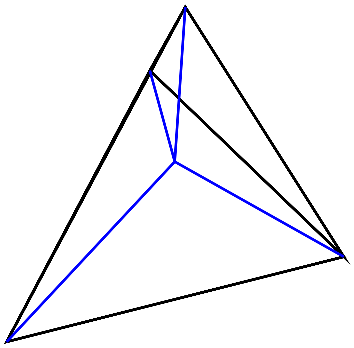
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



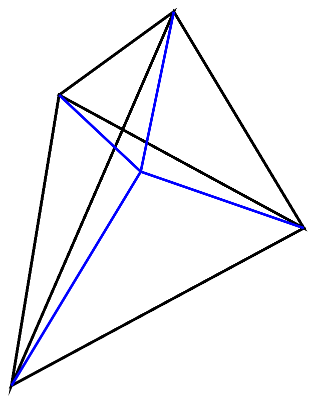
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



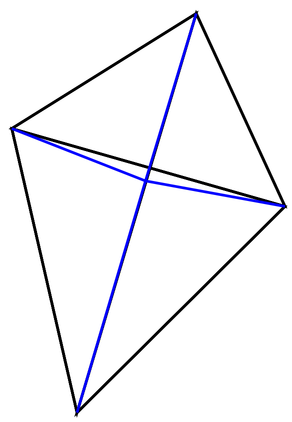
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



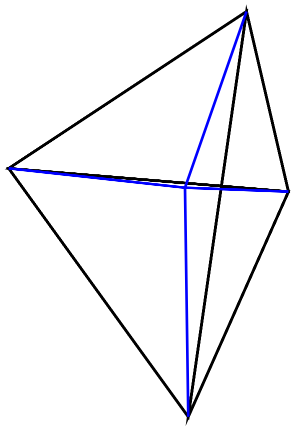
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



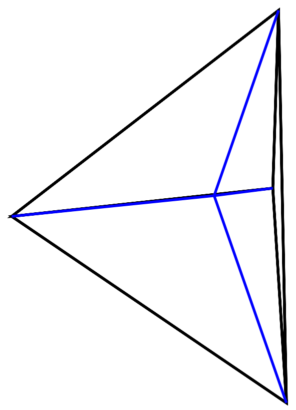
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



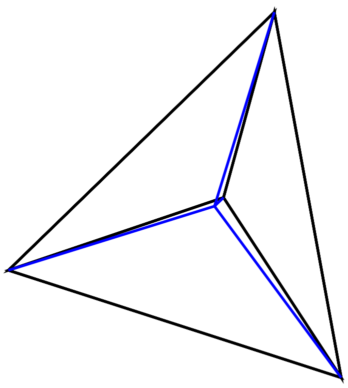
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



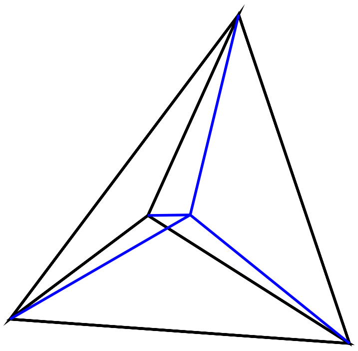
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



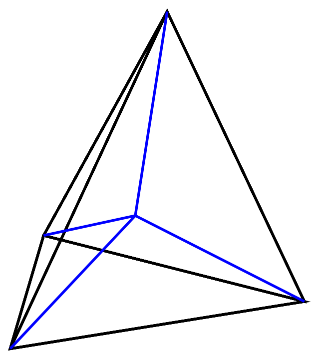
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



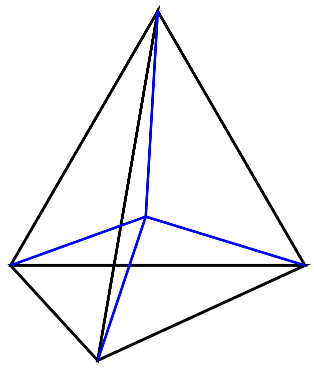
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:



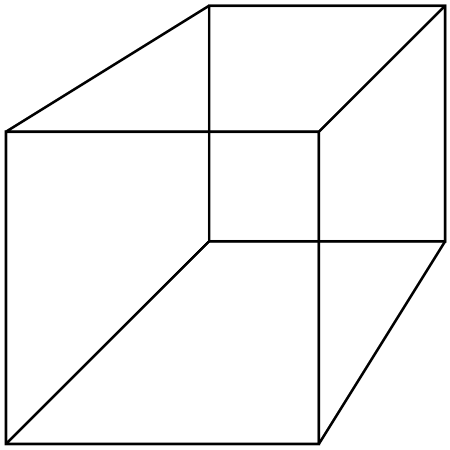
A carbon atom has four valence electrons that are available for bonding with other atoms. When four bonds are formed, the electrons in the bonds repel each other and want to be as far away from one another as possible. The resulting arrangement of the bonds is tetrahedral.

Consider a regular tetrahedron, a polyhedron having four equilateral triangular faces:

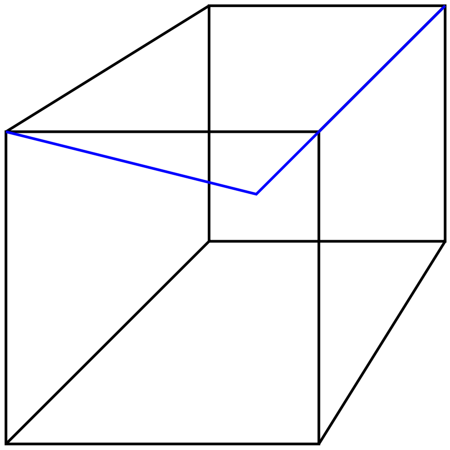


The blue lines extend from the center of the tetrahedron to each of the vertices. They are the radii of the tetrahedron, and they represent the tetrahedral arrangement of bonds around a carbon atom.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

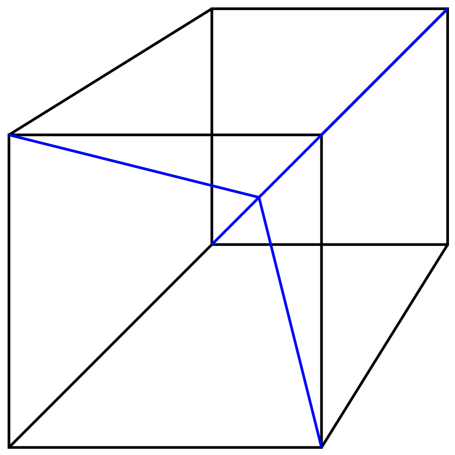


The tetrahedral arrangement of bonds can also be constructed by first considering a cube.



We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

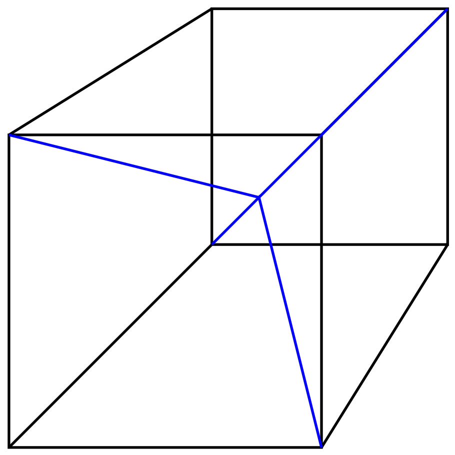


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

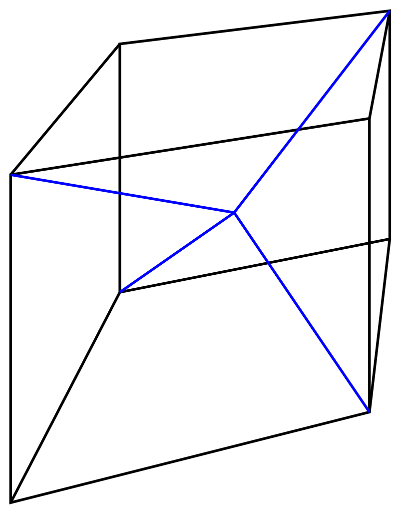


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

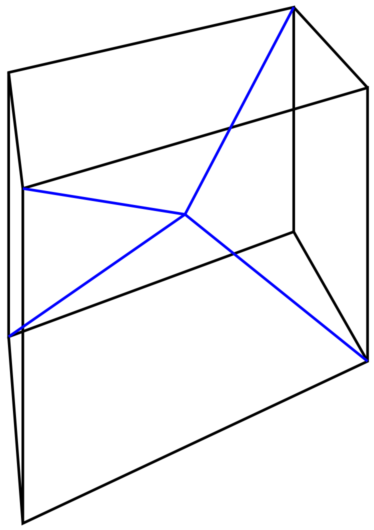


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

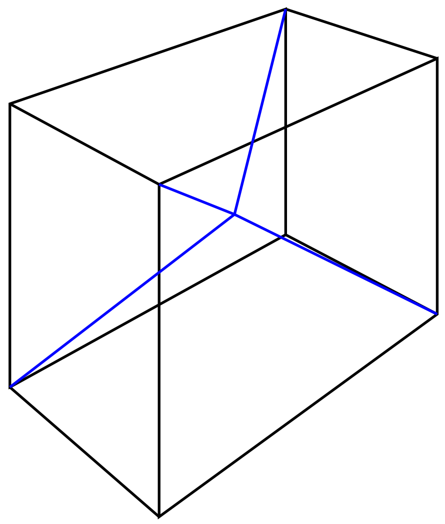


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

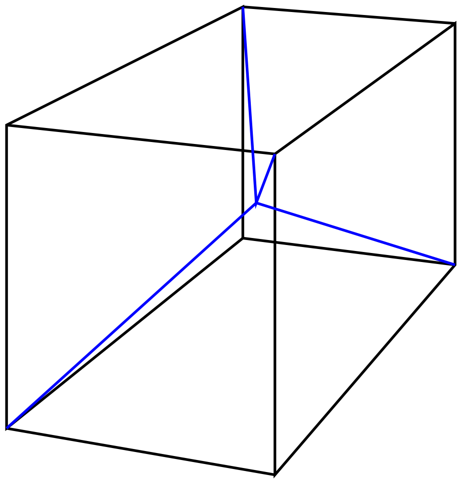


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

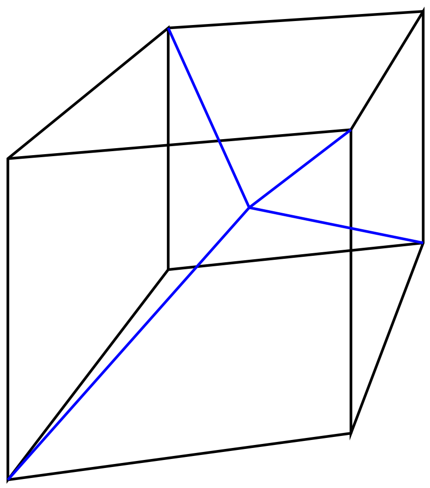


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

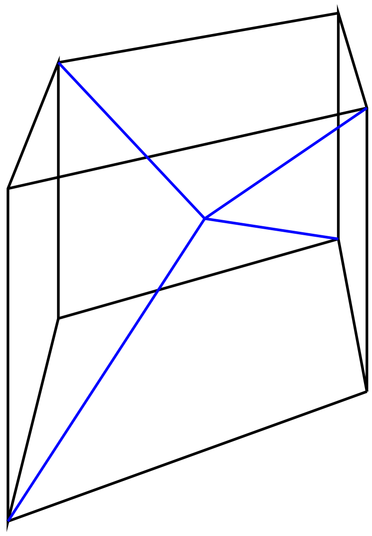


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

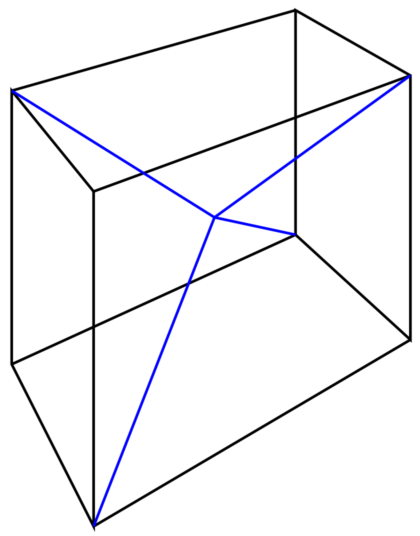


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

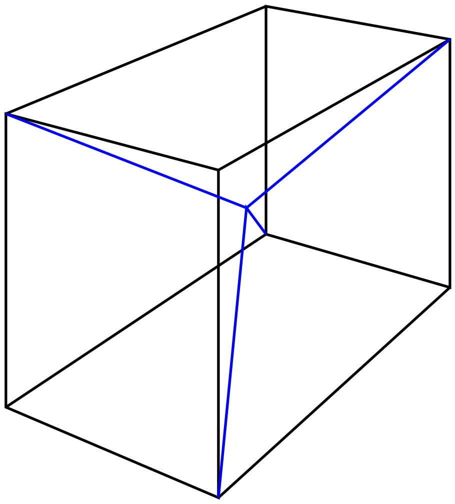


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

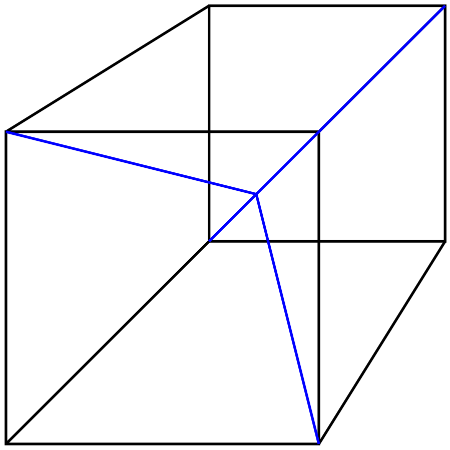


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

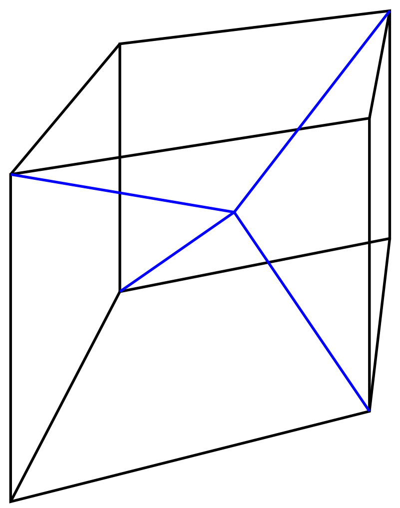


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

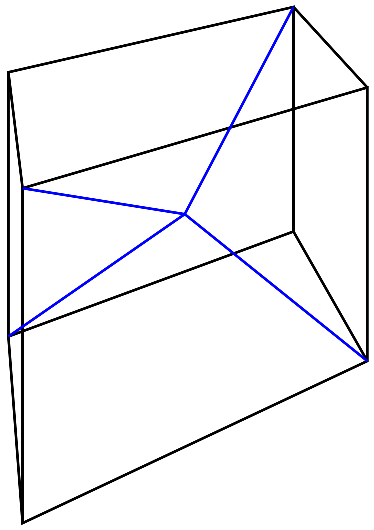


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

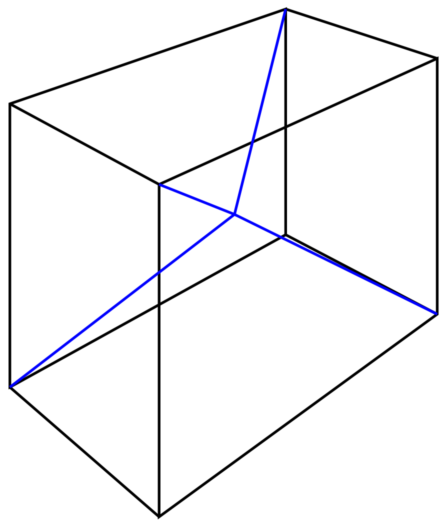


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

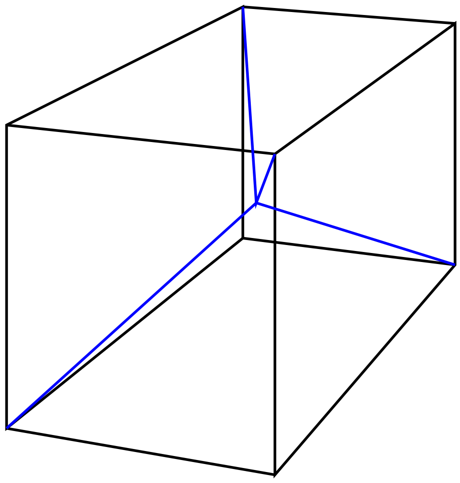


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

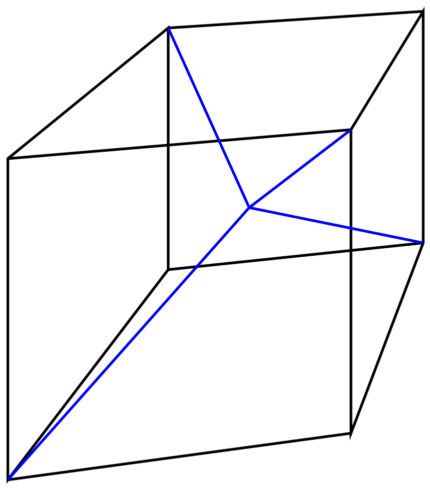


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

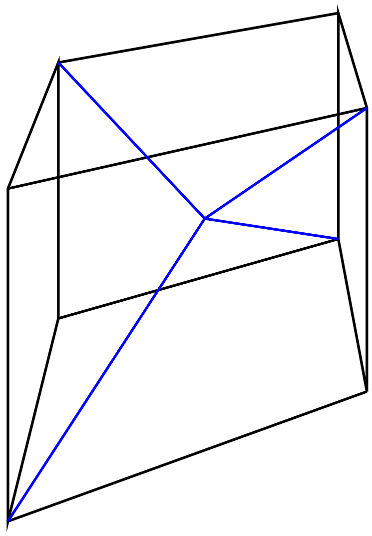


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

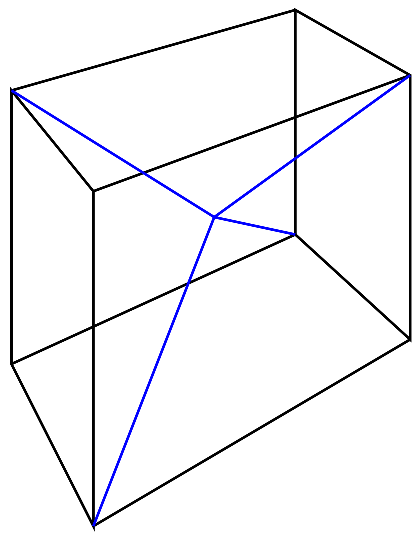


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

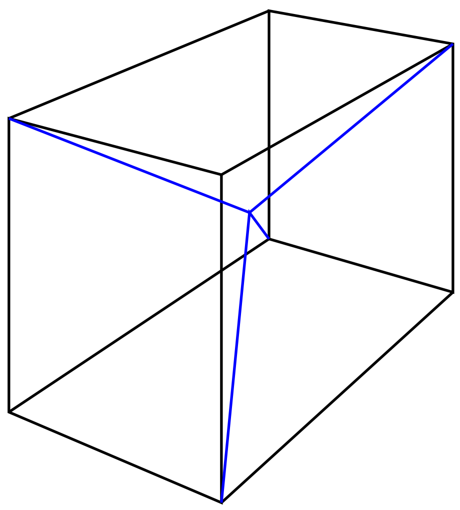


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

These blue lines are radii of the cube.

The tetrahedral arrangement of bonds can also be constructed by first considering a cube.

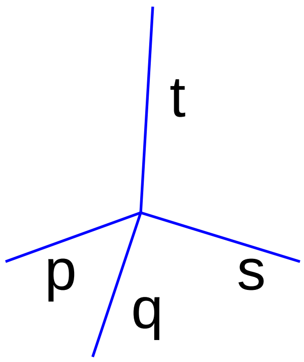


We can first construct two bonds by drawing lines from the center of the cube to two opposite corners of the top face, shown in blue.

We can construct the two remaining bonds by drawing lines from the center of the cube to two opposite corners of the bottom face such that they are not in the same plane as the ones drawn to the top face, again shown in blue.

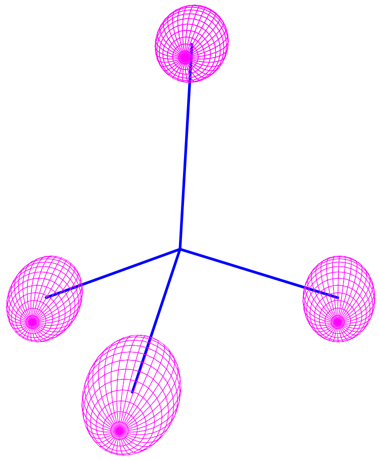
These blue lines are radii of the cube.

What is the angle between the bonds in this tetrahedral arrangement?
Let us label the bonds as vectors p, q, s, and t.



Since p, q, s, and t were represented as the radii of a tetrahedron and then the radii of a cube, we know that their vectors are all of equal length. Consequently, their vector sum is zero.
Then $(a+b+c+d) \cdot a = 0 \cdot a = 0$.
Using the equation $u \cdot v = ||u||\ ||v|| \cos(\theta)$,
$(a+b+c+d) \cdot a = a \cdot a + a \cdot b + a \cdot c + a \cdot d$
$= ||a||\ ||a|| \cos 0 + ||a||\ ||b|| \cos(\theta)$
$+ ||a||\ ||c|| \cos(\theta) + ||a||\ ||d|| \cos(\theta)$
$= L^2 + 3(L^2)\cos(\theta)$ if we let L be the length of each of the vectors.
Then $0 = L^2 + 3(L^2)\cos(\theta)$ gives $\cos(\theta) = -1/3$.
Therefore, the angle between the bonds is $\theta = 109.4712206$ degrees.

If we use pink spheres to represent carbon atoms and blue lines to represent bonds, a carbon atom bonded to four other carbon atoms would look like this:

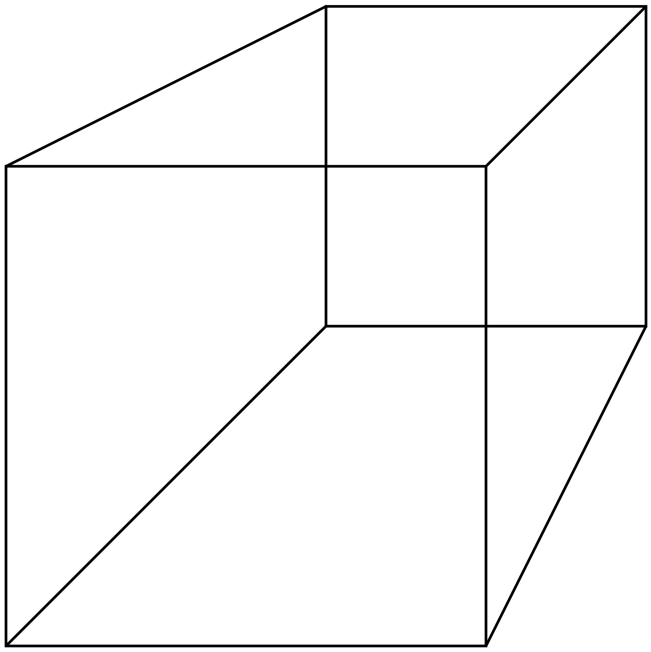


To investigate the crystal structures of diamond and graphite, we will begin by looking at the unit cells of each.

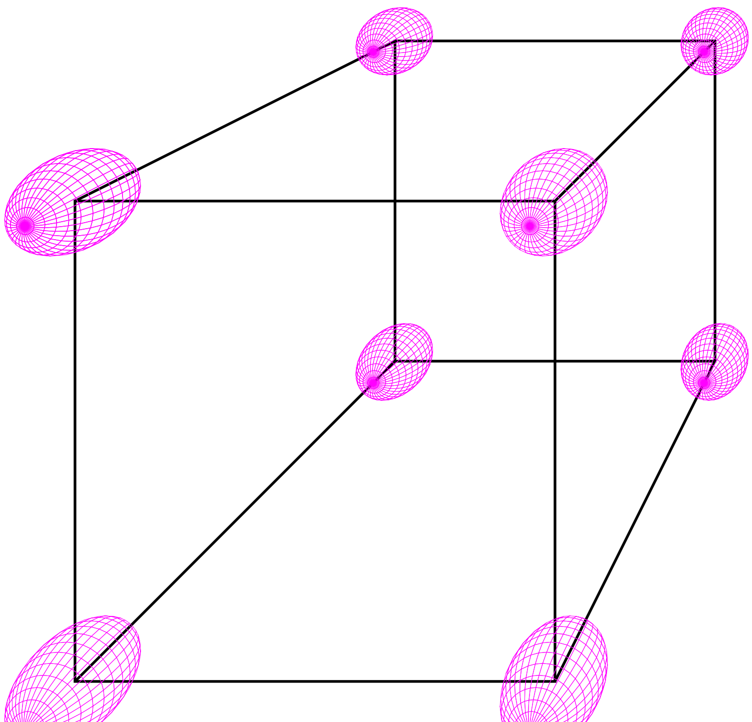
A unit cell is the simplest repeating unit in a crystal structure.

Let us construct the unit cell of the diamond crystal structure...

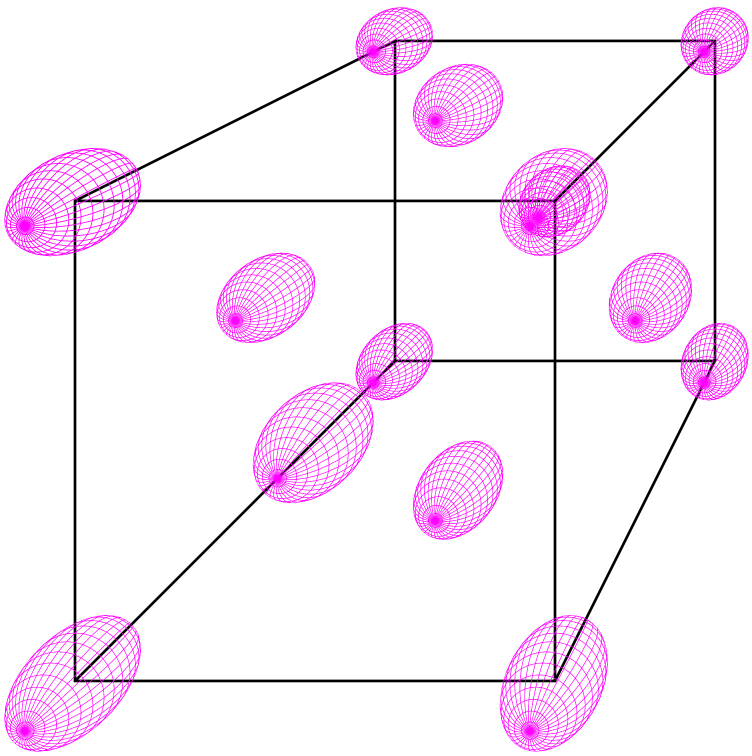
To construct the unit cell of the diamond crystal structure, first construct a cube.



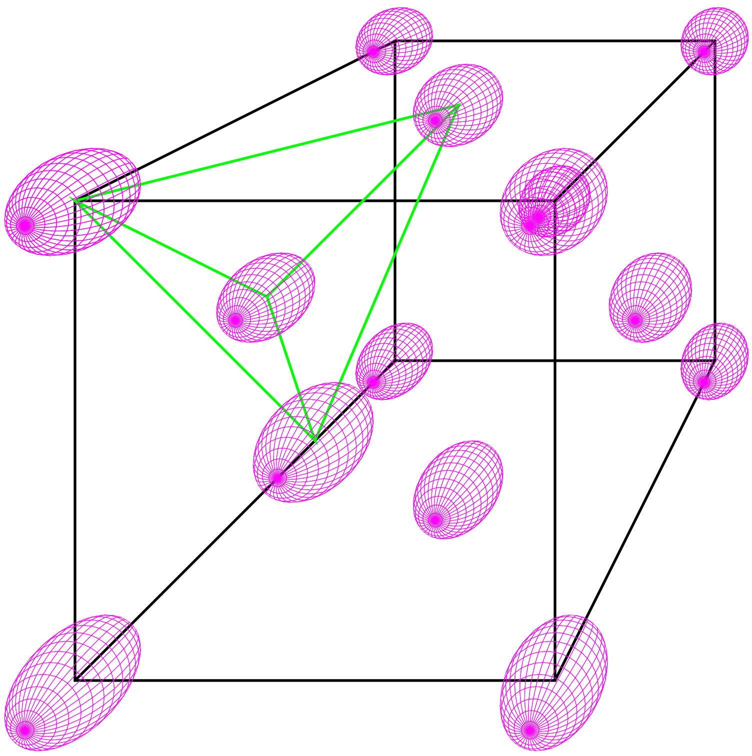
Then place carbon atoms at the corners of the cube, as shown by pink spheres.



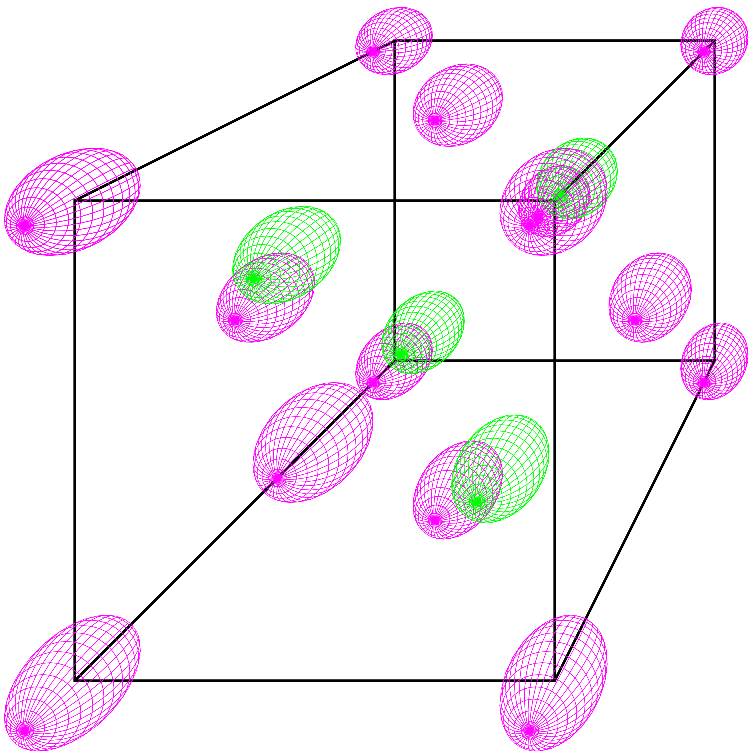
Next place carbon atoms at the center of each of the faces of the cube.



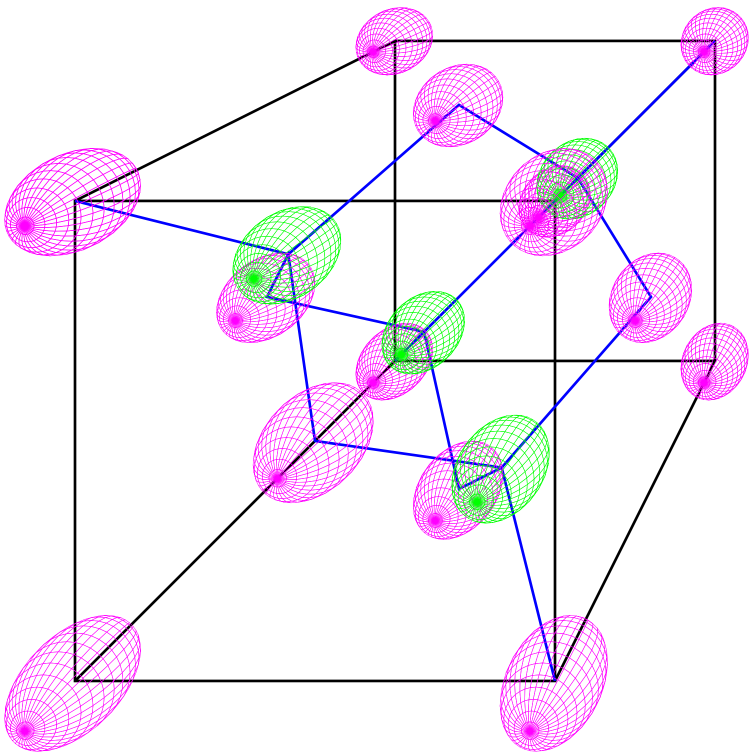
The center of the tetrahedrons formed by each corner atom and its three nearest face-centered neighbours is called a tetrahedral hole.
An example of one of these tetrahedrons is outlined in green.
There are eight tetrahedral holes in the unit cell, one for each corner.



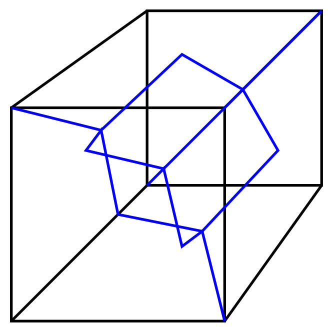
To complete the construction of the diamond crystal unit cell, place carbon atoms in four of the tetrahedral holes, as shown in green for clarity in the image below.



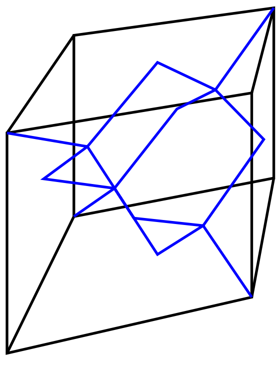
The blue lines show the bonding that occurs between carbon atoms in the diamond crystal structure. Each carbon atom is connected to four other carbon atoms, and the bonds adopt the tetrahedral arrangement.



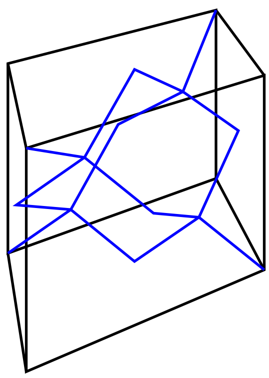
Let us look at the bonds and the boundaries of the unit cell.



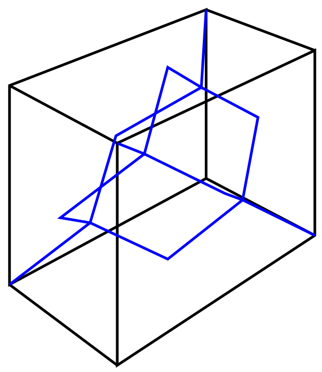
Let us look at the bonds and the boundaries of the unit cell.



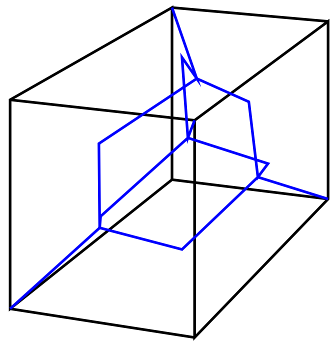
Let us look at the bonds and the boundaries of the unit cell.



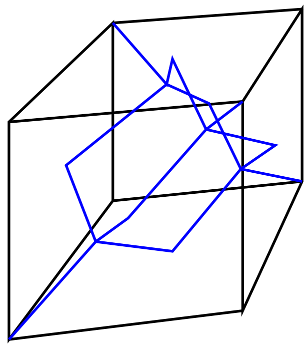
Let us look at the bonds and the boundaries of the unit cell.



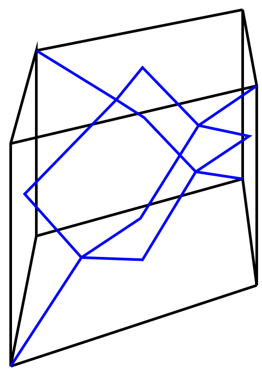
Let us look at the bonds and the boundaries of the unit cell.



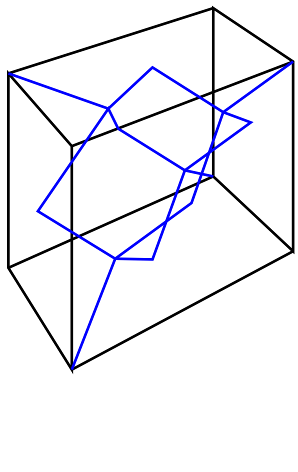
Let us look at the bonds and the boundaries of the unit cell.



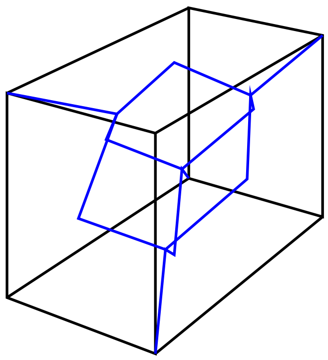
Let us look at the bonds and the boundaries of the unit cell.



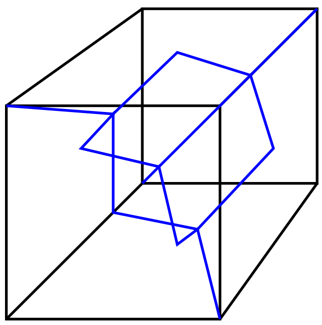
Let us look at the bonds and the boundaries of the unit cell.



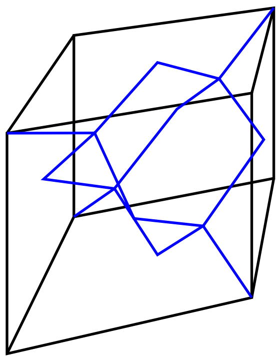
Let us look at the bonds and the boundaries of the unit cell.



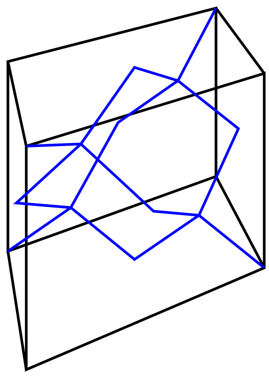
Let us look at the bonds and the boundaries of the unit cell.



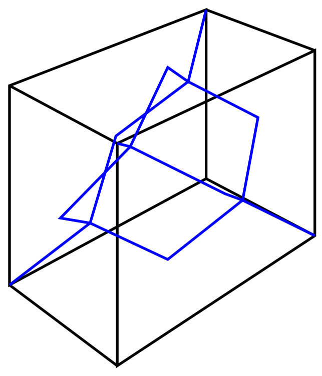
Let us look at the bonds and the boundaries of the unit cell.



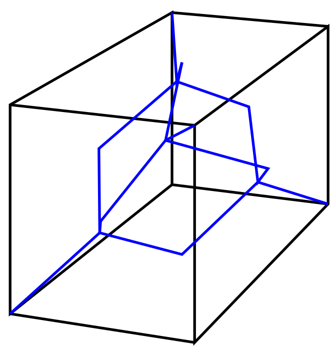
Let us look at the bonds and the boundaries of the unit cell.



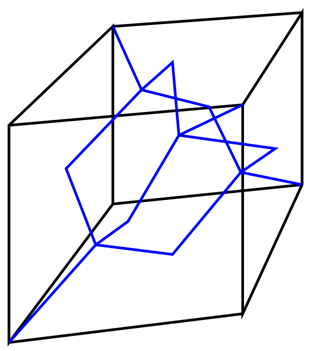
Let us look at the bonds and the boundaries of the unit cell.



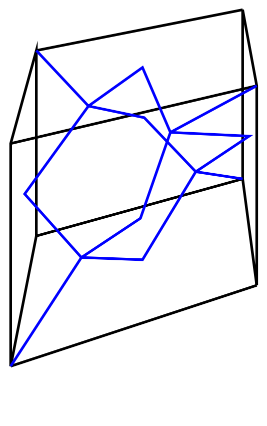
Let us look at the bonds and the boundaries of the unit cell.



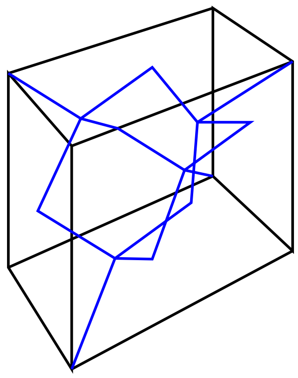
Let us look at the bonds and the boundaries of the unit cell.



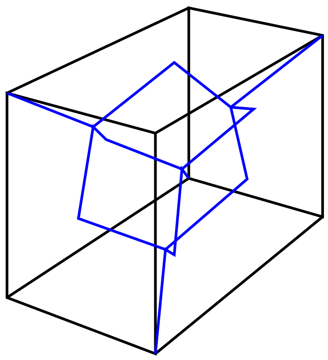
Let us look at the bonds and the boundaries of the unit cell.



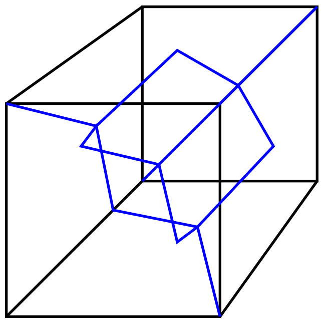
Let us look at the bonds and the boundaries
of the unit cell.



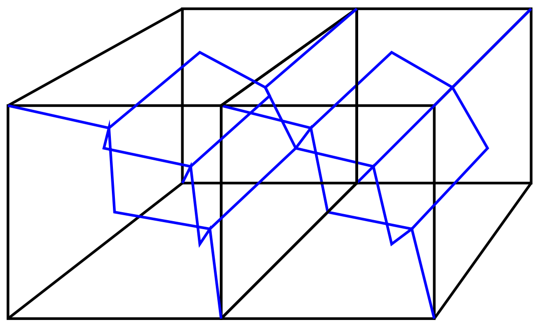
Let us look at the bonds and the boundaries of the unit cell.



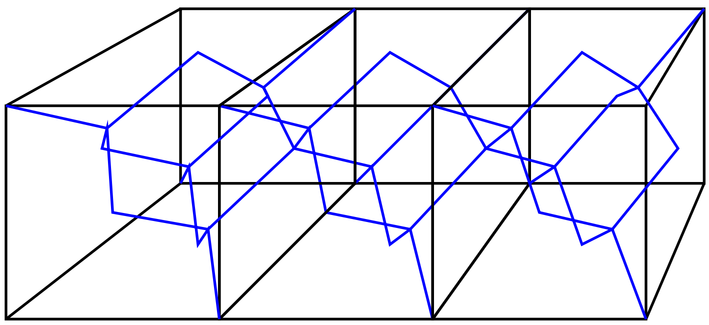
If we duplicate this in different directions...



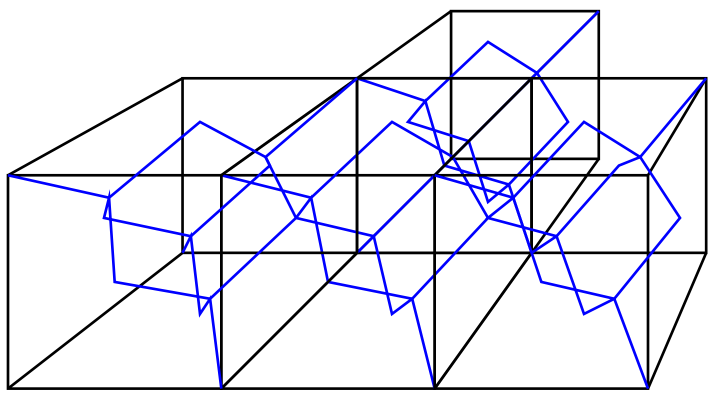
If we duplicate this in different directions...



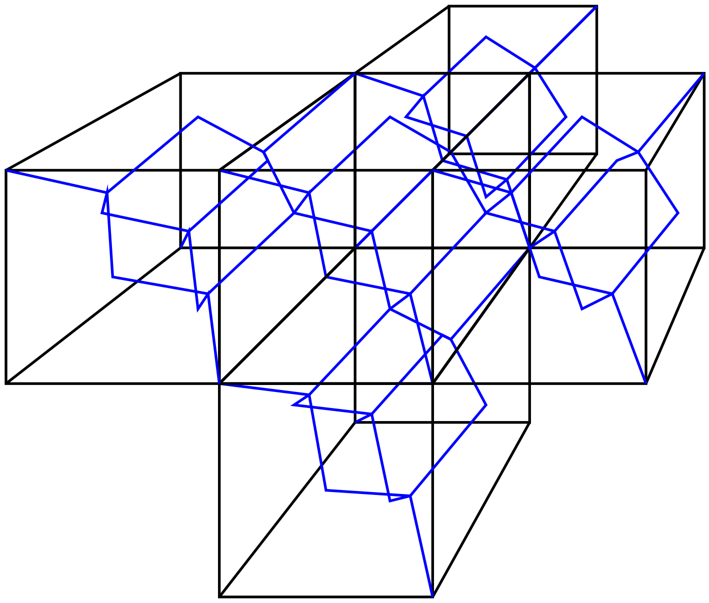
If we duplicate this in different directions...



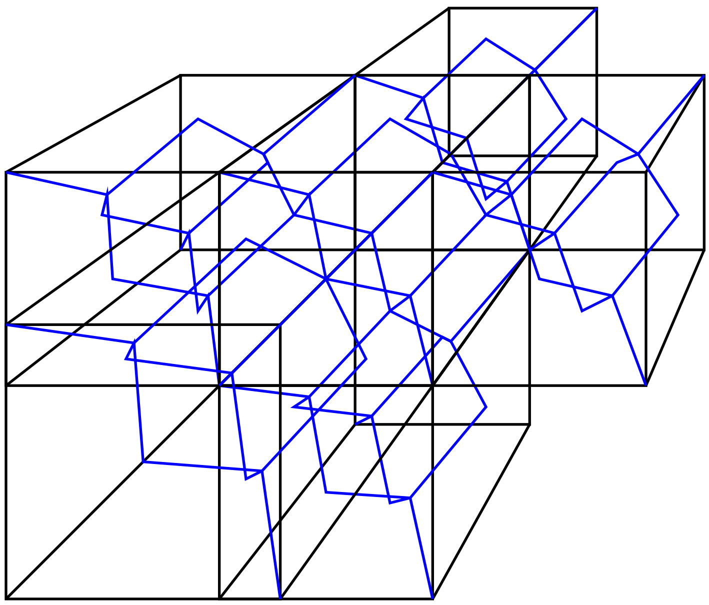
If we duplicate this in different directions...



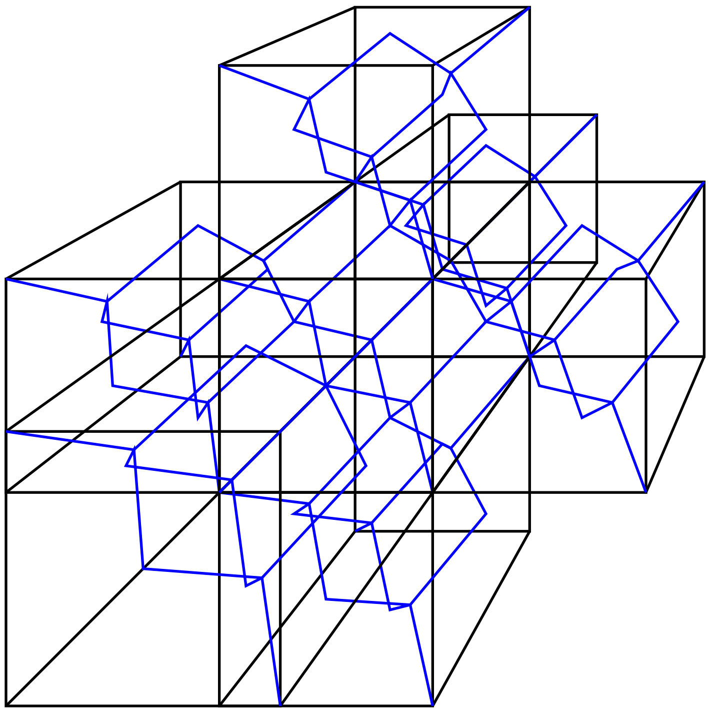
If we duplicate this in different directions...



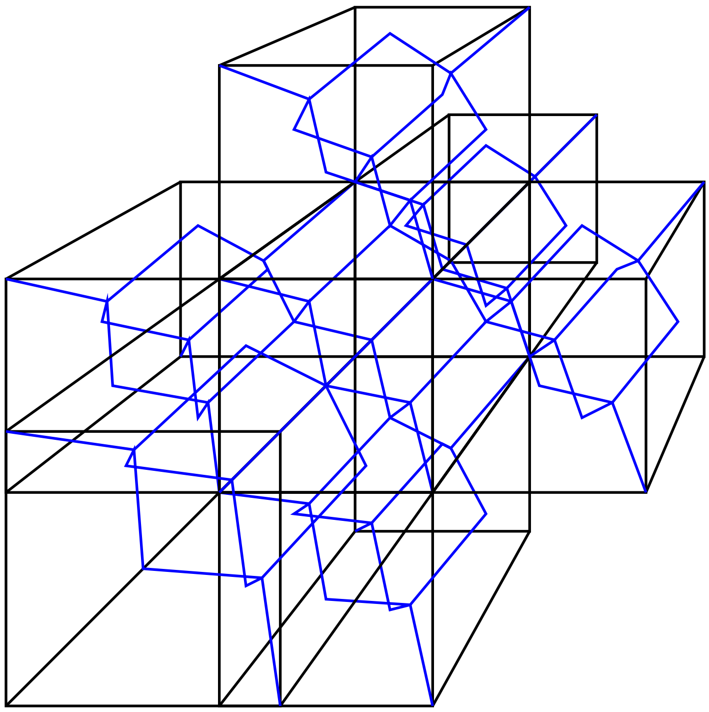
If we duplicate this in different directions...



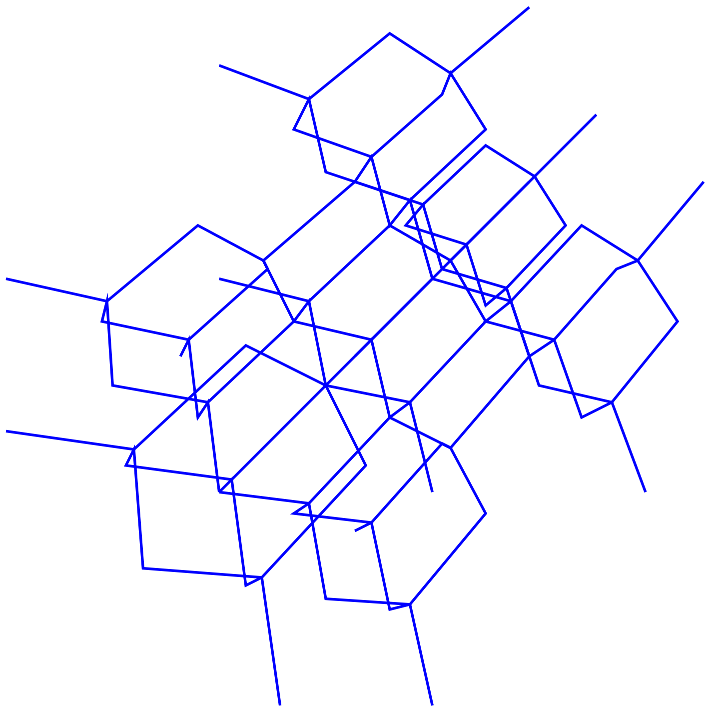
If we duplicate this in different directions...



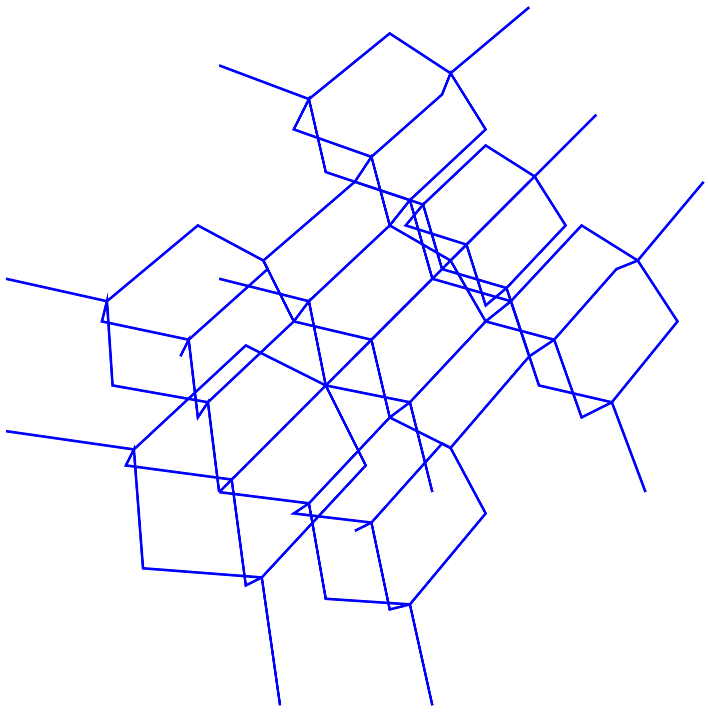
We begin to build the diamond crystal structure.



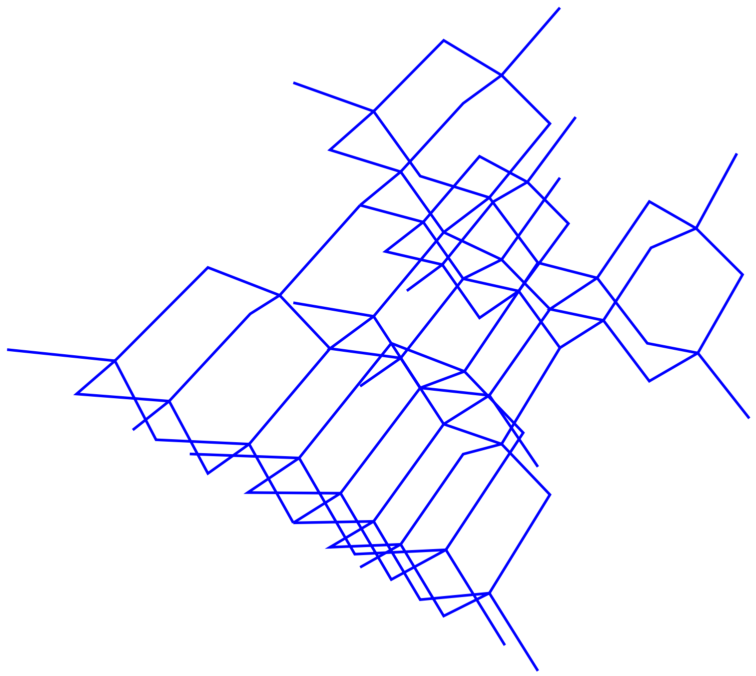
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



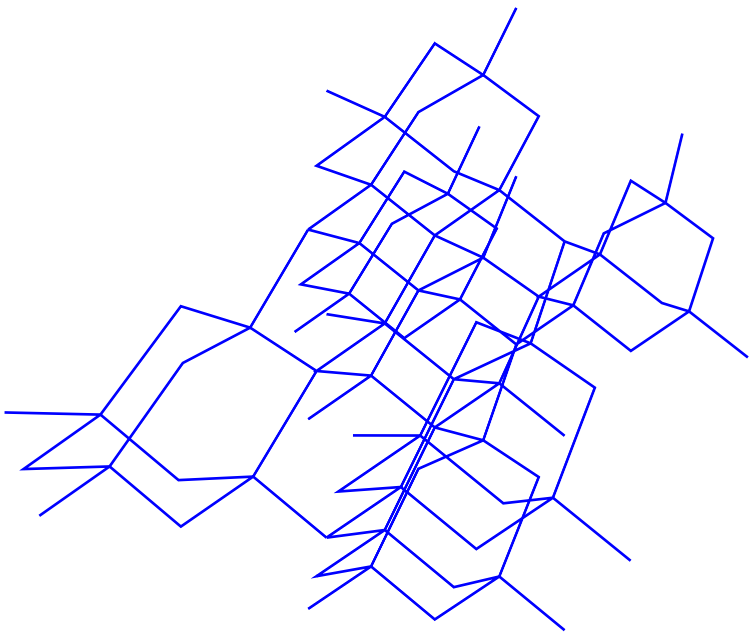
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



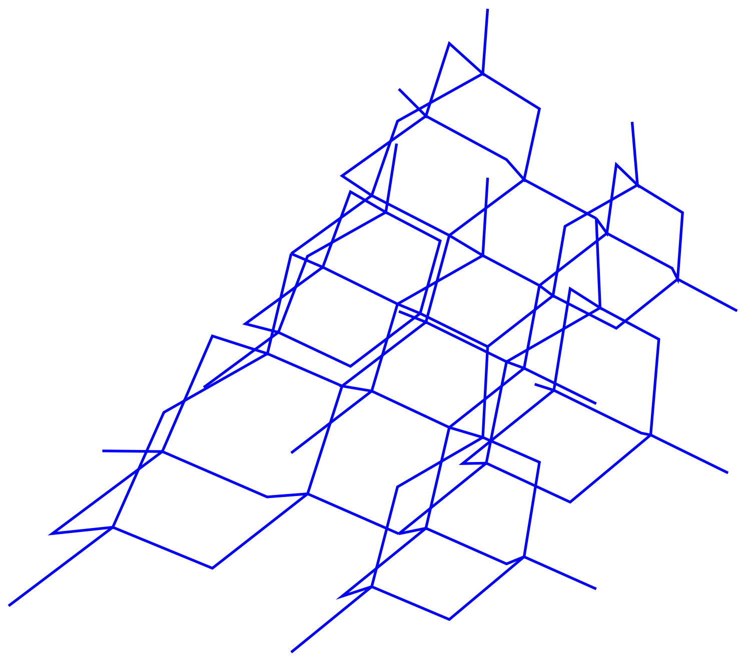
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



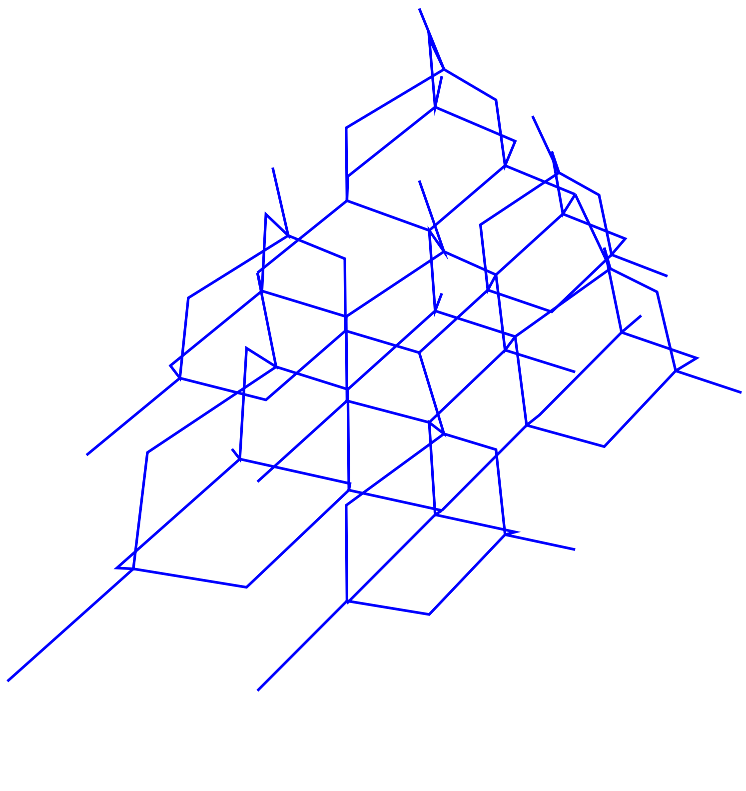
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



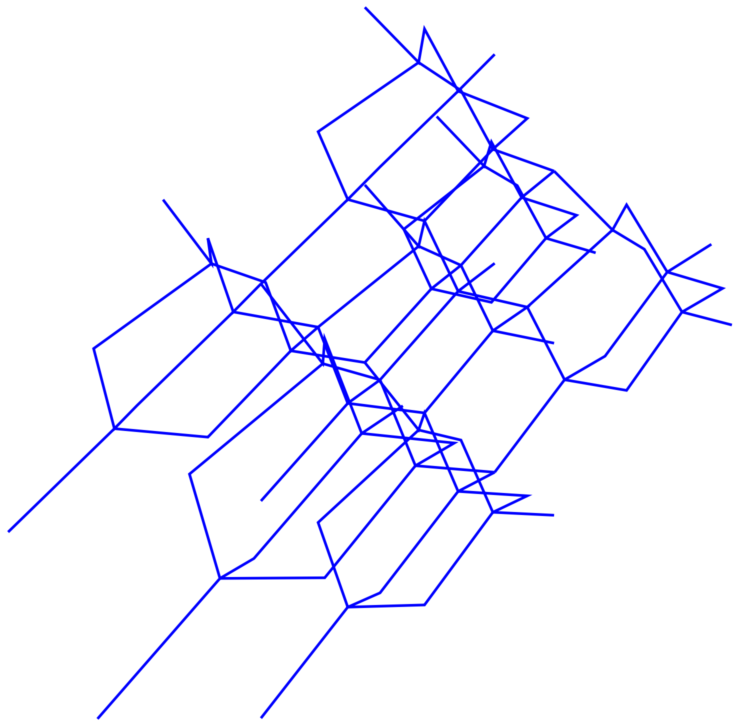
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



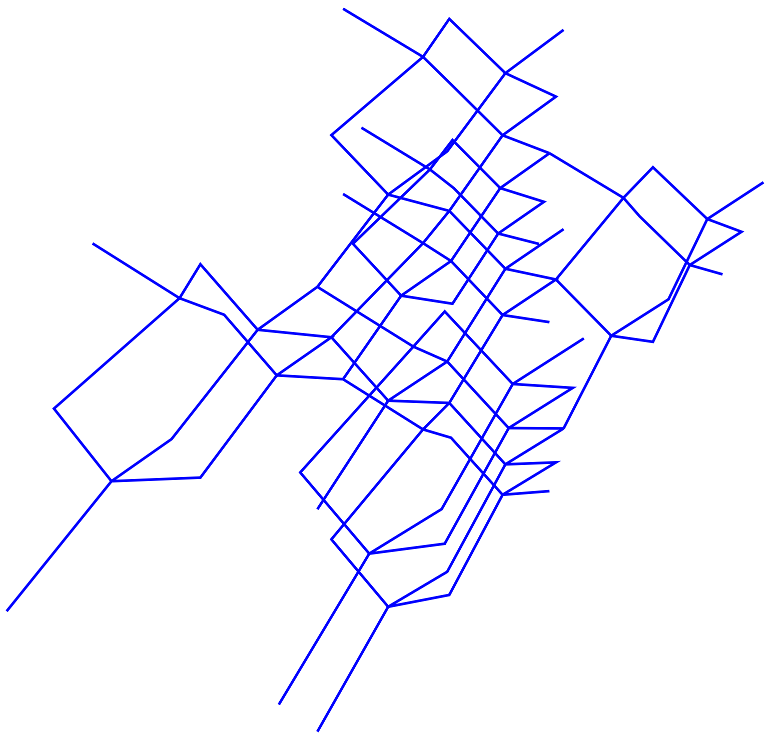
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



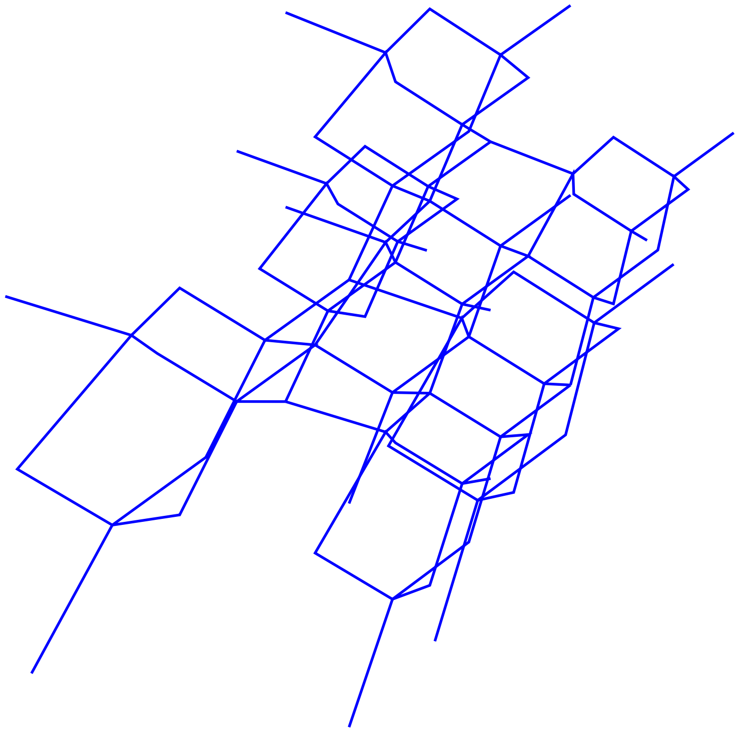
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



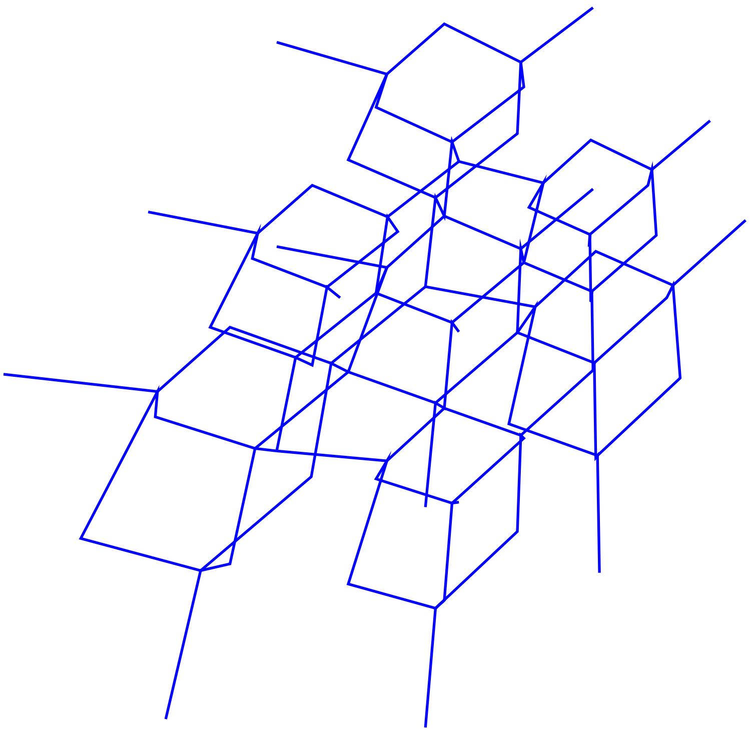
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



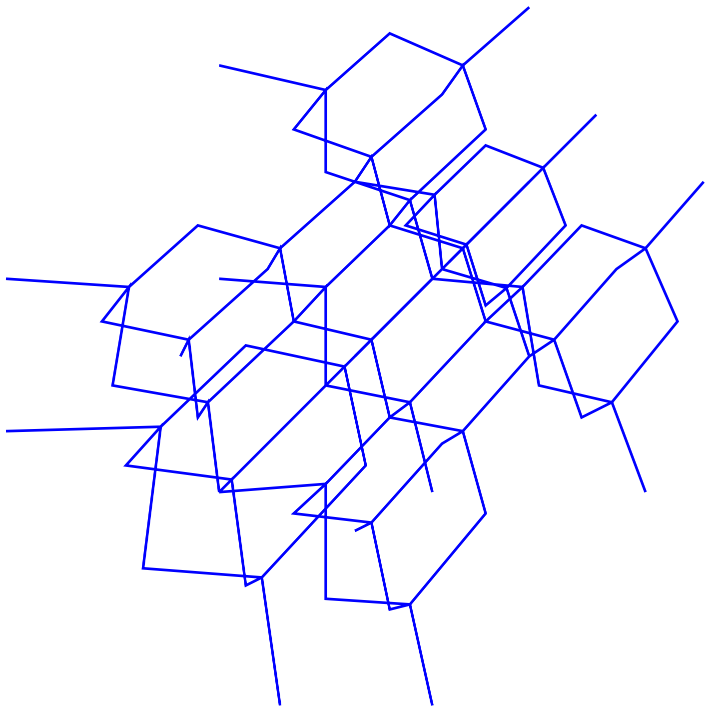
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



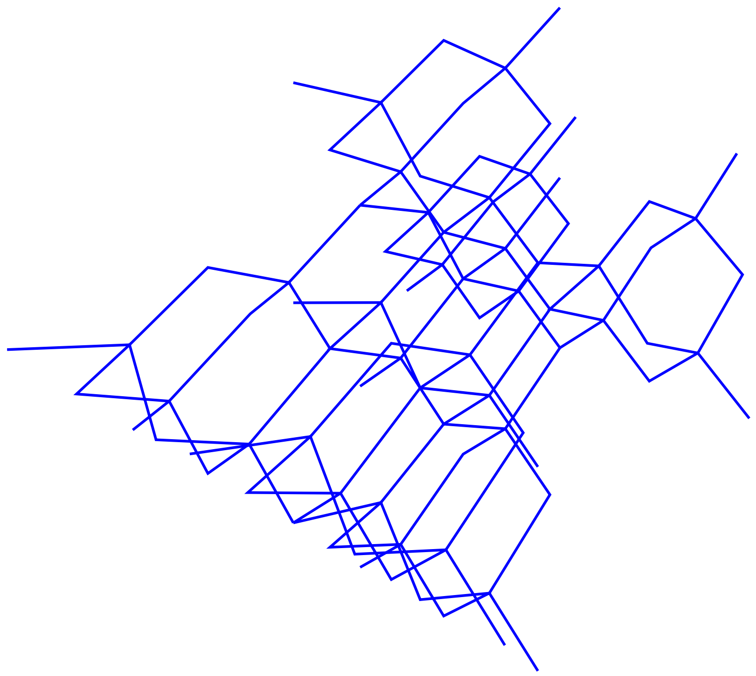
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



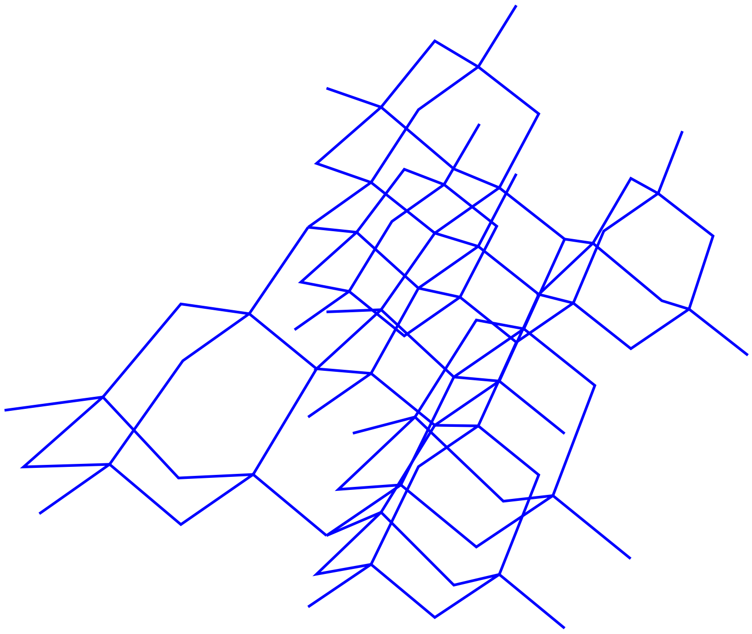
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



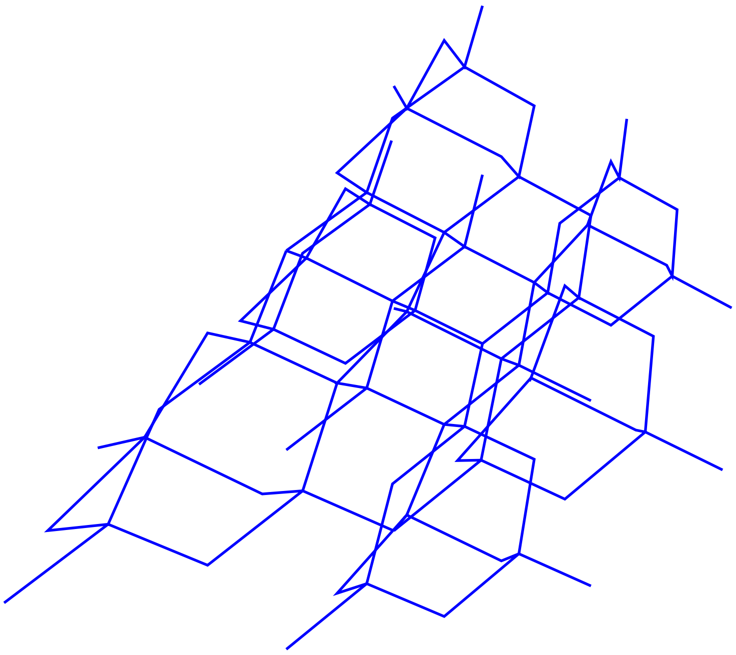
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



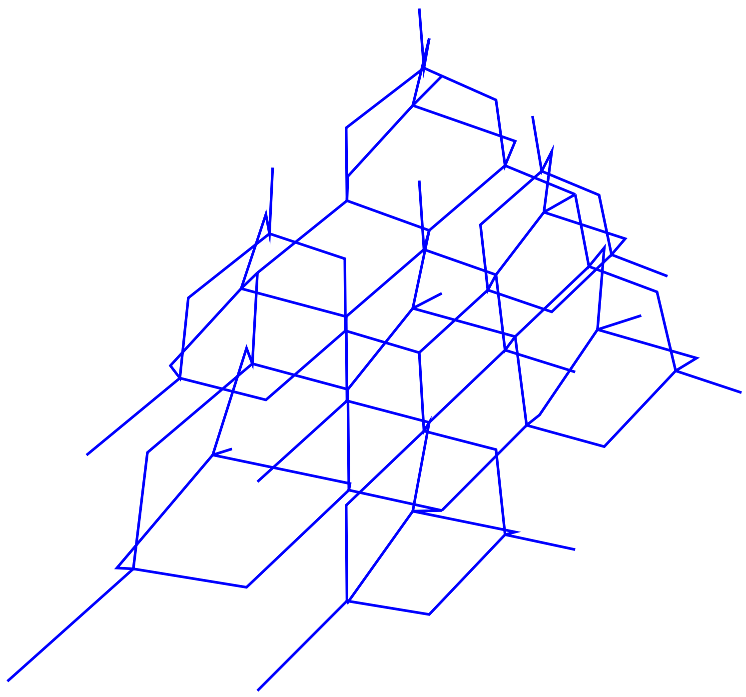
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



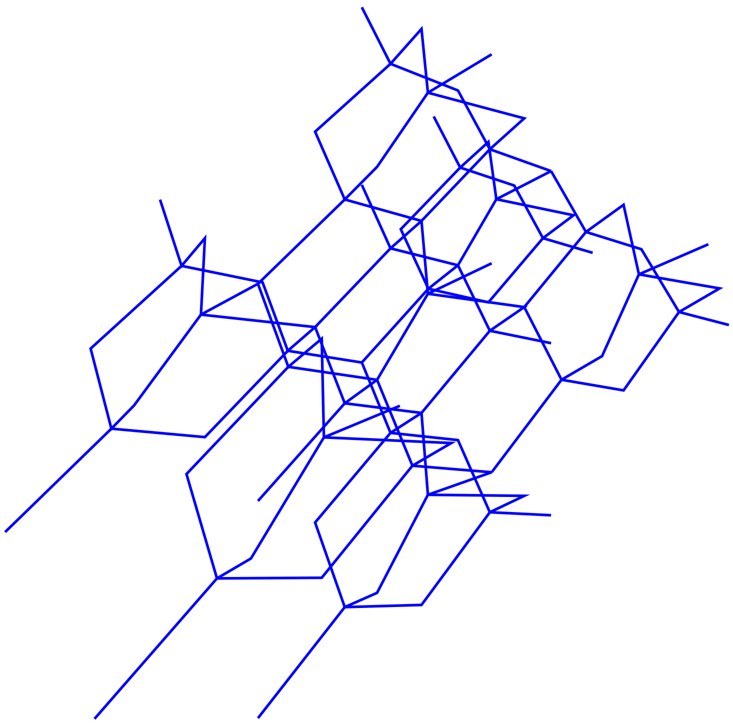
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



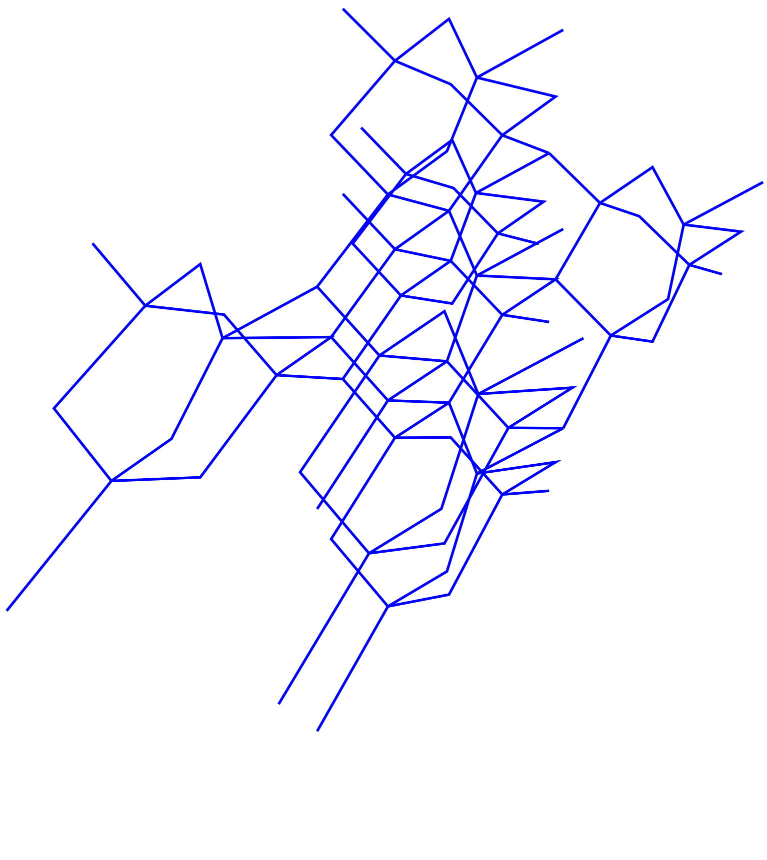
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



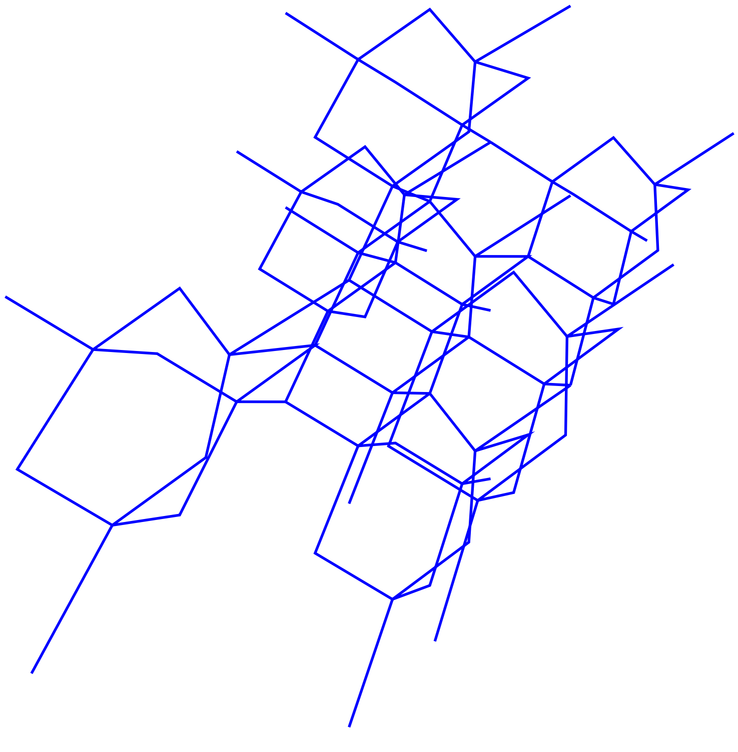
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



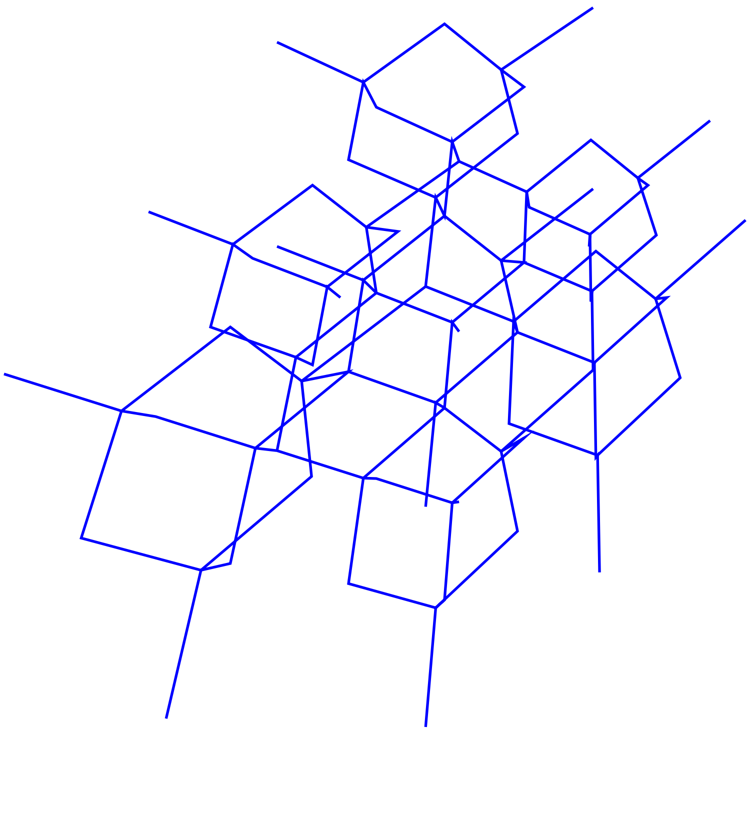
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



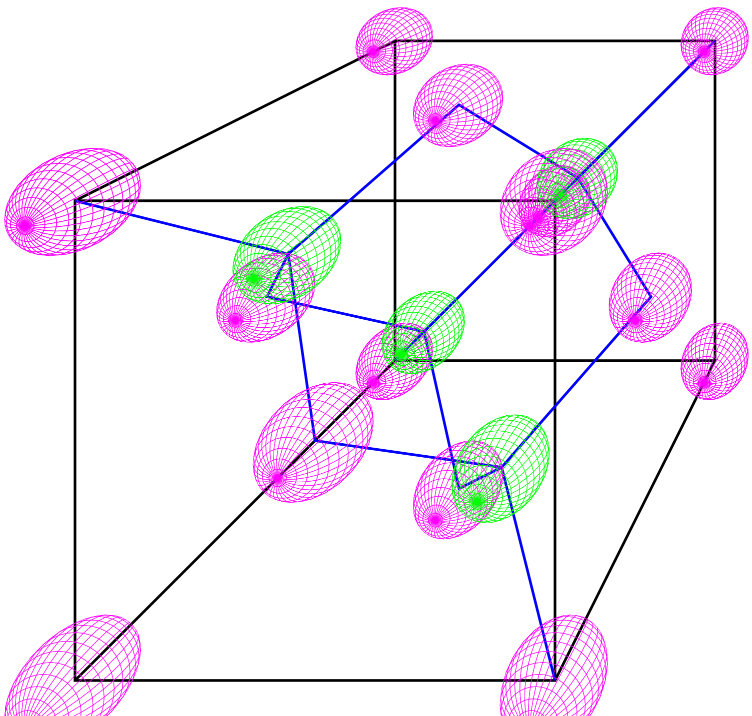
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



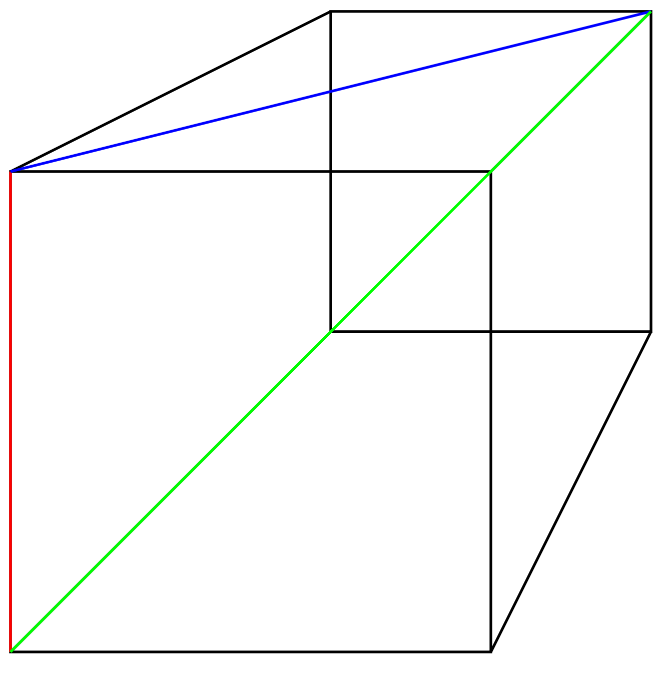
With the boundaries of the unit cell removed, the image below is a small representation of the diamond crystal structure. Carbon atoms sit where the blue bond lines meet.



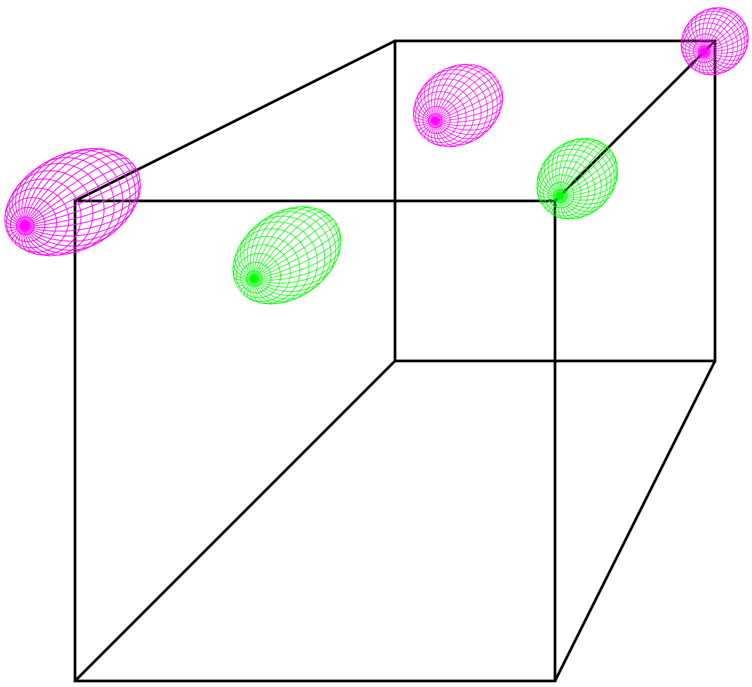
Let us take a look at the unit cell of the diamond crystal again.



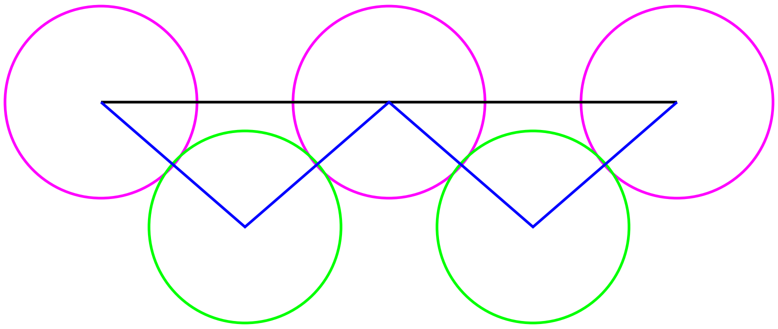
The red line is the edge of the unit cell with length e, the blue line is the face diagonal of the unit cell with length f, and the green line is the body diagonal of the unit cell with length b.



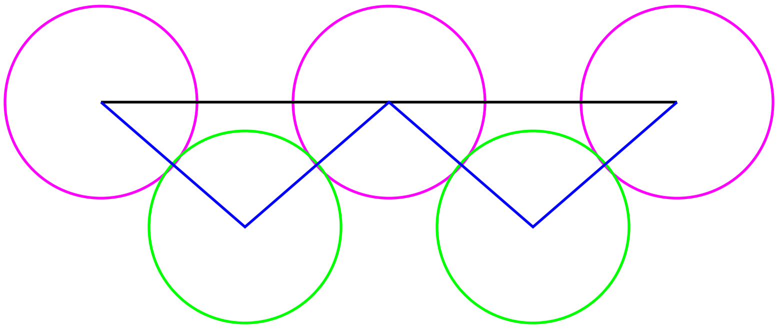
Let us look at a cross-section through the five atoms shown below in order to determine f.



When the carbon atoms in the diamond crystal structure are packed together as much as possible, the atoms we are considering, represented by spheres, actually touch each other. This is shown in the cross-section below.
The black line is the face diagonal of the unit cell.
The blue lines are the bonds between the carbon atoms.



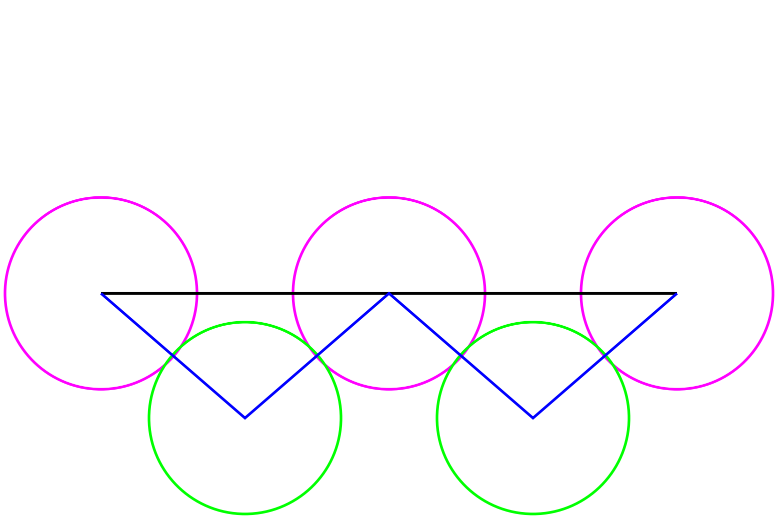
The manner in which carbon atoms form bonds with each other and the length of the bonds are different for different structural arrangements.
Let R represent the radius of a carbon atom when in the diamond crystal structure.
Then each blue bond line has a length of 2R.
Half of the length of the face diagonal is f/2.
The angle at the corner of each triangle below that is at the center of each green atom is 109.4712206 degrees, as we saw earlier, since the bonds are in a tetrahedral arrangement.
Cosine of this angle is -1/3.



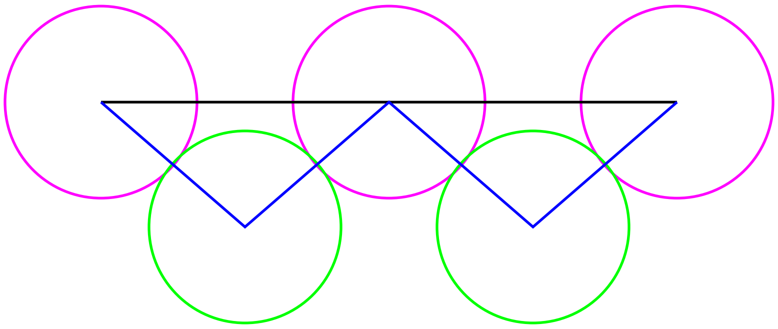
By the cosine rule,

$$(f/2)^2 = (2R)^2 + (2R)^2 - 2(2R)(2R)(-1/3)$$
$$= 4R^2 + 4R^2 - 8R^2(-1/3)$$
$$= 8R^2 + (8/3)R^2$$
$$= (32/3)R^2.$$

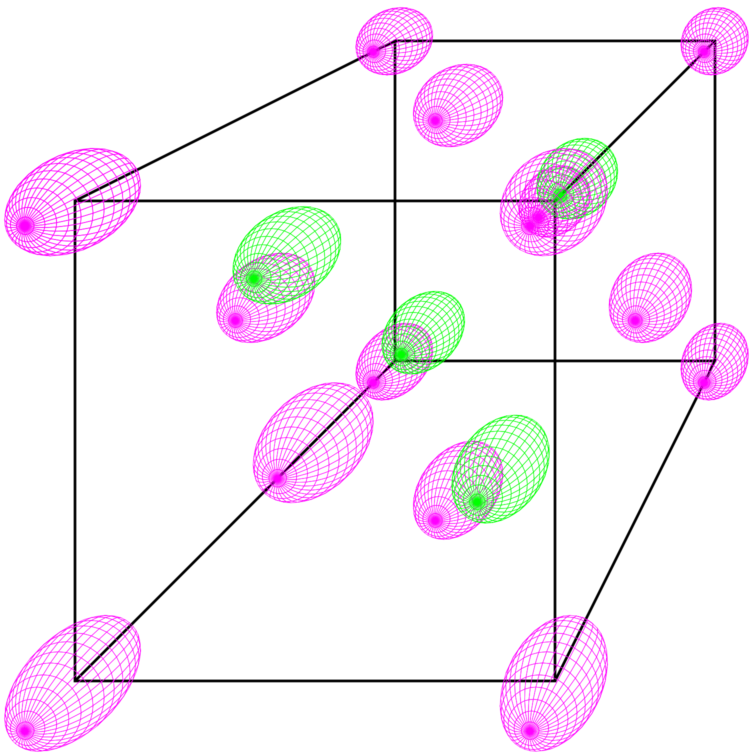
This gives $f/2 = \sqrt{32/3}R$ and $f = 8\sqrt{2/3}R$.



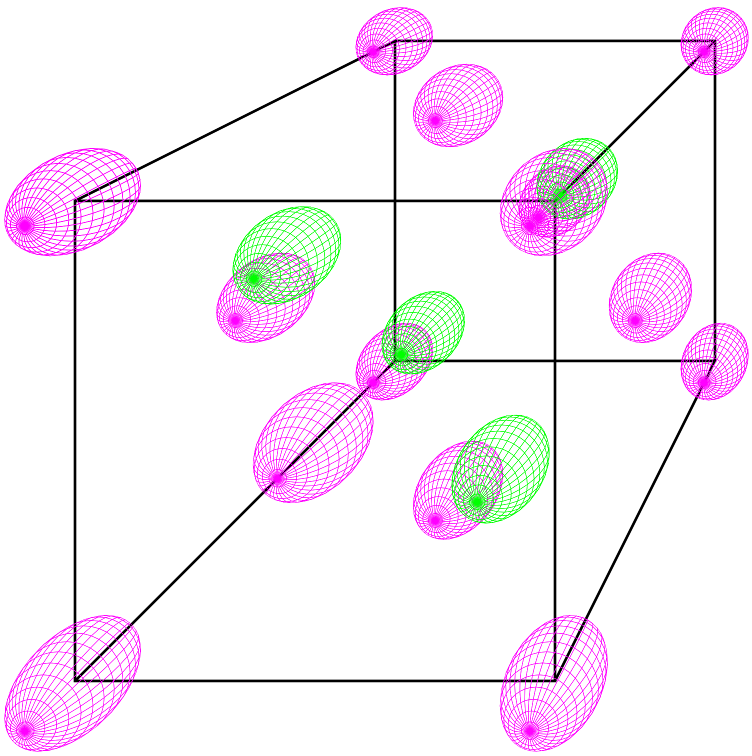
Recall that f is the length of the face diagonal of the unit cell and e is the length of the edge of the unit cell.
By Pythagoras, f^2 = e^2 + e^2 = 2e^2.
Since f = 8sqrt(2/3)R, this gives e = 8R/sqrt(3).



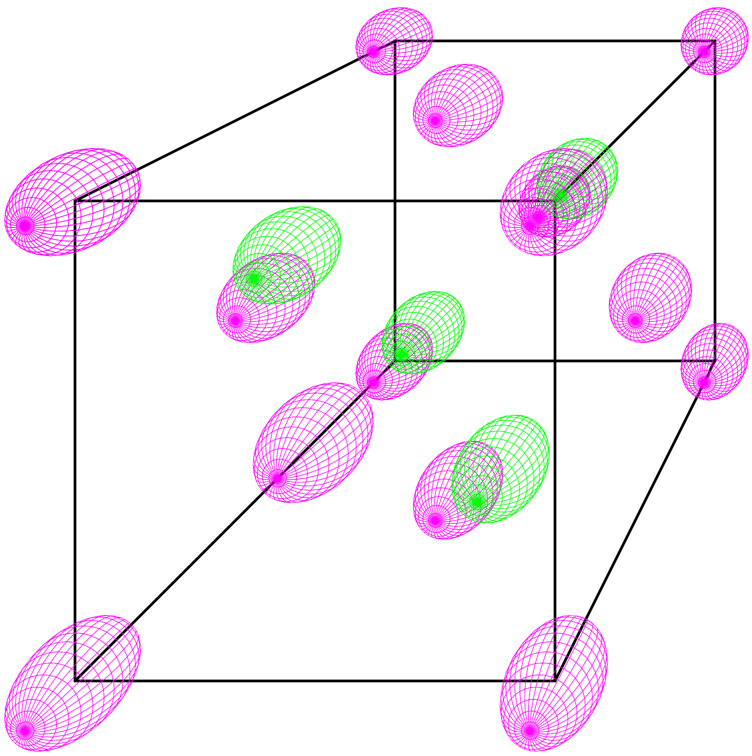
Let us determine the fraction of volume of the unit cell that is occupied by carbon atoms.
The volume of a cube is its width multiplied by its length multiplied by its depth, and we know $e = 8R/\sqrt{3}$ for the unit cell, therefore the volume of the unit cell is $e^3 = 98.53444594(R^3)$.



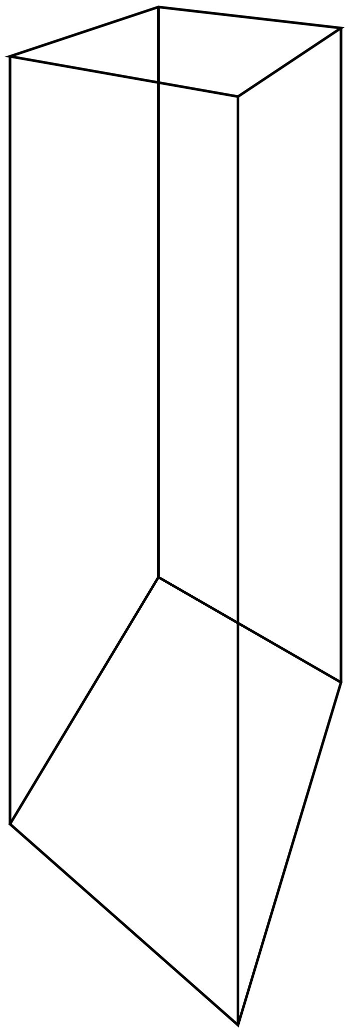
The volume of a carbon atom represented by a sphere is (4/3)(pi)R^3.
The diamond crystal unit cell contains the equivalent of 8 carbon atoms. Atoms in the eight corners of the unit cell provide (1/8)th of an atom each, atoms in the center of each of the six faces provide half of an atom each, and the atoms in the four tetrahedral holes provide 1 atom each.
Therefore, the volume of atoms in the unit cell is equal to (8)(4/3)(pi)R^3 = 33.51032164(R^3).



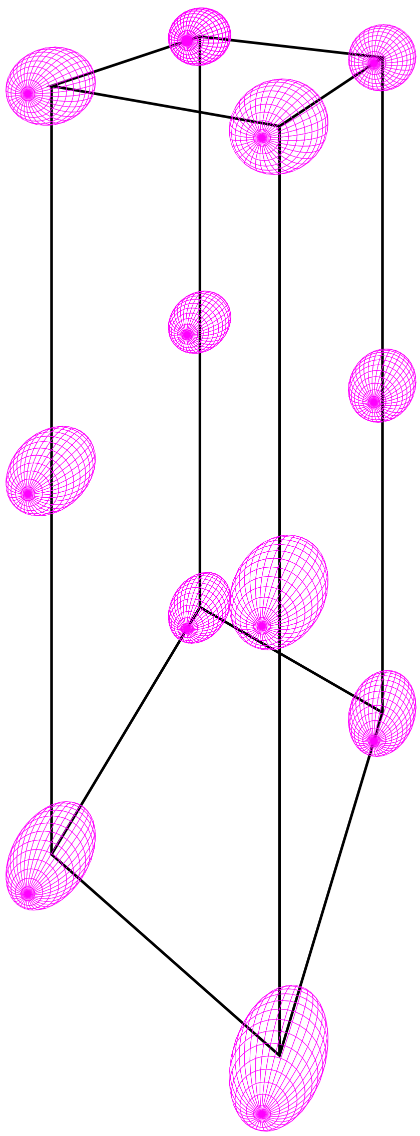
If we take the volume of carbon atoms in the unit cell and divide it by the volume of the unit cell, we obtain the fraction of volume of the unit cell occupied by carbon atoms to be 0.34.



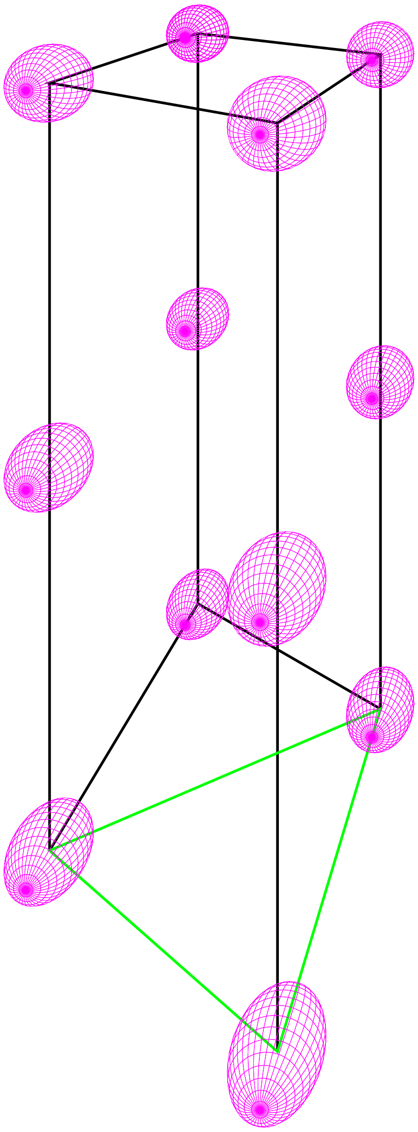
Let us now take a look at graphite.
To construct the unit cell of the graphite crystal structure, start with a parallelepiped that looks like the following:



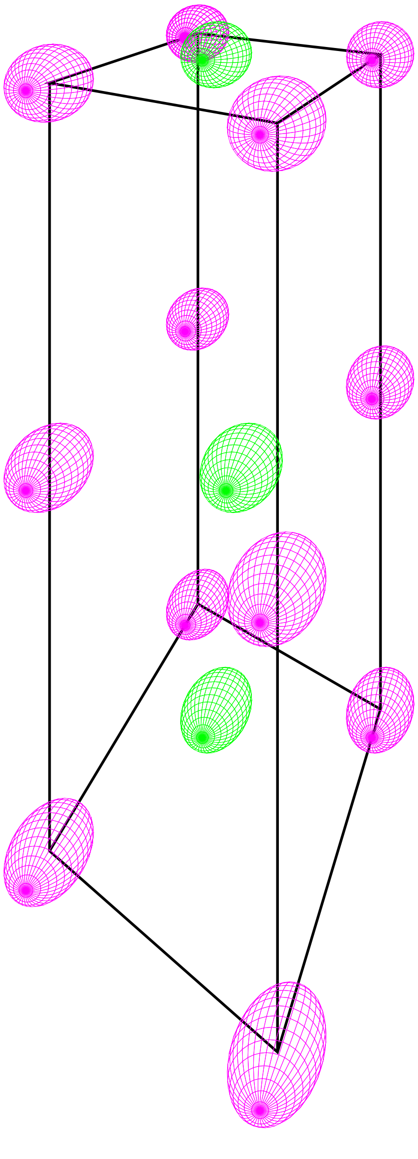
Place carbon atoms at the corners of the parallelepiped, as well as at the midpoints of the vertical edges.



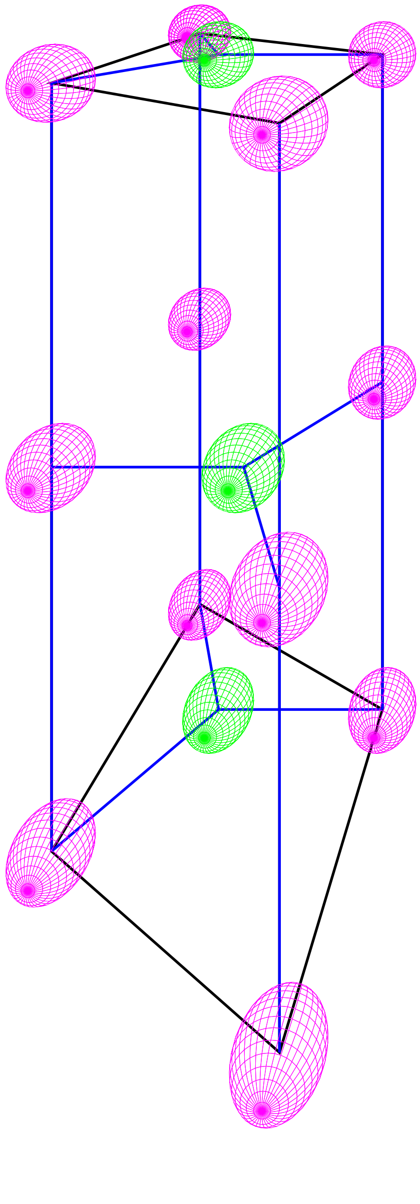
Each carbon atom on the back vertical edge and the front vertical edge of the unit cell with its two nearest neighbours form an equilateral triangle. An example of one of these equilateral triangles is outlined in green. There are six of these equilateral triangles in the unit cell, one for each carbon atom on the front and back vertical edges.



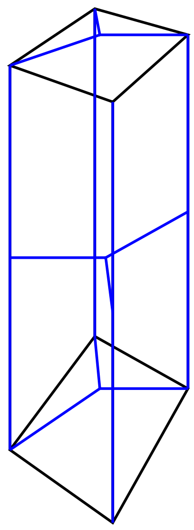
To complete the construction of the unit cell, place carbon atoms at the center of three of these equilateral triangles, as shown in green for clarity.



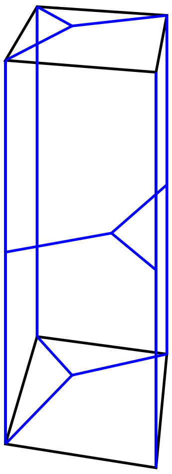
The bonding between carbon atoms that occurs in this graphite unit cell is shown in blue.



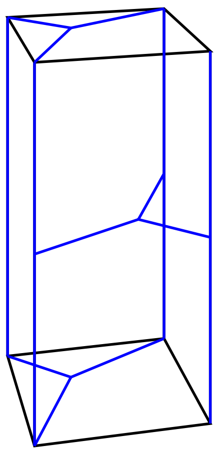
Let us now look at the bonds and the boundaries of the unit cell.



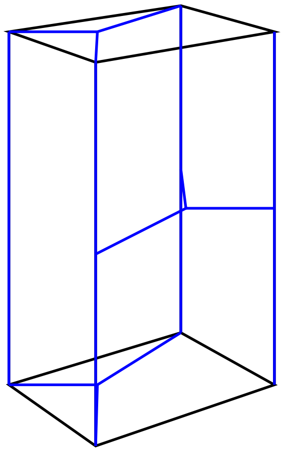
Let us now look at the bonds and the boundaries of the unit cell.



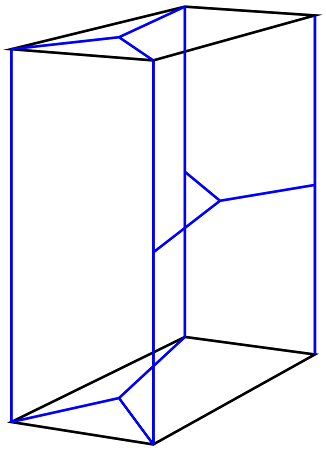
Let us now look at the bonds and the boundaries of the unit cell.



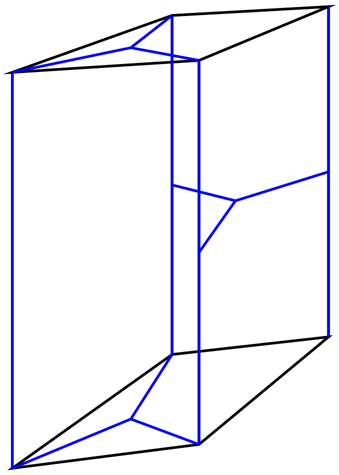
Let us now look at the bonds and the boundaries of the unit cell.



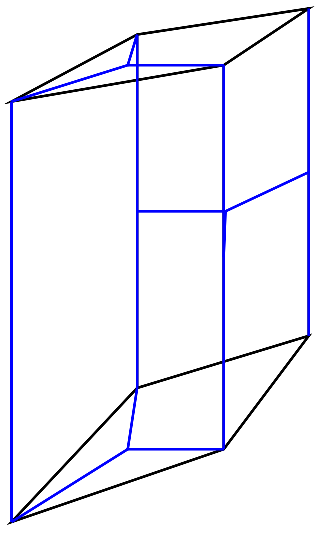
Let us now look at the bonds and the boundaries of the unit cell.



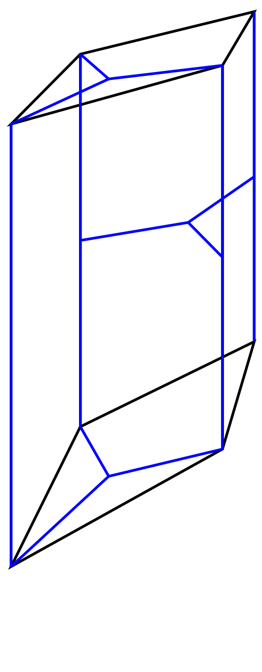
Let us now look at the bonds and the boundaries of the unit cell.



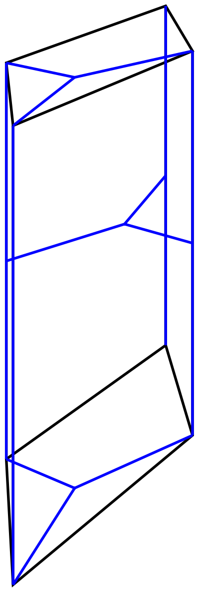
Let us now look at the bonds and the boundaries of the unit cell.



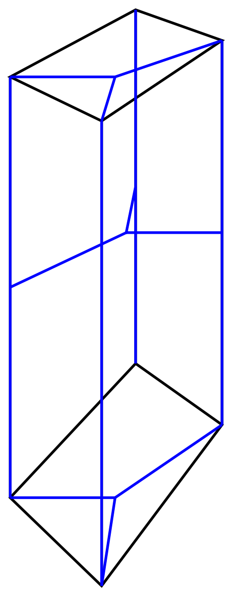
Let us now look at the bonds and the boundaries of the unit cell.



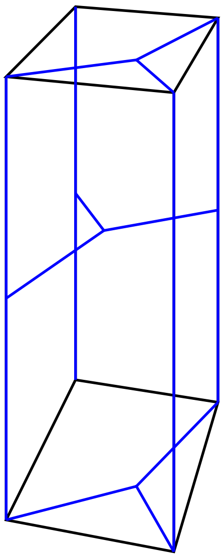
Let us now look at the bonds and the boundaries of the unit cell.



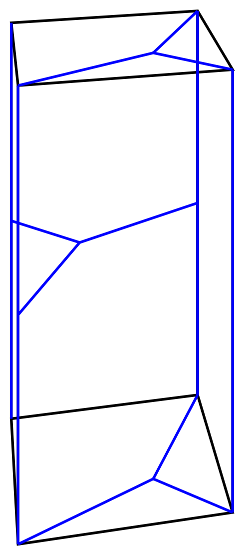
Let us now look at the bonds and the boundaries of the unit cell.



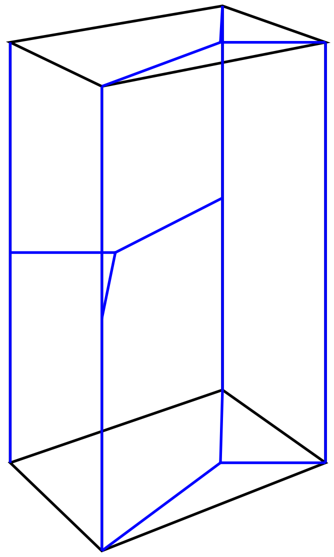
Let us now look at the bonds and the boundaries of the unit cell.



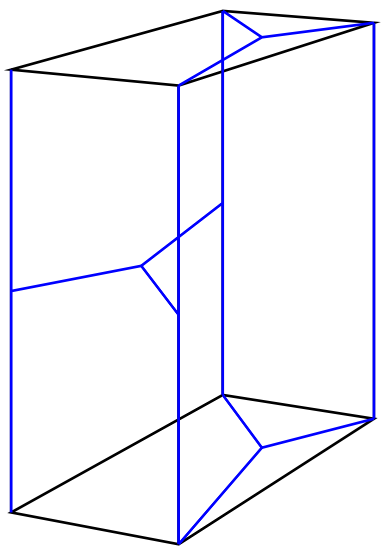
Let us now look at the bonds and the boundaries of the unit cell.



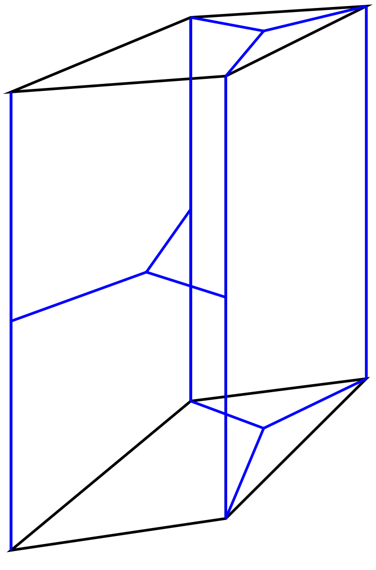
Let us now look at the bonds and the boundaries of the unit cell.



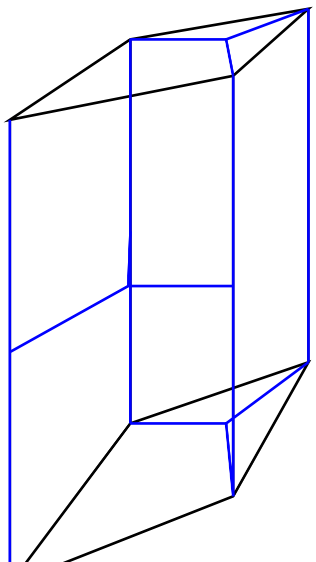
Let us now look at the bonds and the boundaries of the unit cell.



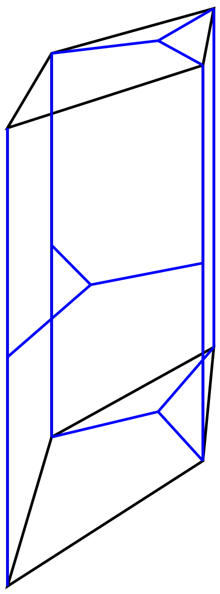
Let us now look at the bonds and the boundaries of the unit cell.



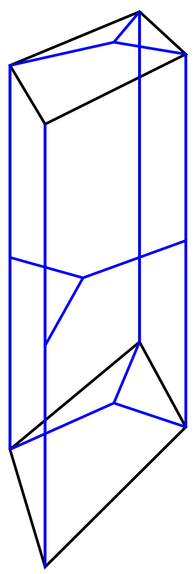
Let us now look at the bonds and the boundaries of the unit cell.



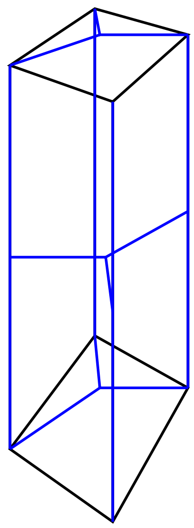
Let us now look at the bonds and the boundaries of the unit cell.



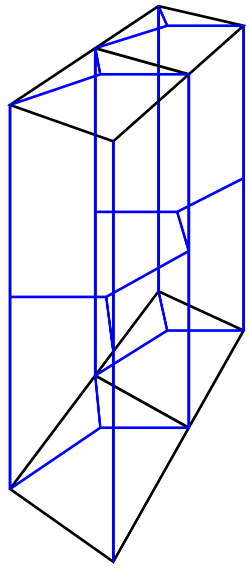
Let us now look at the bonds and the boundaries of the unit cell.



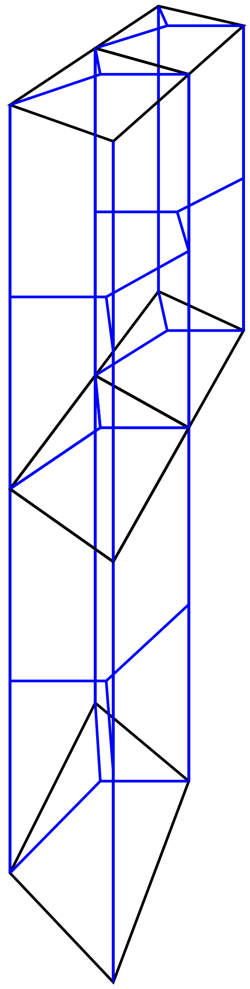
If we duplicate this in different directions...



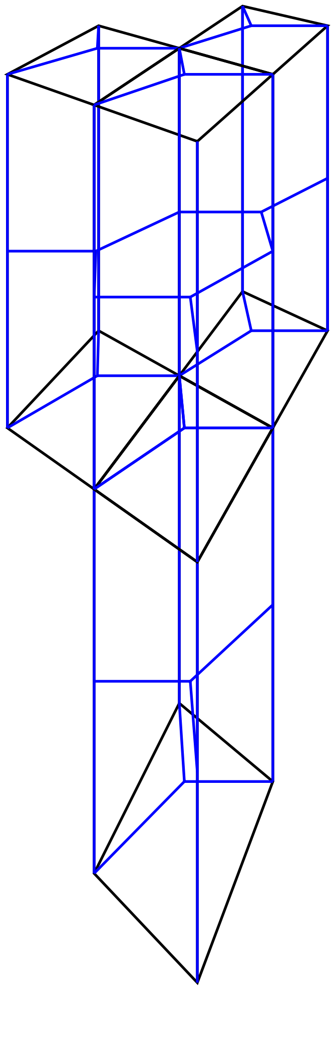
If we duplicate this in different directions...



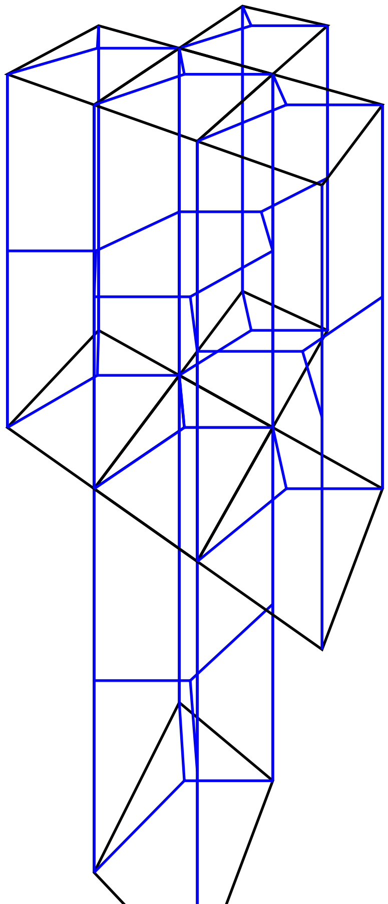
If we duplicate this in different directions...



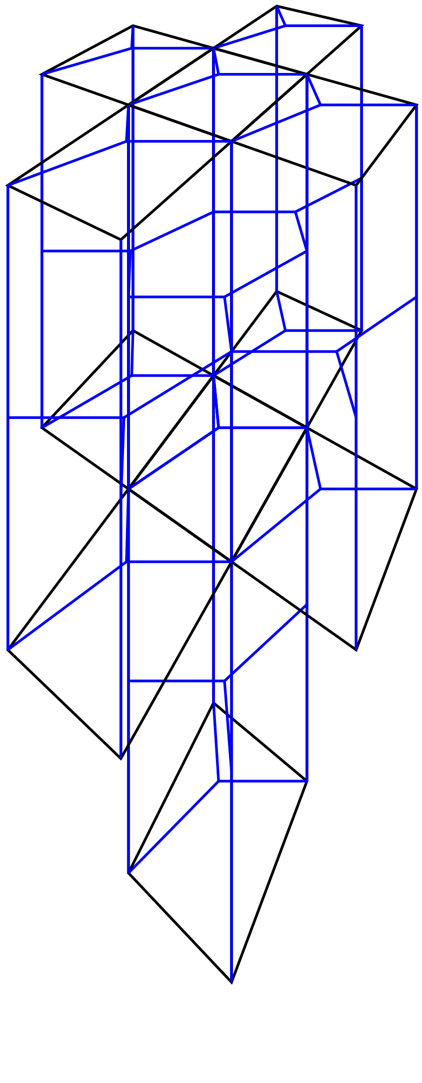
If we duplicate this in different directions...



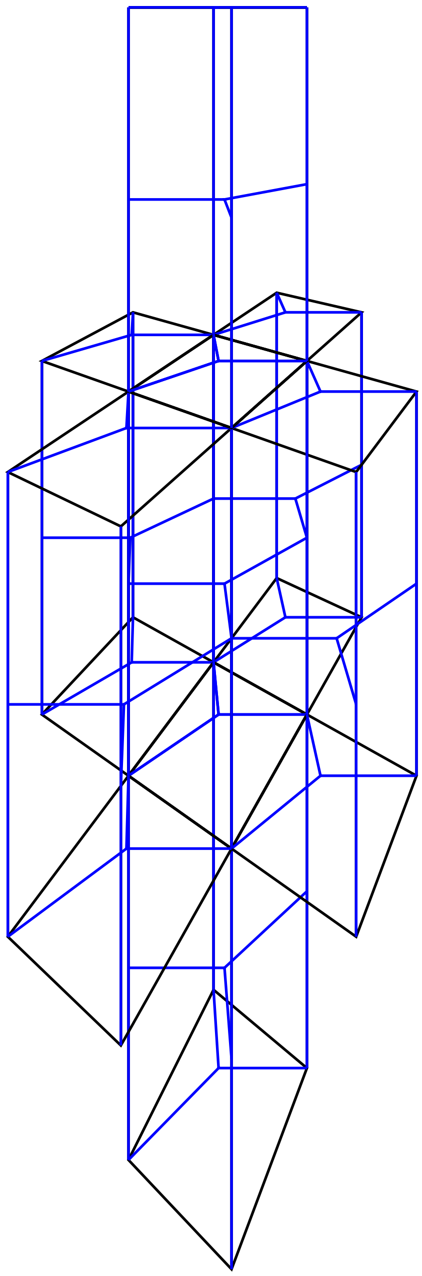
If we duplicate this in different directions...



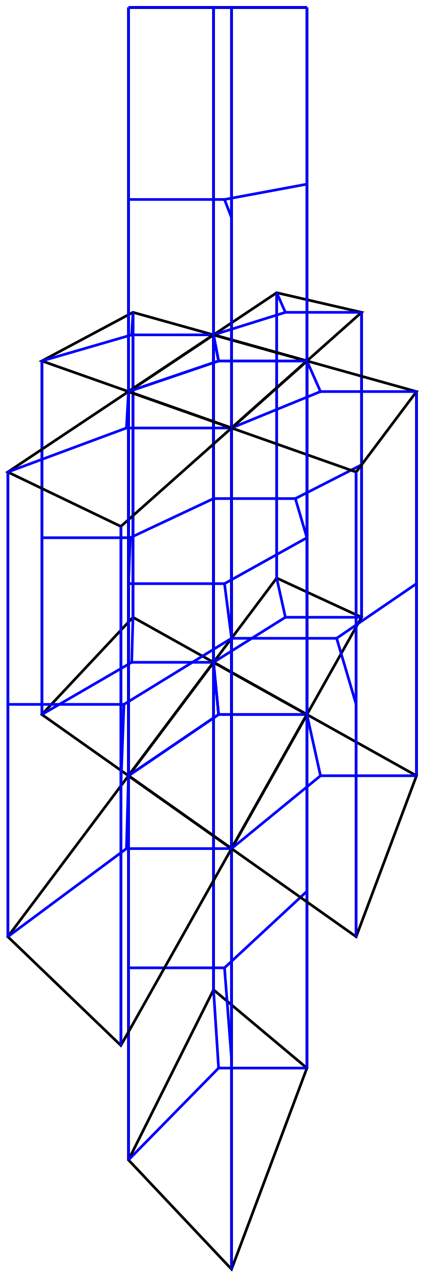
If we duplicate this in different directions...



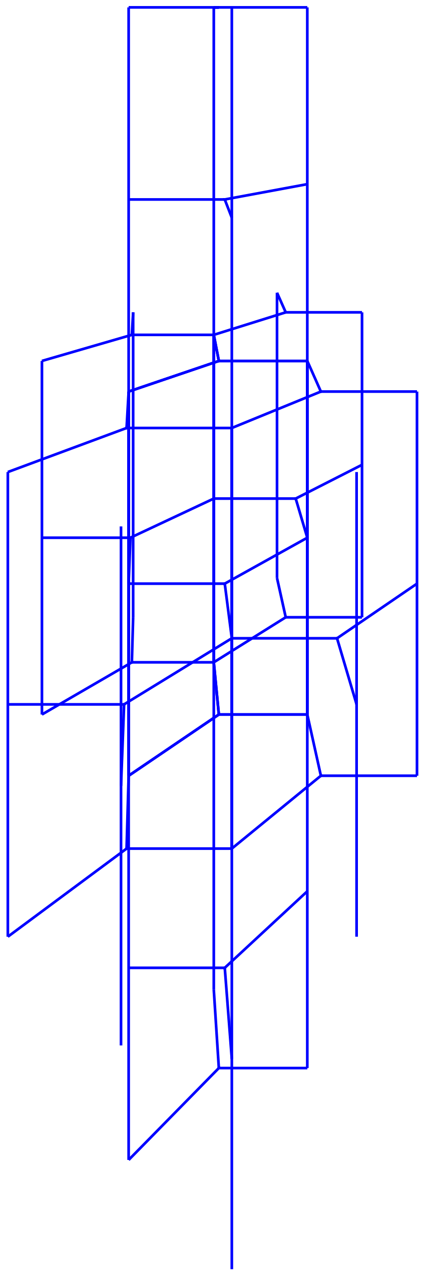
If we duplicate this in different directions...



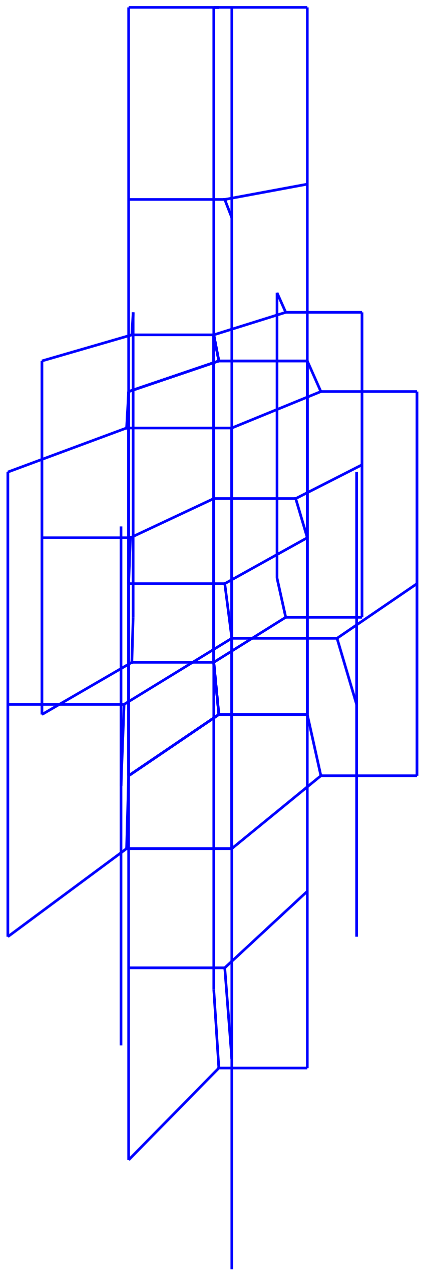
We begin to build the graphite crystal structure.



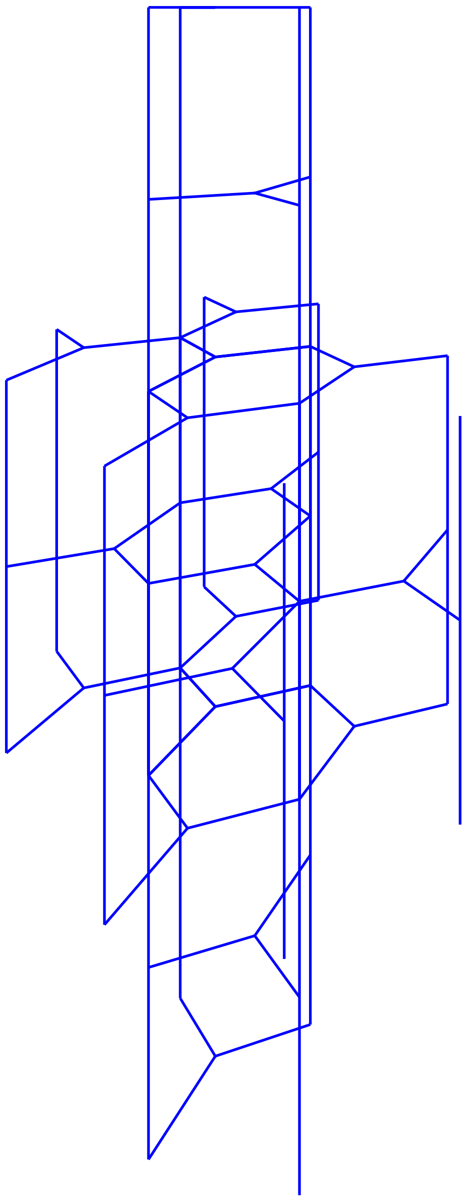
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



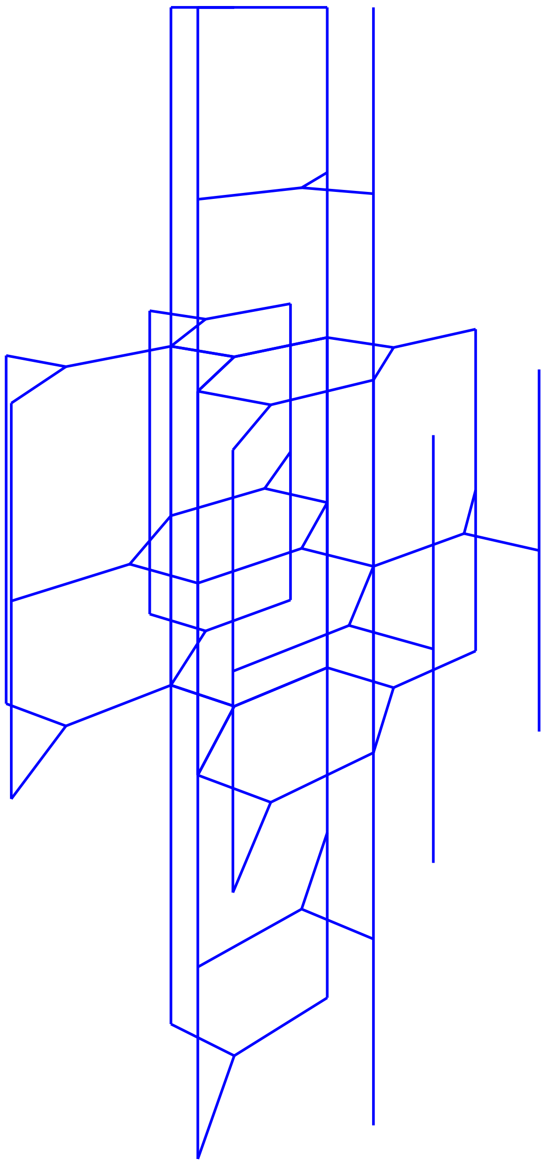
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



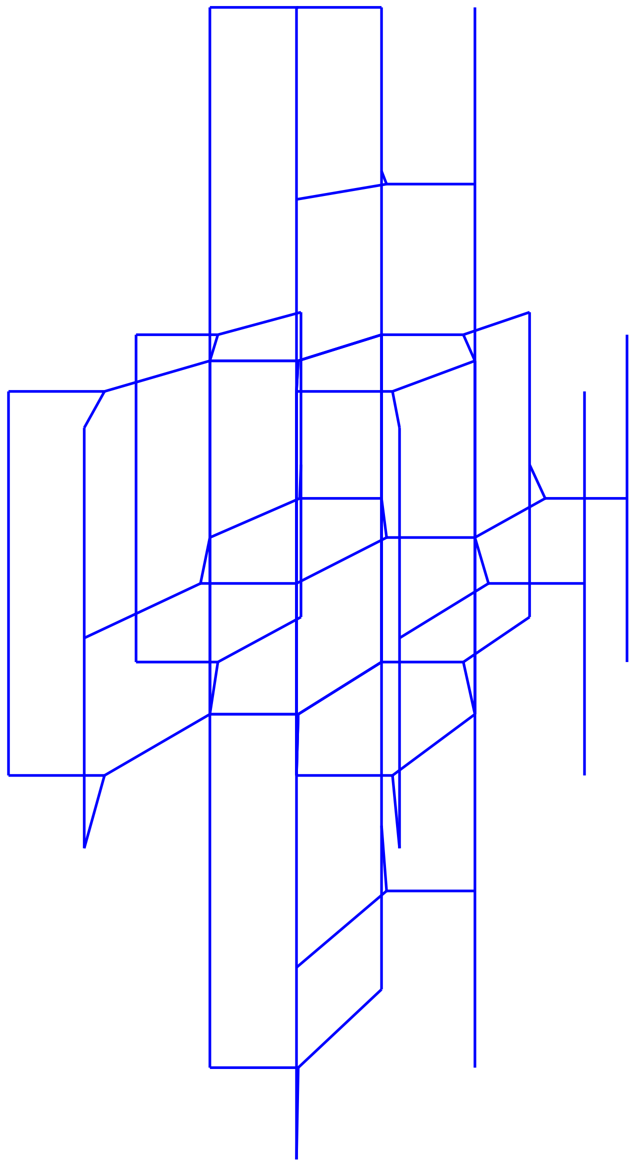
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



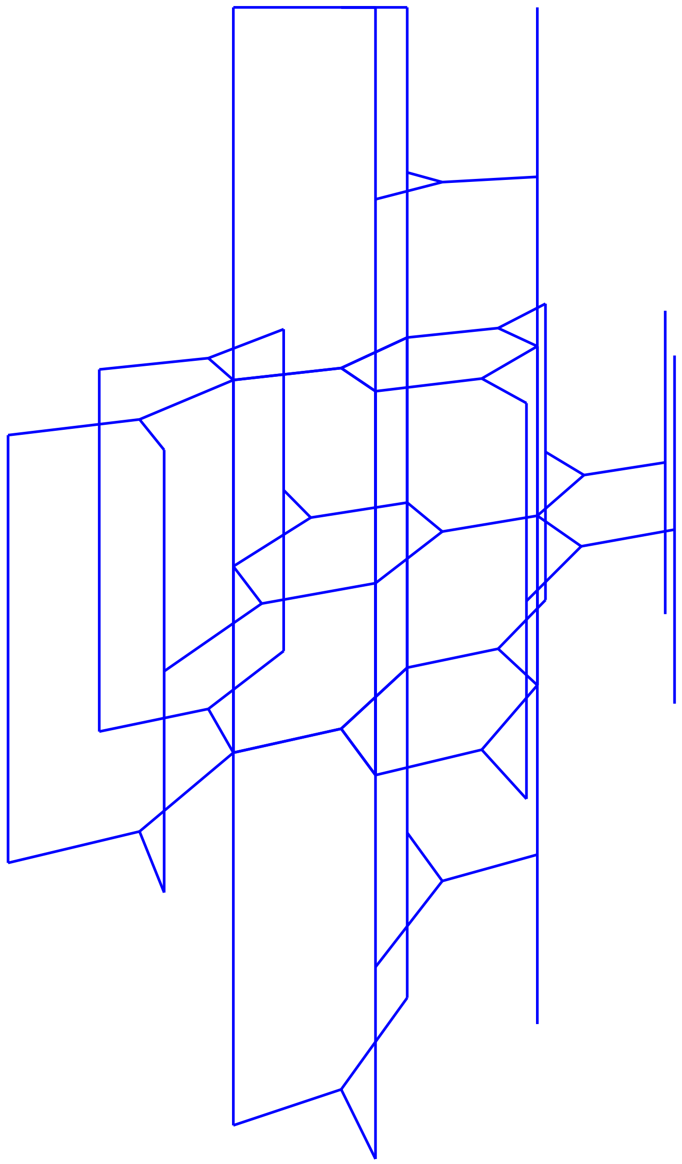
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



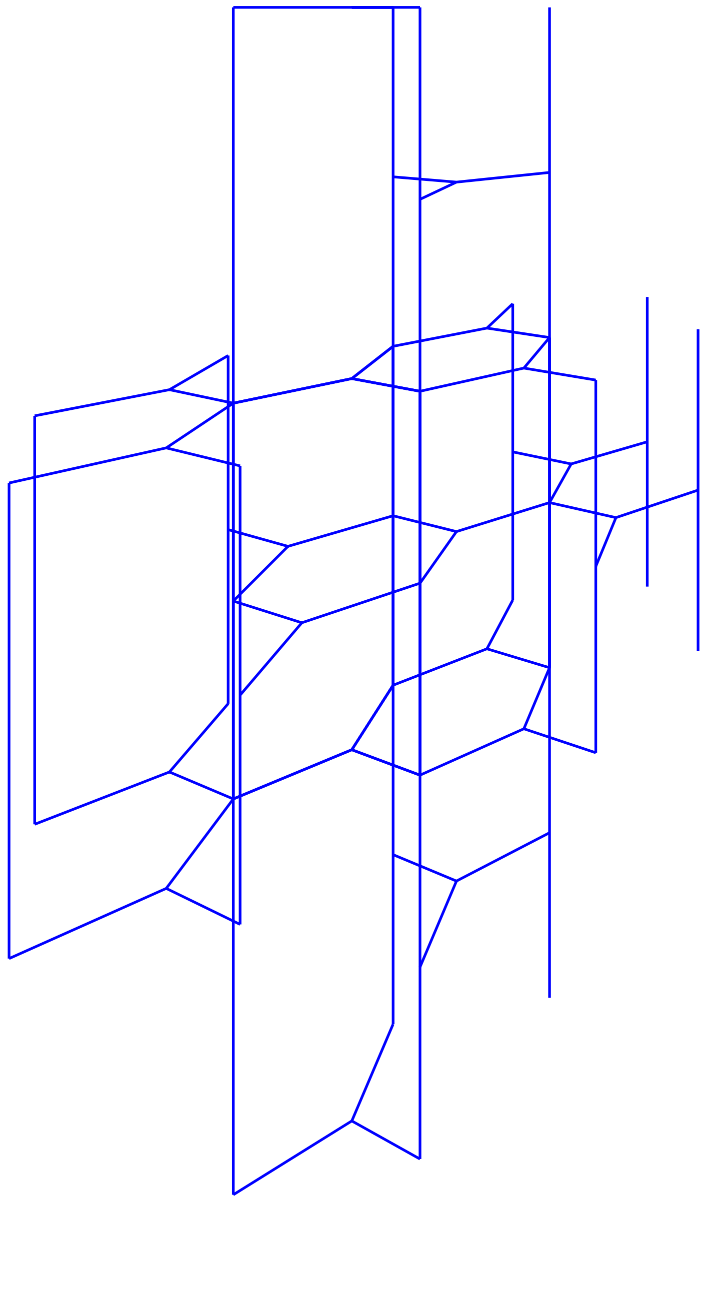
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



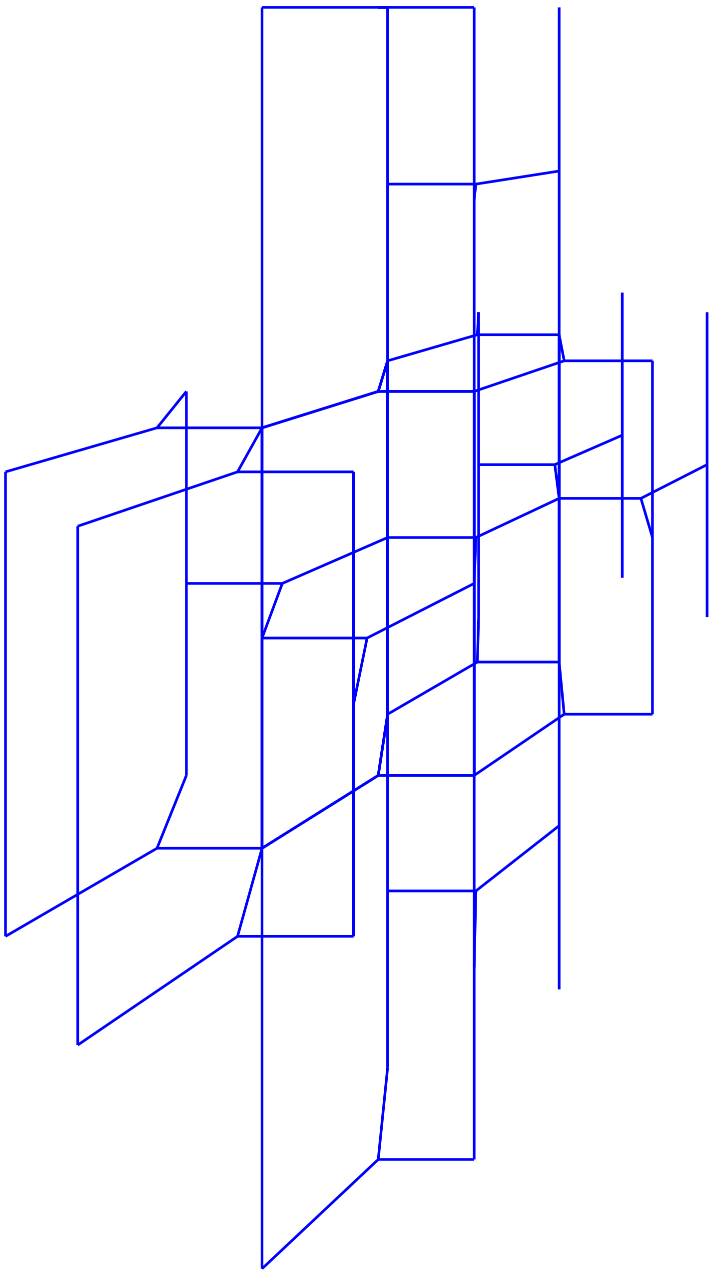
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



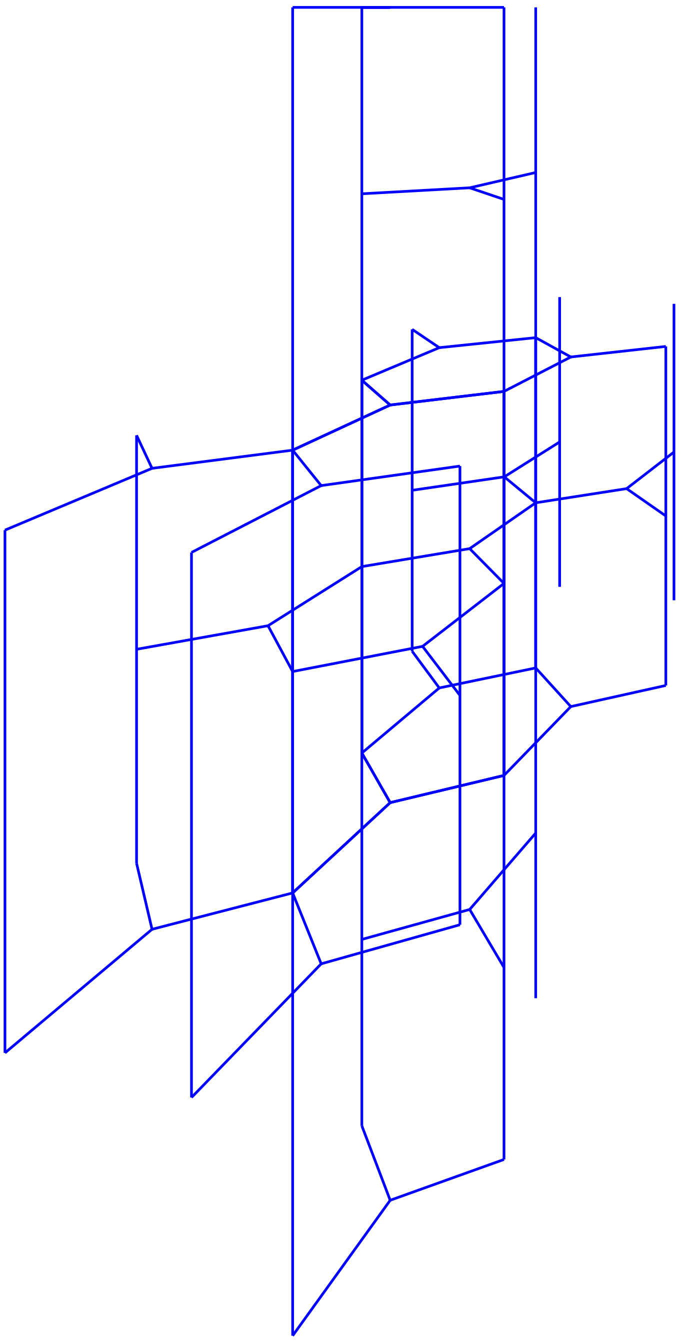
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



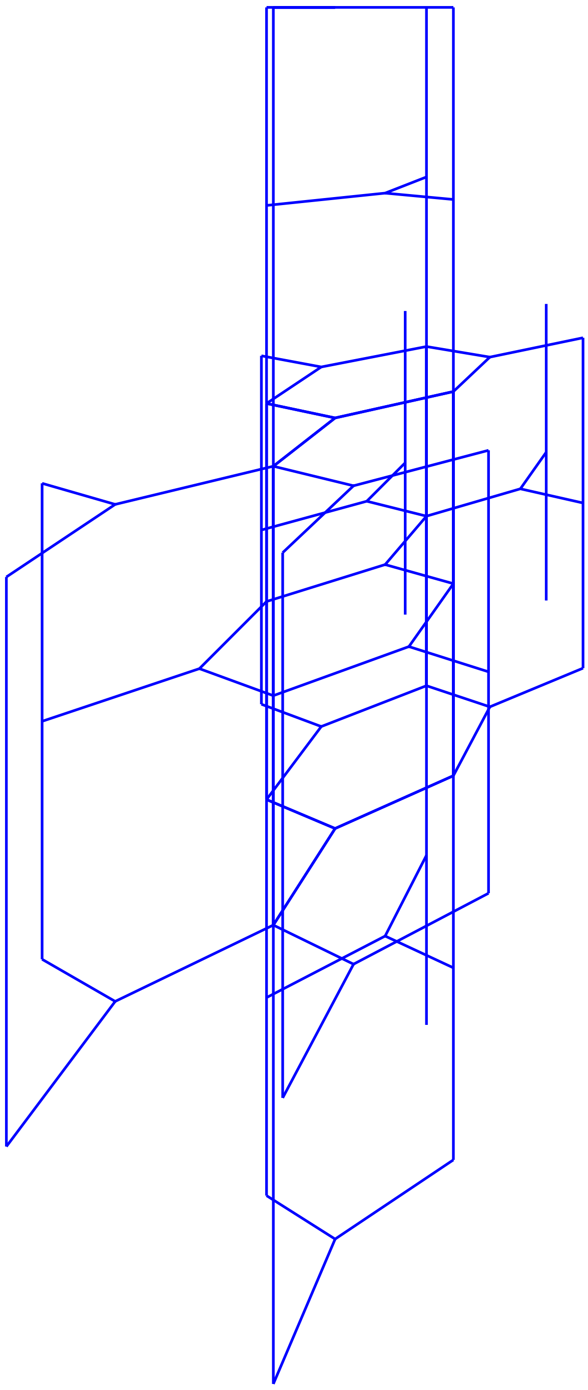
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



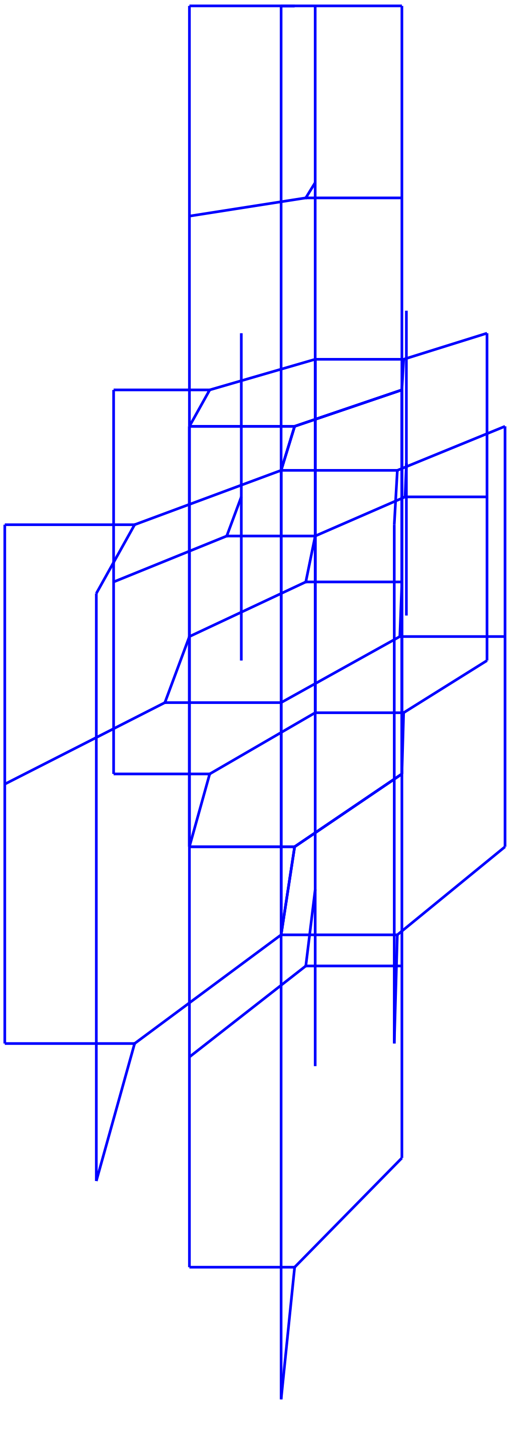
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



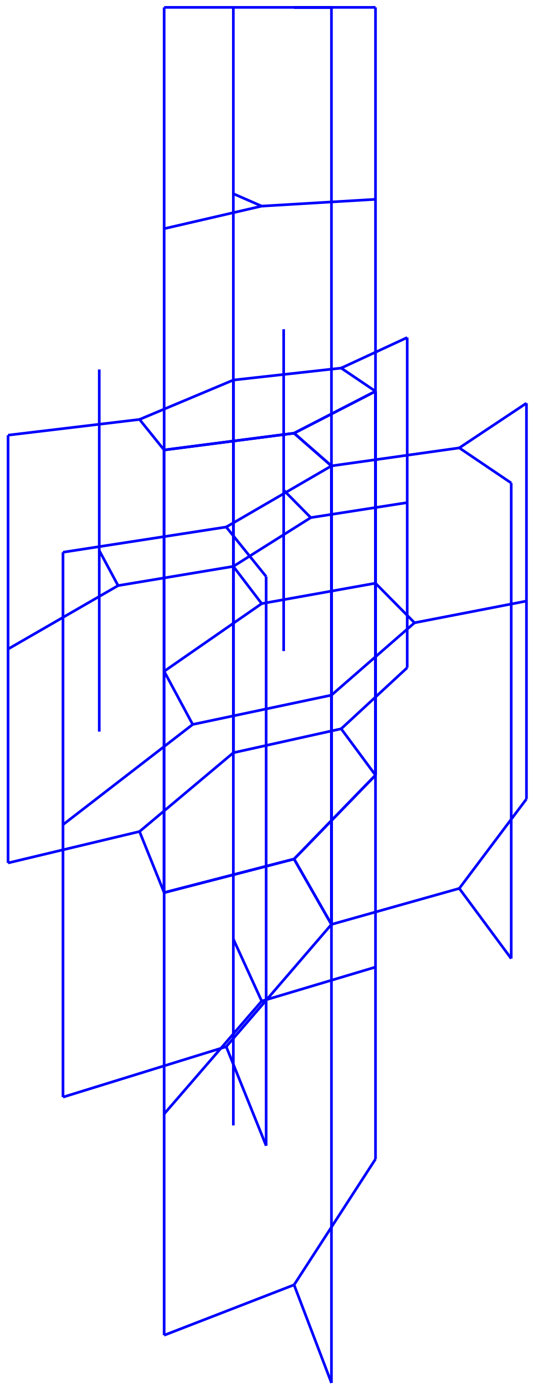
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



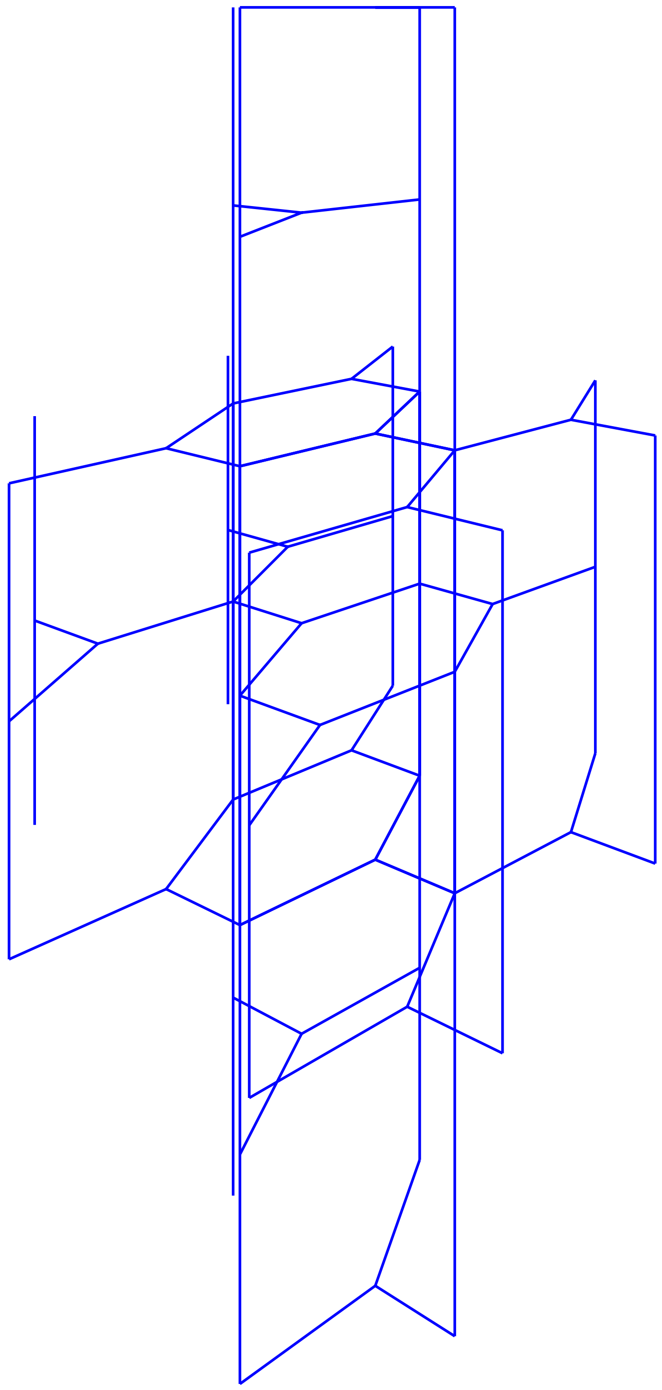
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



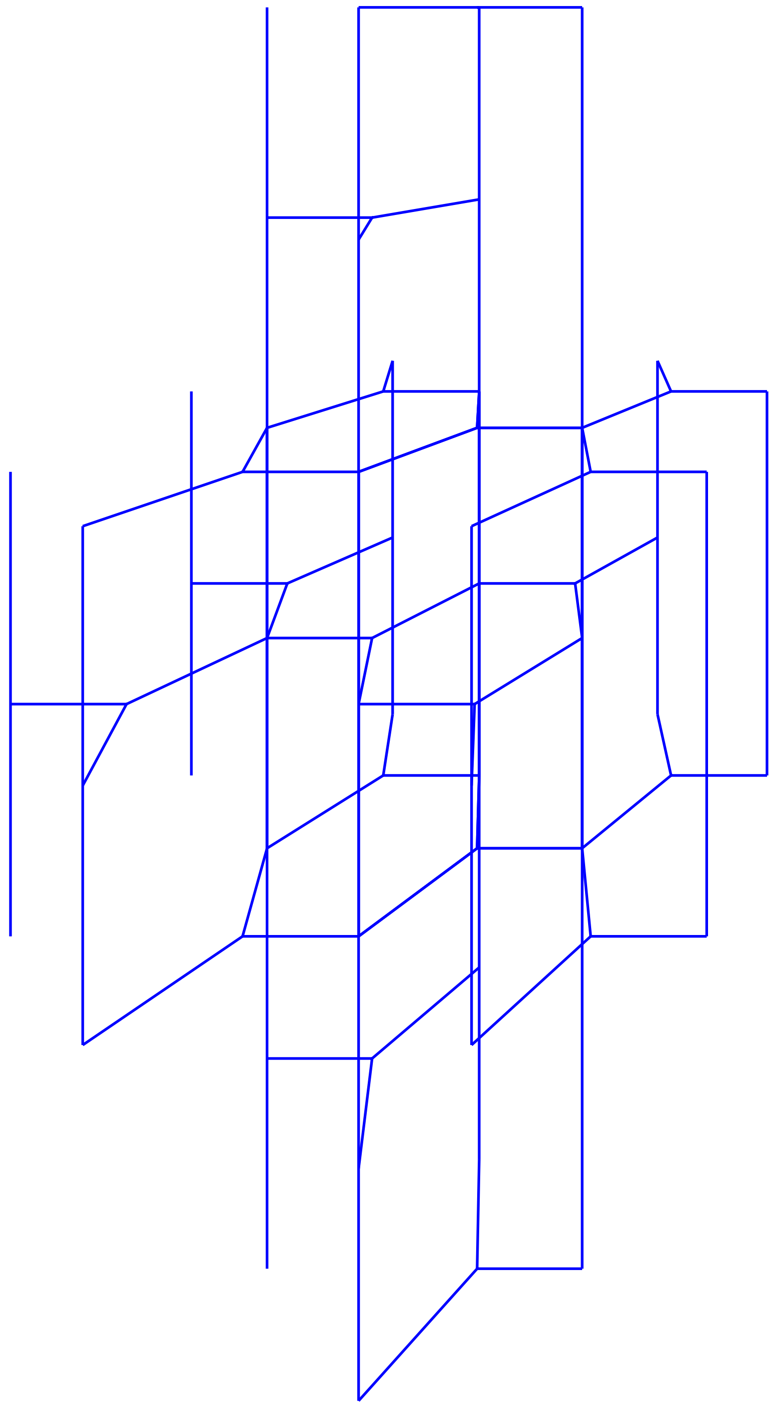
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



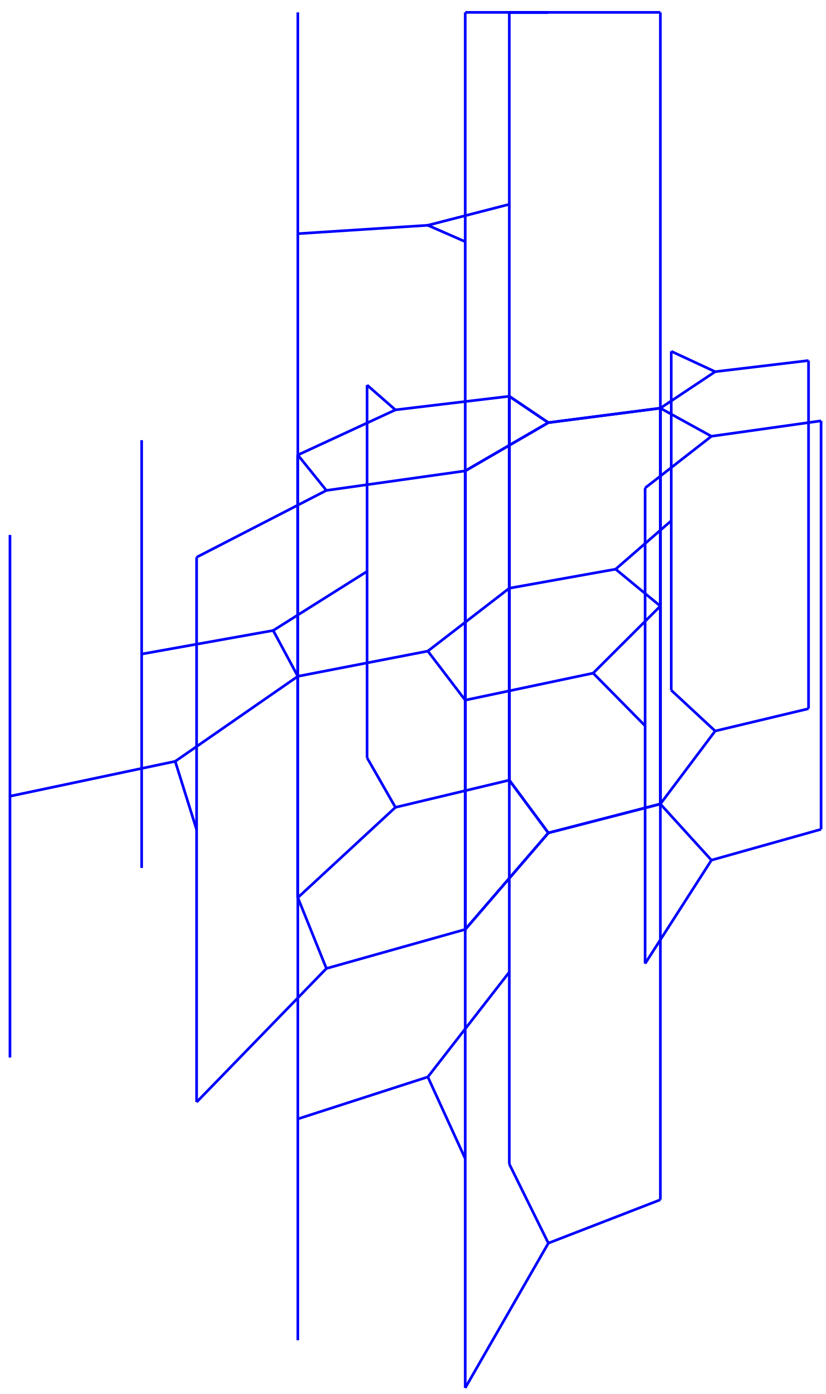
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



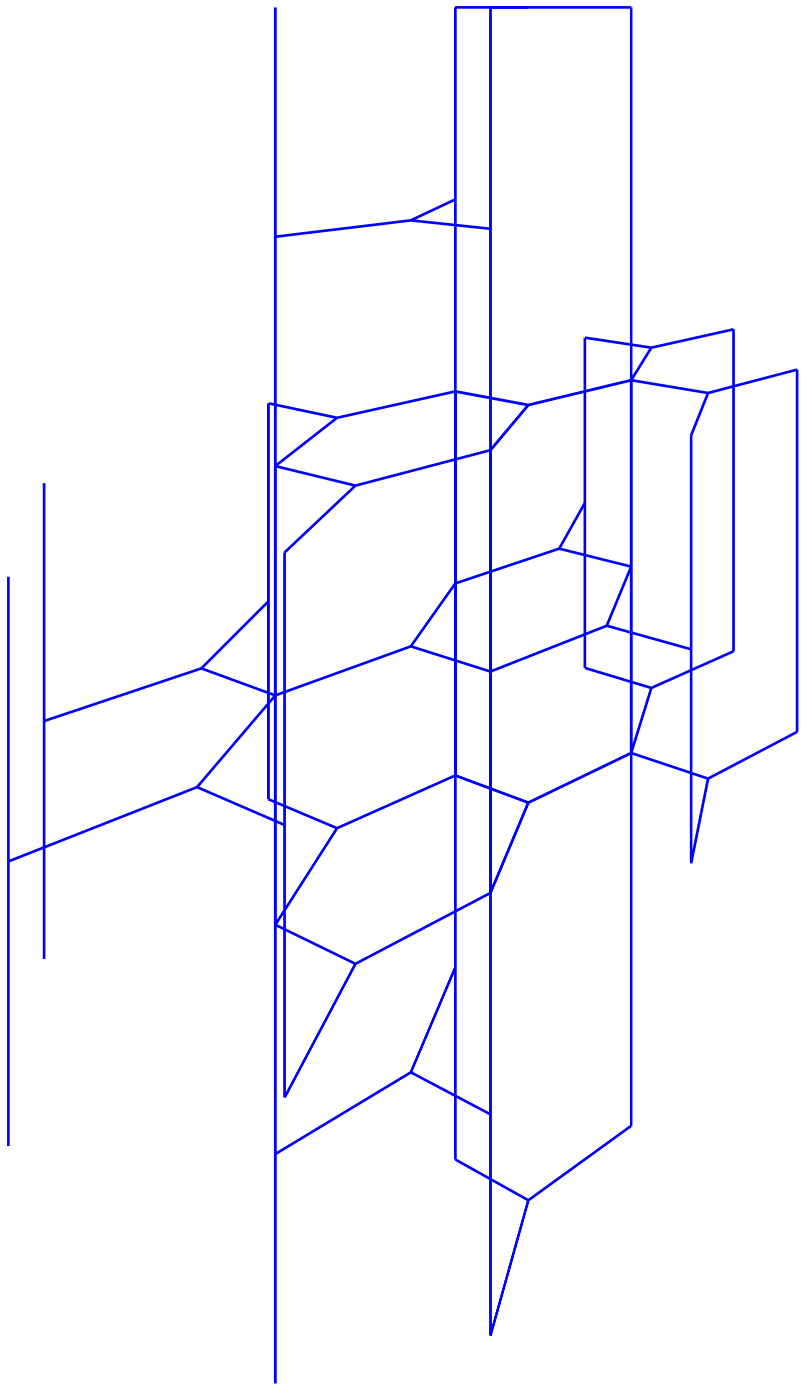
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



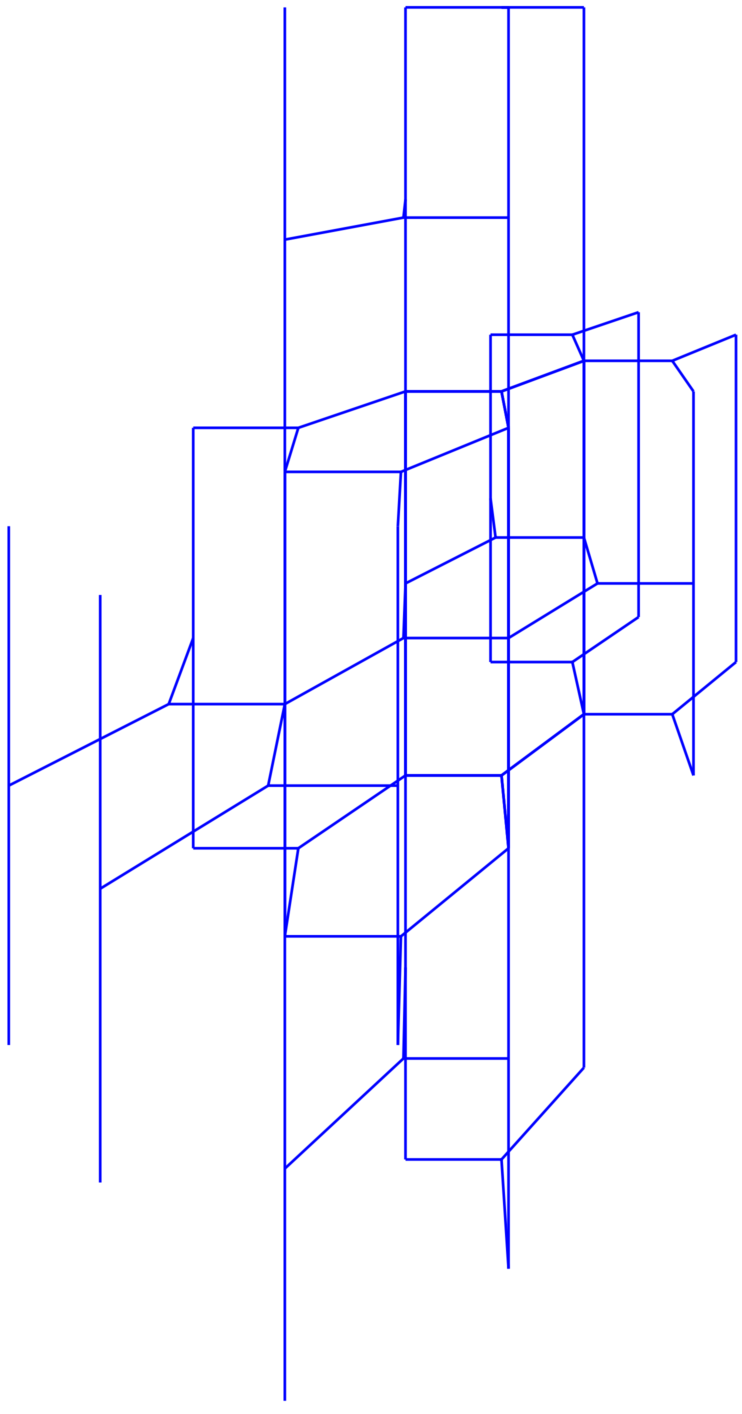
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



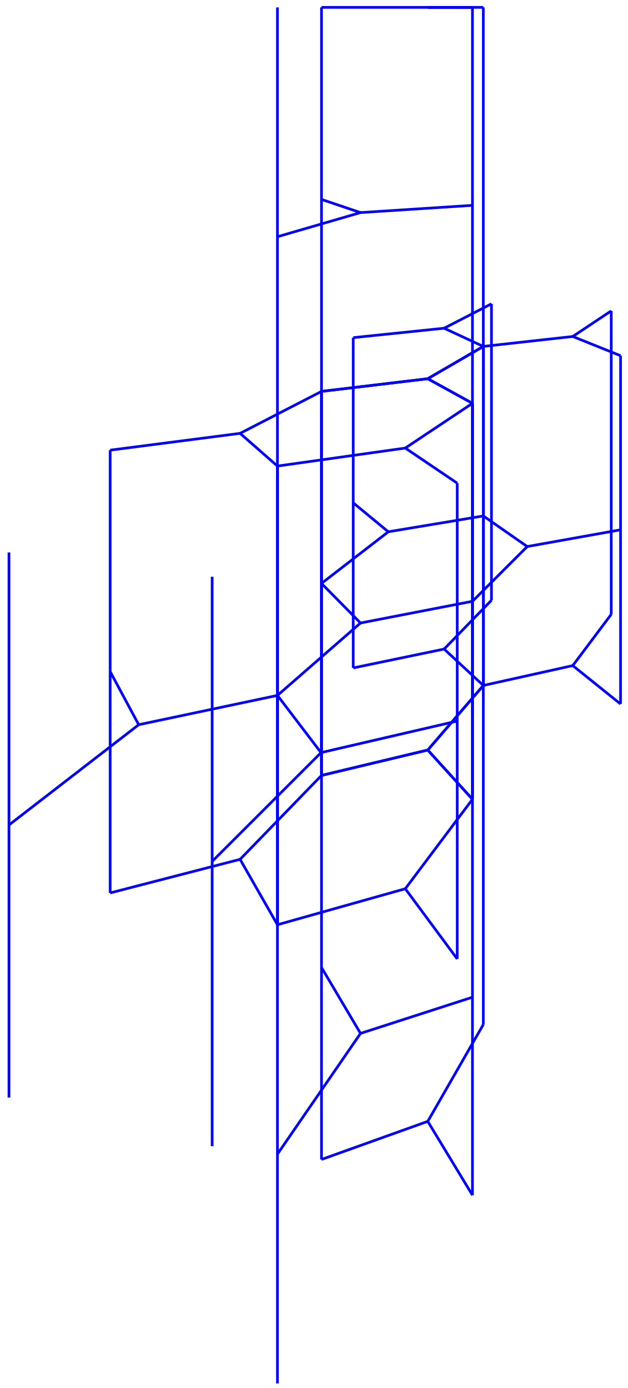
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



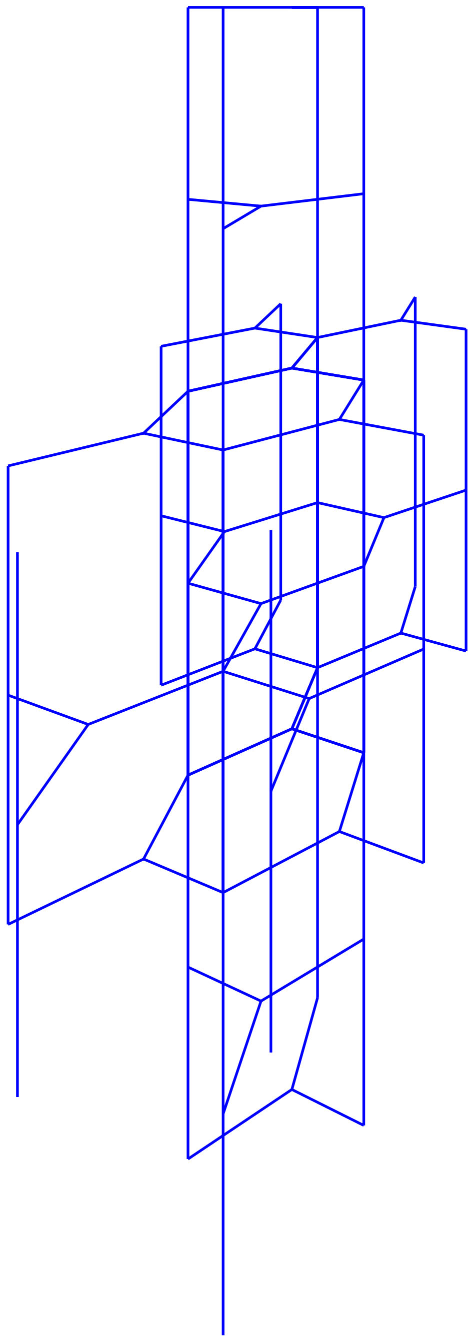
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



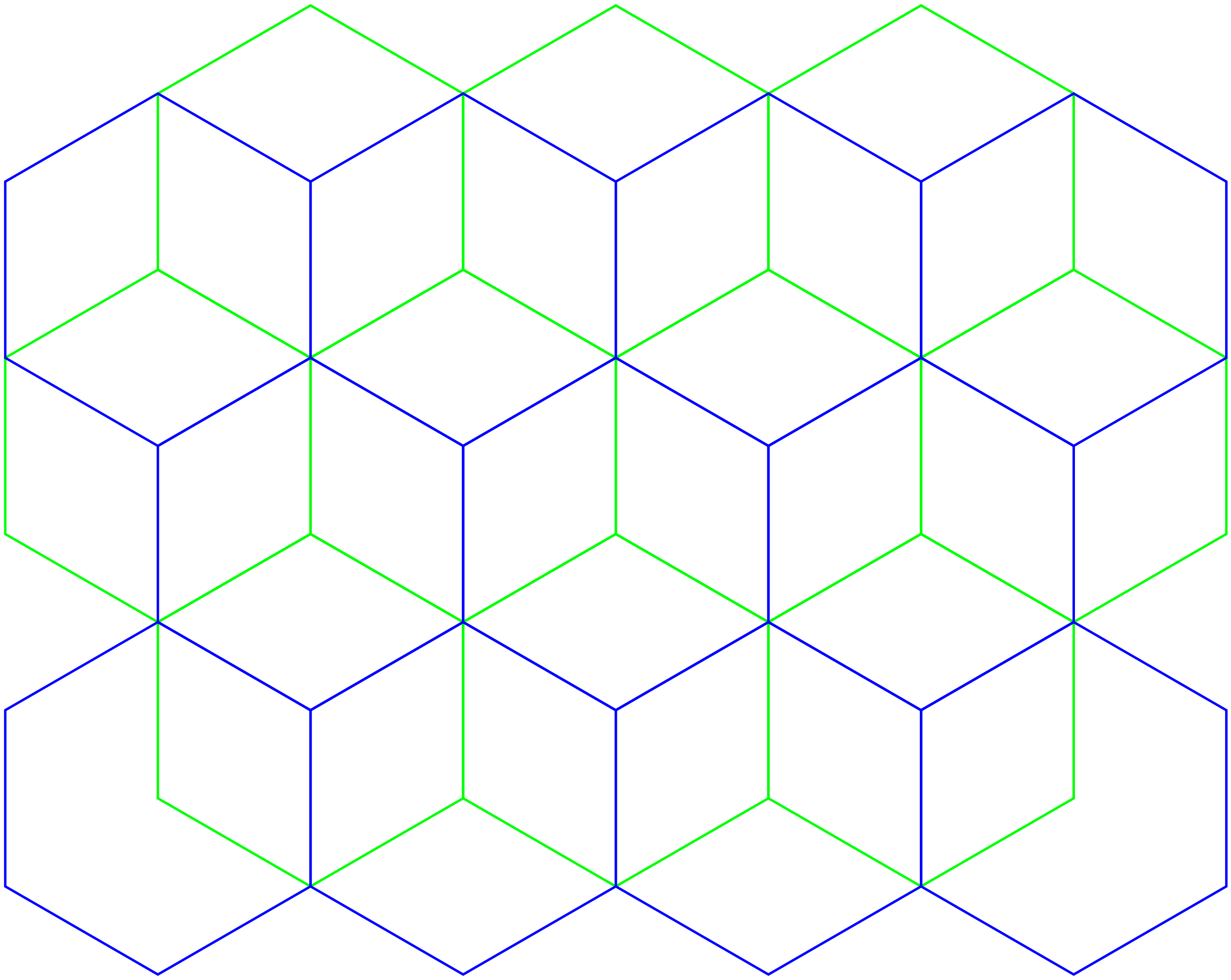
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



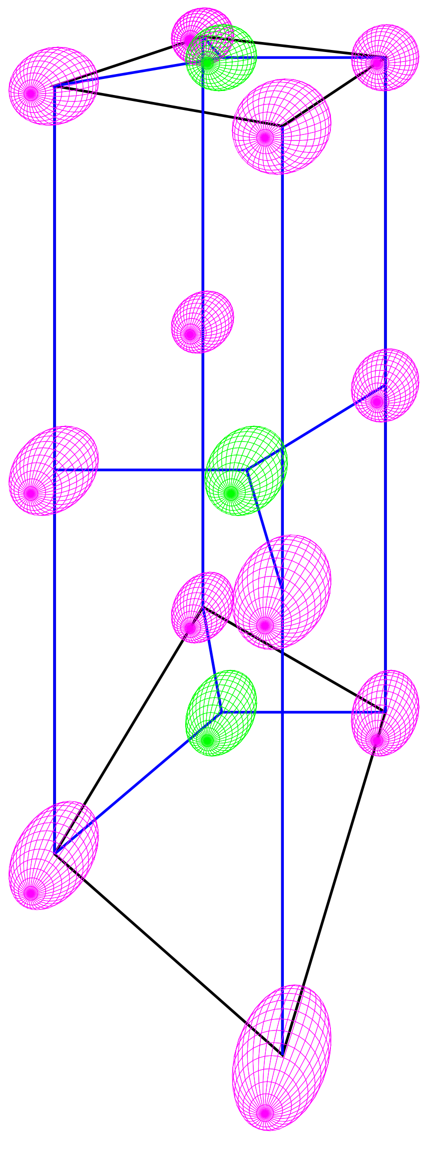
With the boundaries of the unit cell removed, the image below is a small representation of the graphite crystal structure. Carbon atoms sit where the blue bond lines meet.



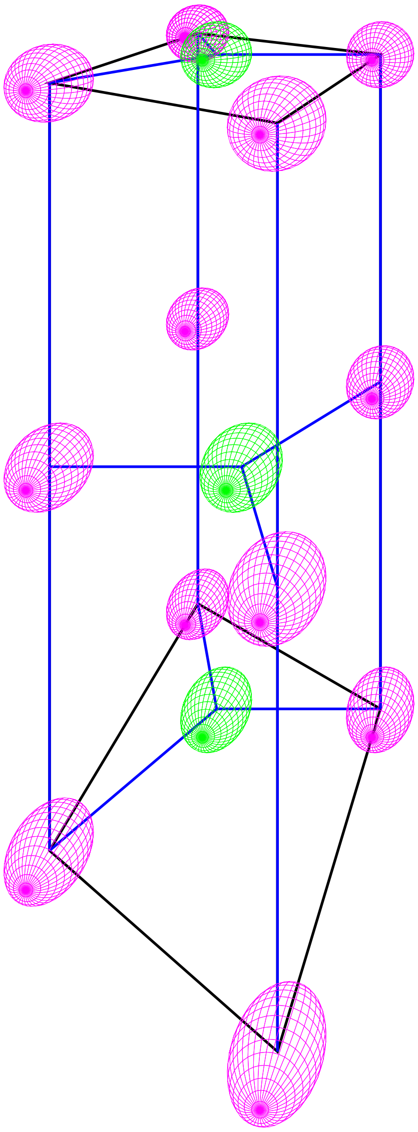
In fact, the graphite crystal structure is arranged in layers, where each layer is a honeycomb-like arrangement of bonds. Below in blue are bonds in one layer of the crystal, and in green are bonds in the next layer below.



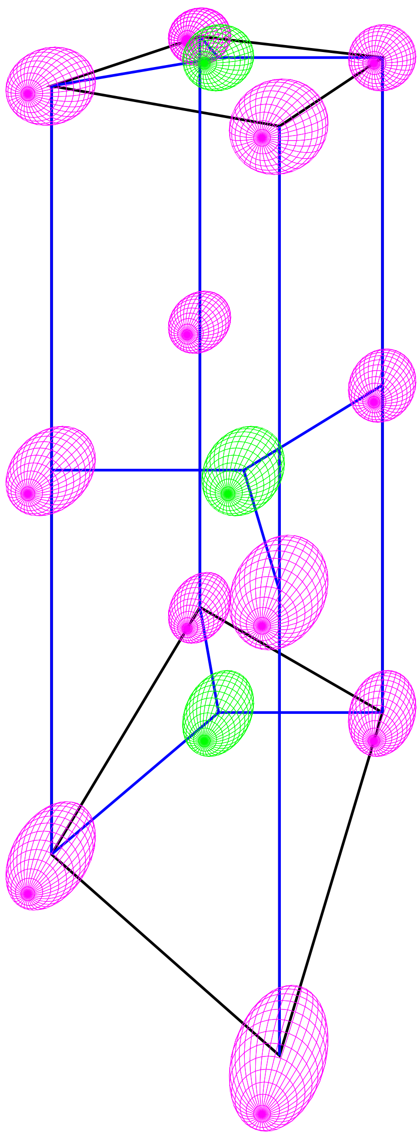
Let us take a look again at the unit cell of the graphite crystal.



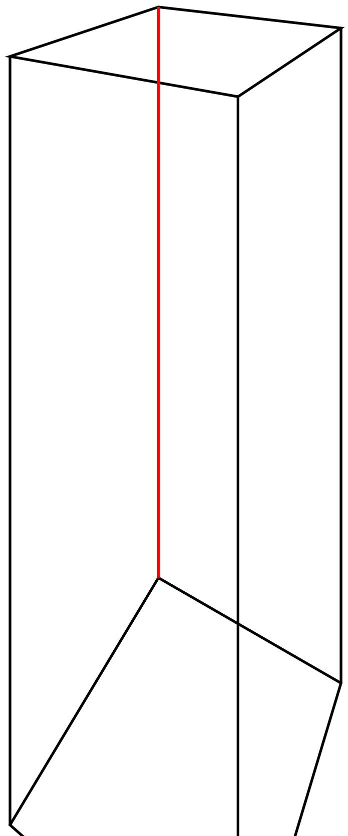
The atoms are not bonded to each other in a tetrahedral arrangement. We also note that the distance between two horizontal layers of the unit cell is greater than the distance between bonded atoms within a horizontal layer.



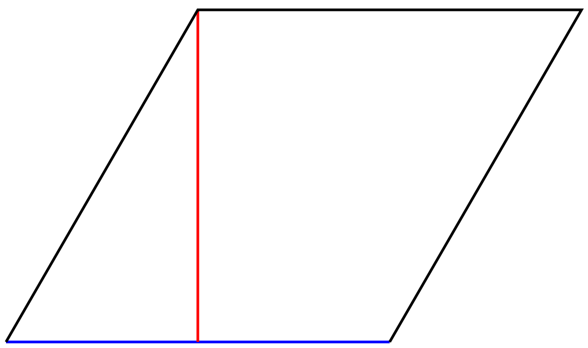
We can consider the bonded atoms, represented by spheres, within a horizontal layer to be actually touching each other. In the diagram below, these spheres are shown not to be touching simply to allow for the structure to be viewed more easily. Recall that bond lengths are different for different structural arrangements. Hence, we define a new variable Q to be the radius of a carbon atom in a graphite crystal. This is different from R, which was the radius of a carbon atom in a diamond crystal.



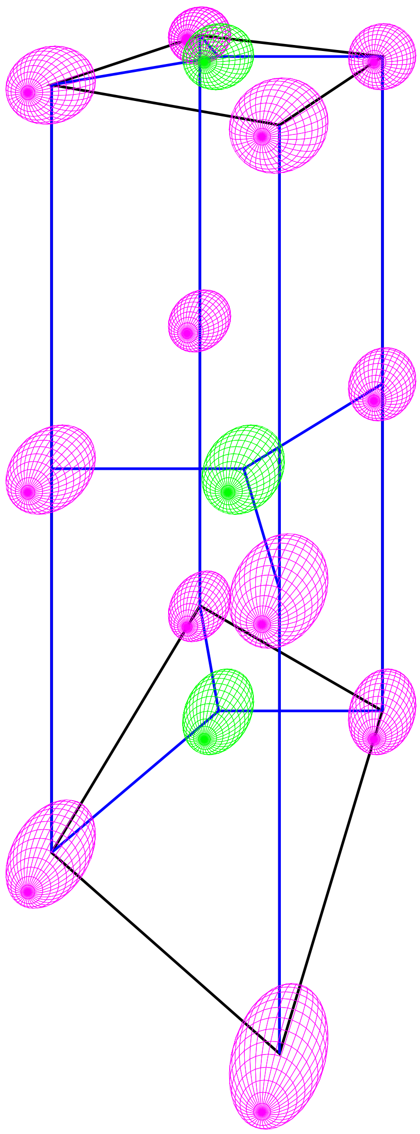
Literature values give that the height of the graphite unit cell, which is the length of the red line in the diagram below, is equal to about 10Q.



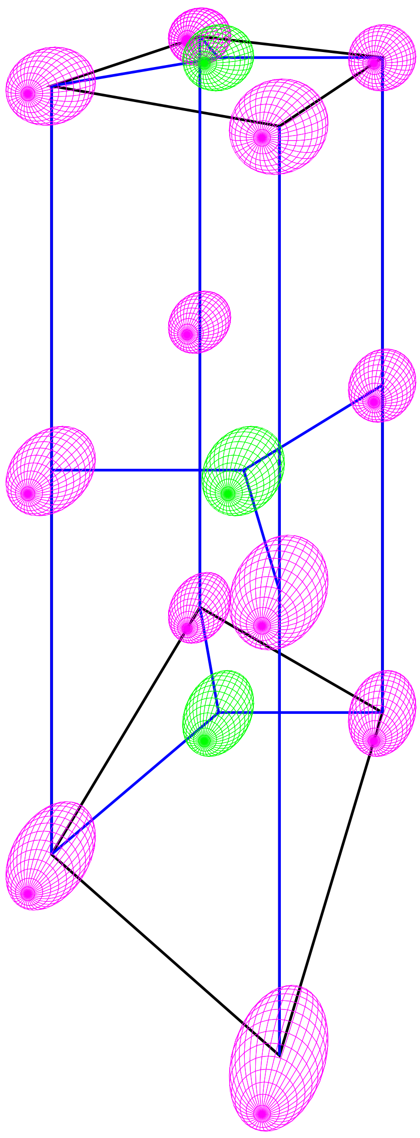
Consider the parallelogram that makes up the top and bottom surfaces of the graphite unit cell. Literature values give that it has a base of about (29/8)Q.
In the image below, the blue line is the base of the parallelogram and the red line is the height of the parallelogram. All sides of the parallelogram are of equal length.
If the height is represented by h, then by Pythagoras, h^2 + ((29/16)Q)^2 = ((29/8)Q)^2.
This gives that the height of the parallelogram is h = (29/16)(sqrt3)Q.



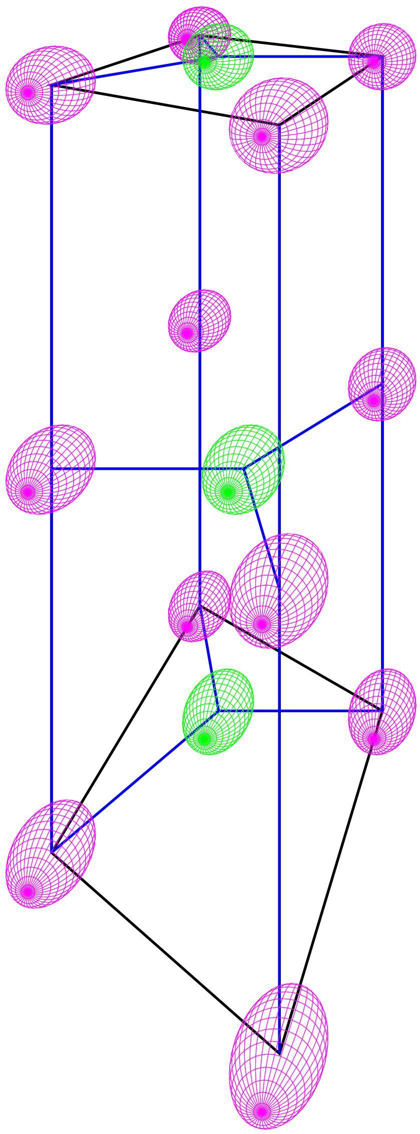
The volume of the graphite unit cell is equal to the base of the parallelogram that makes up the bottom surface multiplied by the height of the parallelogram that makes up the bottom surface multiplied by the height of the unit cell. It is therefore equal to (29/8)Q(29/16)(sqrt3)Q(10)Q = 113.8011507(Q^3).



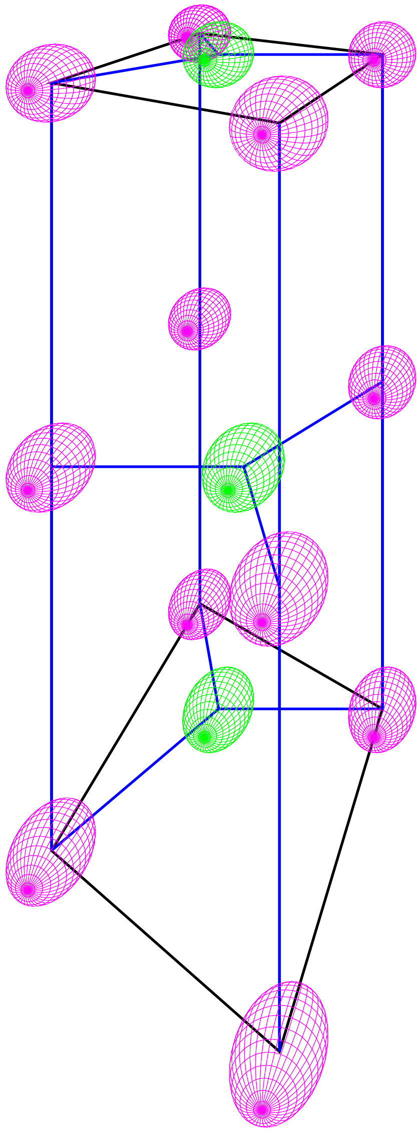
The graphite unit cell contains the equivalent of 4 carbon atoms. The atoms at the corners of the unit cell when put together contribute the equivalent of 1 atom. The atoms at the midpoints of the vertical edges when put together contribute the equivalent of 1 atom. The green atoms at the top and bottom surfaces each contribute half an atom. The green atom in the middle contributes 1 atom.



The volume of a carbon atom as a sphere is equal to (4/3)(pi)(Q^3). Thus, the volume of carbon atoms in the graphite unit cell is (4)(4/3)(pi)(Q^3) = 16.75516082(Q^3).



If we divide the volume of carbon atoms in the graphite unit cell by the volume of the graphite unit cell, we obtain the fraction of volume of the unit cell that is occupied by carbon atoms. It is equal to 0.147.



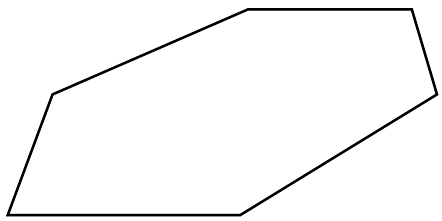
We have now seen some significant differences in the structures of diamond and graphite.

The fraction of volume of the diamond unit cell that is occupied by atoms is 0.34 while the fraction of volume of the graphite unit cell that is occupied by atoms is 0.147 which is much lower. Therefore, diamond is a denser material than graphite.

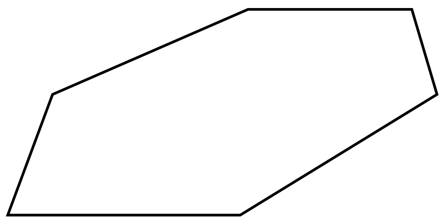
The carbon atoms in diamond are bonded in a tetrahedral arrangement while the carbon atoms in graphite are bonded in planes of honeycomb-like arrangements. The diamond structure is therefore very rigid as opposed to the graphite structure whose planes are weakly held together and can be made to slide. This accounts for the extreme strength and resistance to compression of diamond, and for the flakiness of graphite.

At room temperature and pressure, the arrangement of carbon atoms in graphite is actually more stable than the arrangement of carbon atoms in diamond. It is only at high temperature and pressure that diamond is more stable than graphite, and graphite is converted to diamond.

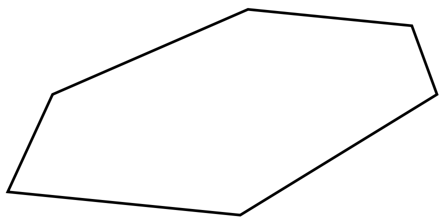
The details of the conversion of graphite into diamond are still somewhat unknown, but one possibility is that at high temperature and pressure, the planes of graphite are distorted so that the bonds adopt the tetrahedral arrangement that occurs in diamond. Shown below is a perspective view of one hexagon of bonds from a plane of the graphite crystal structure.



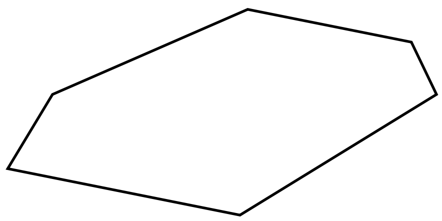
Now, shown below is the distortion of this hexagon. We can see that the bonds are distorted to make the angle between them equal to that in a tetrahedral arrangement. Thus, the planar arrangement of bonds in graphite is converted to a tetrahedral arrangement similar to that in diamond.



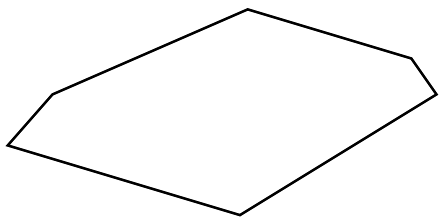
Now, shown below is the distortion of this hexagon. We can see that the bonds are distorted to make the angle between them equal to that in a tetrahedral arrangement. Thus, the planar arrangement of bonds in graphite is converted to a tetrahedral arrangement similar to that in diamond.



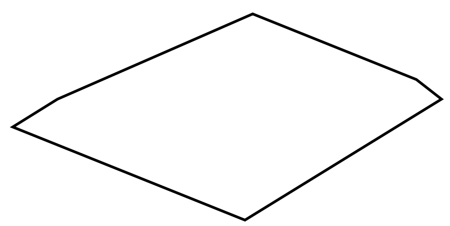
Now, shown below is the distortion of this hexagon. We can see that the bonds are distorted to make the angle between them equal to that in a tetrahedral arrangement. Thus, the planar arrangement of bonds in graphite is converted to a tetrahedral arrangement similar to that in diamond.



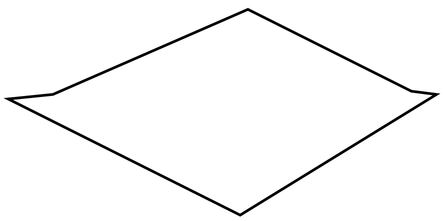
Now, shown below is the distortion of this hexagon. We can see that the bonds are distorted to make the angle between them equal to that in a tetrahedral arrangement. Thus, the planar arrangement of bonds in graphite is converted to a tetrahedral arrangement similar to that in diamond.



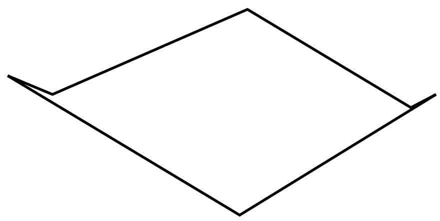
Now, shown below is the distortion of this hexagon. We can see that the bonds are distorted to make the angle between them equal to that in a tetrahedral arrangement. Thus, the planar arrangement of bonds in graphite is converted to a tetrahedral arrangement similar to that in diamond.



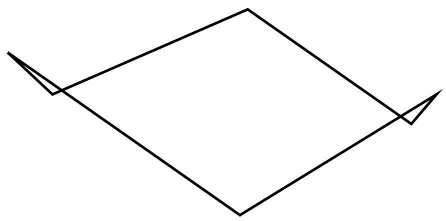
Now, shown below is the distortion of this hexagon. We can see that the bonds are distorted to make the angle between them equal to that in a tetrahedral arrangement. Thus, the planar arrangement of bonds in graphite is converted to a tetrahedral arrangement similar to that in diamond.



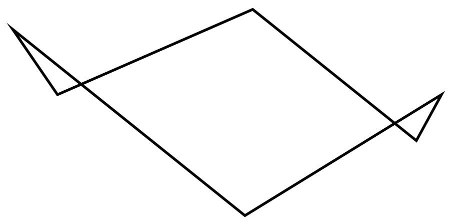
Now, shown below is the distortion of this hexagon. We can see that the bonds are distorted to make the angle between them equal to that in a tetrahedral arrangement. Thus, the planar arrangement of bonds in graphite is converted to a tetrahedral arrangement similar to that in diamond.



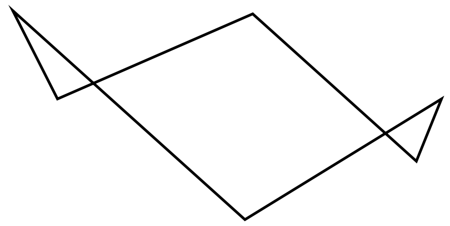
Now, shown below is the distortion of this hexagon. We can see that the bonds are distorted to make the angle between them equal to that in a tetrahedral arrangement. Thus, the planar arrangement of bonds in graphite is converted to a tetrahedral arrangement similar to that in diamond.



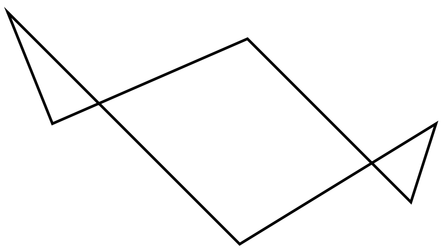
Now, shown below is the distortion of this hexagon. We can see that the bonds are distorted to make the angle between them equal to that in a tetrahedral arrangement. Thus, the planar arrangement of bonds in graphite is converted to a tetrahedral arrangement similar to that in diamond.



Now, shown below is the distortion of this hexagon. We can see that the bonds are distorted to make the angle between them equal to that in a tetrahedral arrangement. Thus, the planar arrangement of bonds in graphite is converted to a tetrahedral arrangement similar to that in diamond.



Now, shown below is the distortion of this hexagon. We can see that the bonds are distorted to make the angle between them equal to that in a tetrahedral arrangement. Thus, the planar arrangement of bonds in graphite is converted to a tetrahedral arrangement similar to that in diamond.



Since we are at the surface of the Earth where temperature and pressure are not high enough to make diamond more stable than graphite, our diamonds are actually transforming into graphite! Fortunately, this change occurs very slowly...
so slowly that we can still claim that, relatively speaking, a diamond lasts forever.

THE END

References:

"Diamond and Graphite". <http://www.enmu.edu/academics/excellence/museums/miles-mineral/diamond-and-graphite.shtml> Maintained by the Eastern New Mexico University, updated July 20th, 2002.

Pierson, Hugh O. "Handbook of Carbon, Graphite, Diamond and Fullerenes". Park Ridge, NJ: Noyes Publications, 1993. Pages 44-46, 247-249.

Reynolds, W. N. "Physical Properties of Graphite". London: Elsevier Publishing Co. Ltd., 1968. Pages 1-4.

"The Hexagonal Diamond (Lonsdaleite) Structure". <http://cst-www.nrl.navy.mil/lattice/struk/hexdia.html> Maintained by the Naval Research Laboratory Center for Computational Materials Science, updated Oct. 21, 2004.

Ubbelohde, A. R., and Lewis, F. A. "Graphite and its Crystal Compounds". London: Oxford University Press, 1960. Pages 1-2.

Wyckoff, Ralph W. G. "Crystal Structures". Second Edition, Volume 1. New York: John Wiley & Sons, Inc., 1963. Pages 26-27.