L4: Symmetry and crystal classes

Friday, July 24, 2020 16:15

Time on task: about 2 hours to review the material - MUCH MORE for practice!
(Material posted on August 31st, office hours: Monday Sept 14th and Wednesday Sept 16th)

Goals:

Upon completion of this lecture, you should be able to:

1. Identify the elements of symmetry in a 2D pattern
2. Identify the elements of symmetry in a 3D structure
3. Fully describe the seven crystal systems and their diagnostic symmetry
4. Give the Herman Mauguin symbol of the crystal
5. Determine the crystal class of a crystal

This lecture is complemented with your Problem set #2 (due on Friday Sept 25th) and your lab#3 (due on Friday Sept 18th)

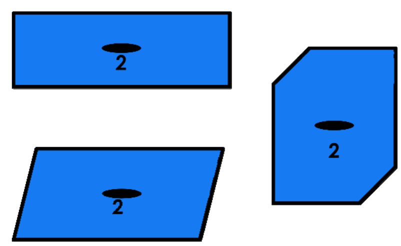
You now know how to describe the unit cell of a crystal, its crystal system and its crystal lattice. We are now going to introduced the elements of symmetry we can find in the crystal structure. Identify the elements of symmetry of a minerals is the best way to determine its crystal system (and crystal class - see lecture 4). However, because symmetries are sometimes (often) hard to see in 3D, we will, once again, start by working with 2D patters.

1. 2D symmetry

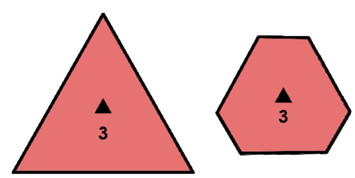
A Symmetry operation is an operation on an object that results in no change in the appearance of the object.
In 2D, there are **3 types of symmetry operations**: **rotation, reflection, and inversion**. Below, I list all the symmetry operations that can exist in crystalline structure.

1.1. Rotational symmetry

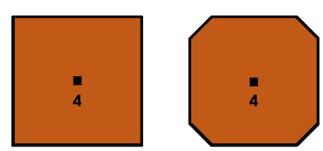
- **2-fold rotation axis**: identical after a rotation of 180° (360/180 = 2)
  symbol: filled oval, 2 or A_2



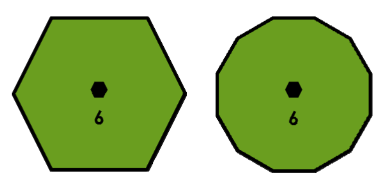
- **3-fold rotation axis** = identical after a rotation of 120° (360/120 = 3)
  symbol: filled triangle, 3 or A_3



- **4-fold rotation axis:** identical after a rotation of 90° (360/90 = 4)
  symbol: filled square, 4 or A_4

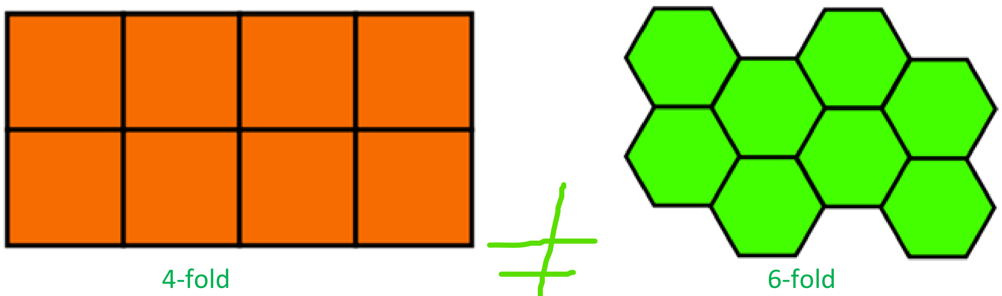


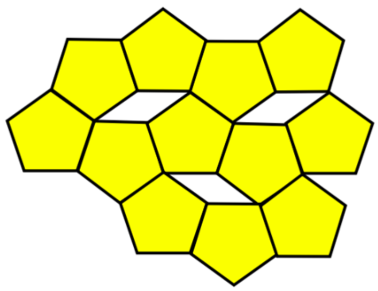
- **6-fold rotation axis** = identical after a rotation of 60° (360/60 = 6)
  symbol: filled hexagon or A_6



5-fold, 7-fold, 8-fold or higher do not exist in crystal structures. **Can you guess why?**

e.g.,





5-fold

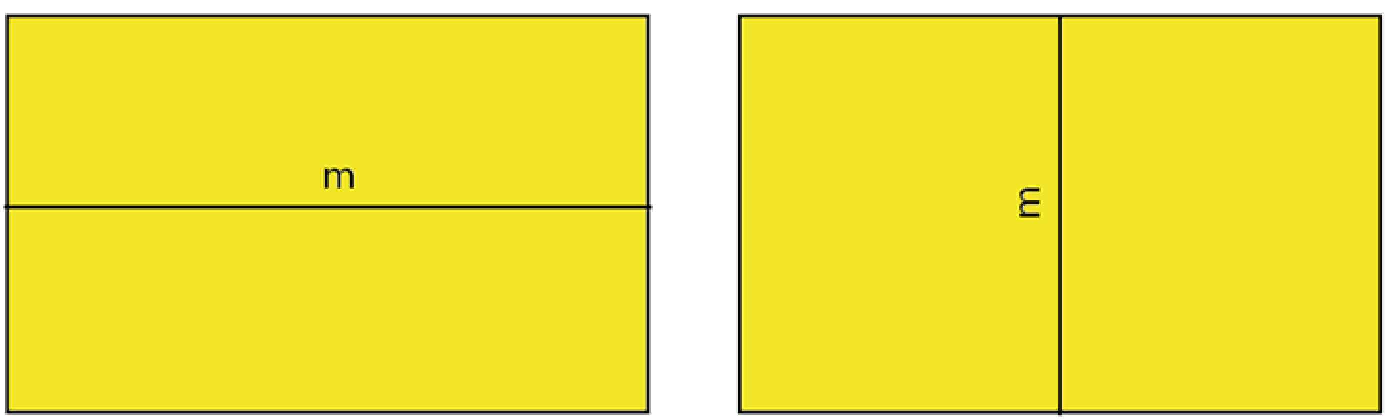
Because it's impossible to fill the space with such symmetries. Voids in crystals are not stable.

- **Notation:**

A_2 **A_3** **A_4** **A_6**

1.2. Mirror symmetry

A mirror plan gives the exact reflection on other side of the plan: same distance, same component/atoms/molecules. A mirror plane, and is symbolized with the letter "**m"** and with a solid line.

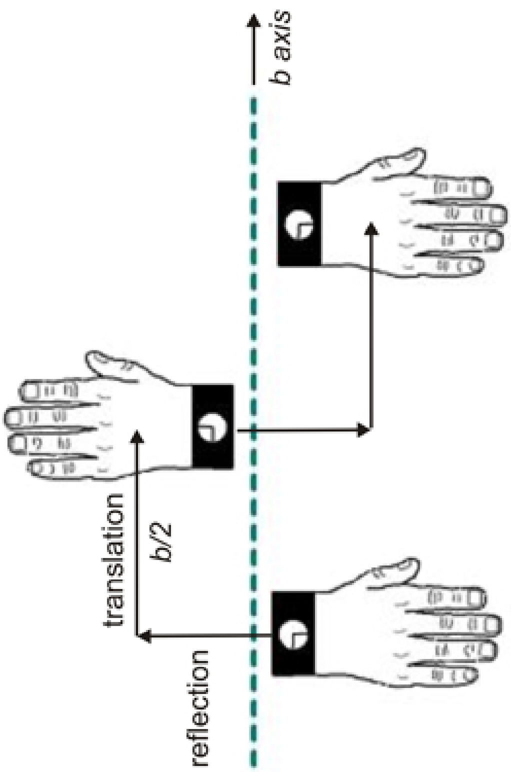


1.3. Center of symmetry.

A center of symmetry is an inversion through a point, symbolized with the letter **"i"**. In 2D, a center of the symmetry and a 2-fold rotation axis have the same effect.

1.4. Glide = translation + mirror

Glide planes are often represented with a dashed line.

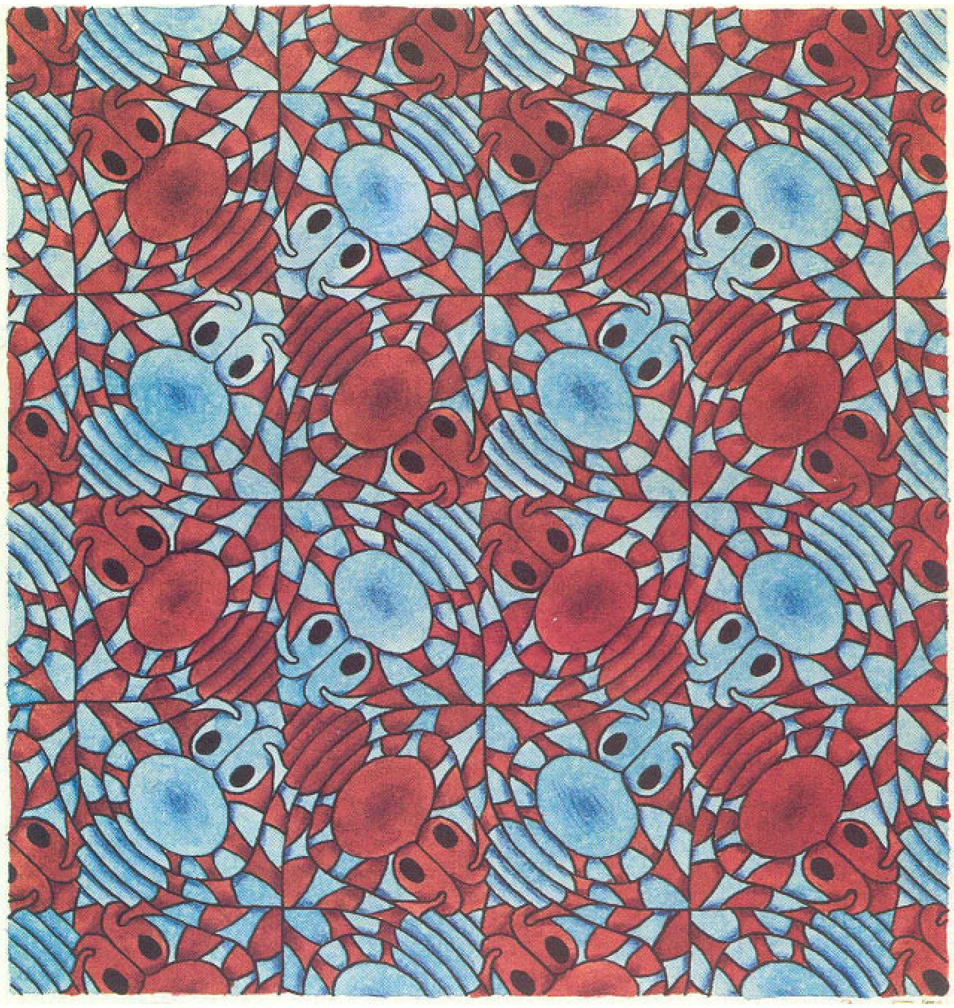


From M. Kastner, T. Medlock & K. Brown

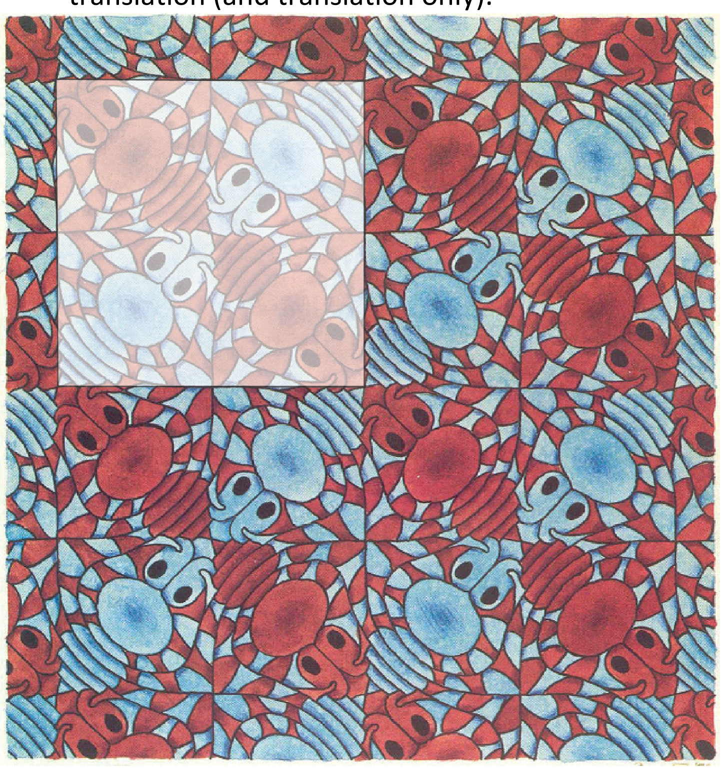
1.5. Intro to PS2

Patterns (2D structures) and minerals (3D structures) can show a vast combination of elements of symmetry. Patterns are the combination of the element of symmetry present in your motif (i.e, ions, molecules, atoms of groups of molecules,… present at each lattice point) and the elements of symmetry present in your lattice. Visualizing element of symmetry can be extremely challenging. **The only way to make progresses is to practice.** Let's first look at an example together first.

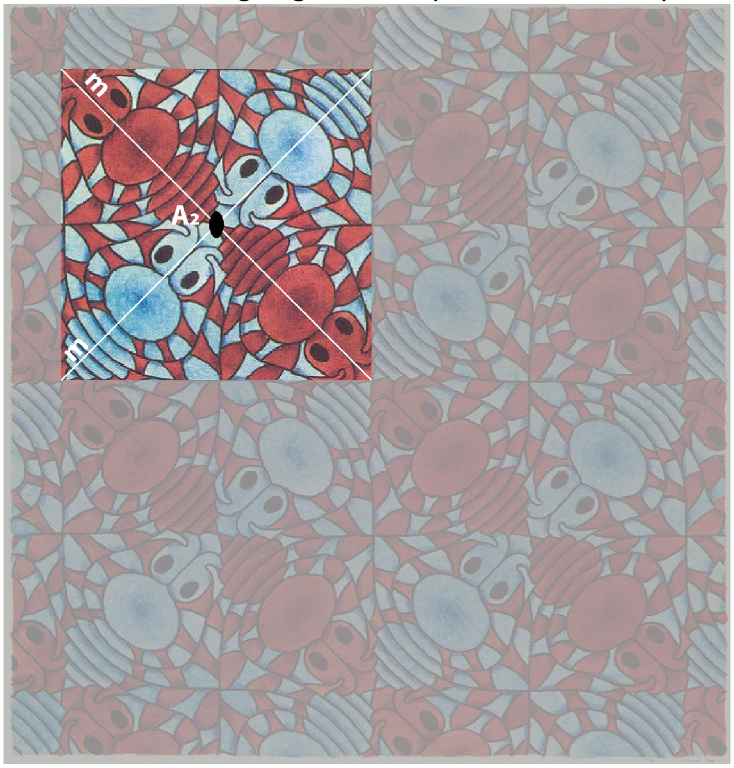
Let's look at the pattern bellow:



- First, we are going to look for the smallest motif (i.e., the part of the pattern that is repeated by translation (and translation only).



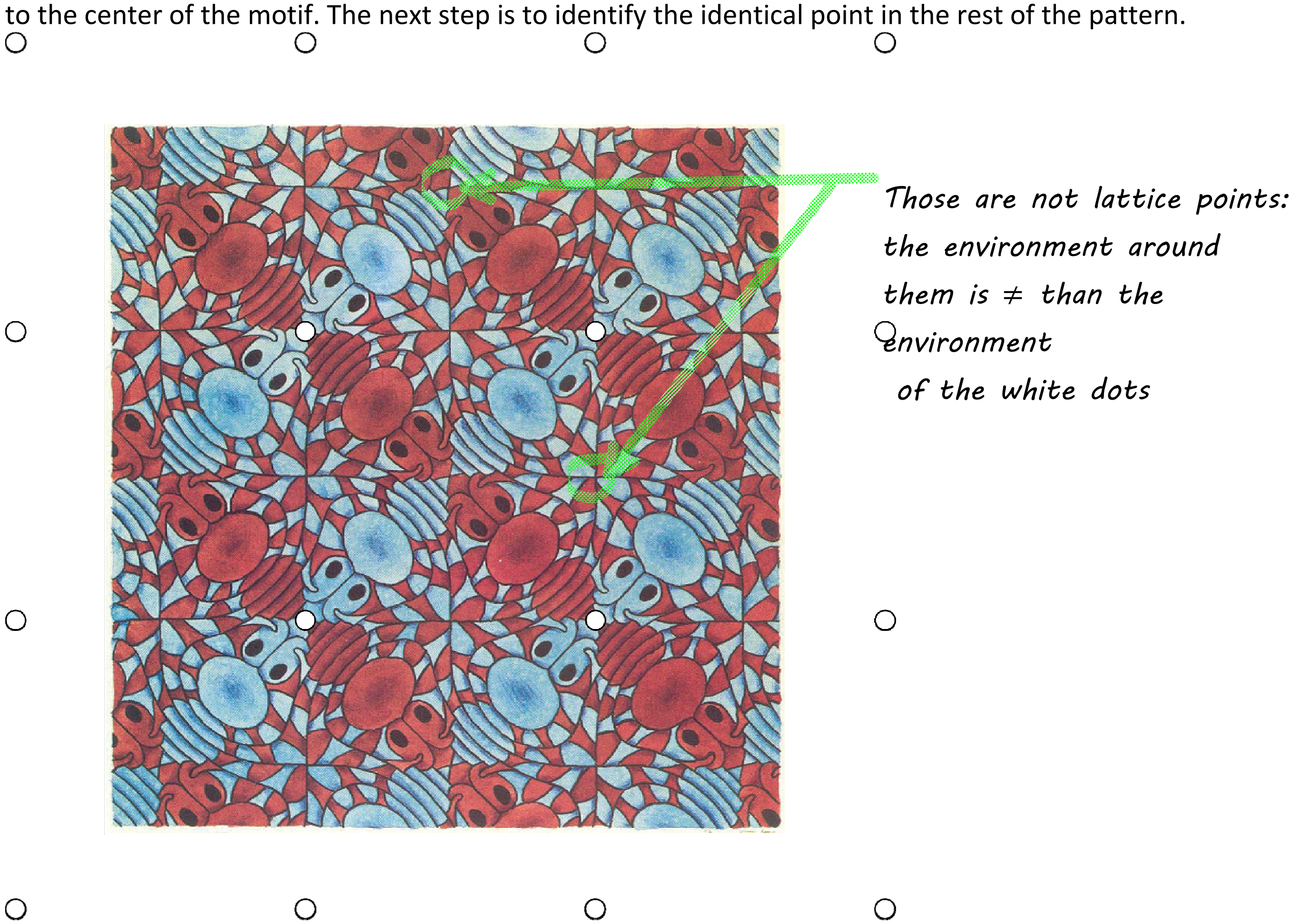
- Then we are going to identify the element of symmetry in the motif:



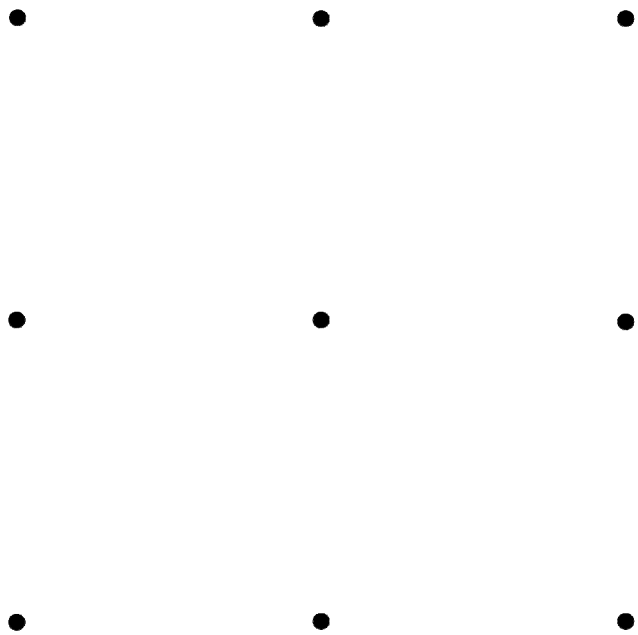
The motif shows two perpendicular mirror and a 2-fold rotation axis.

- We can now look at the element of symmetry of the crystal lattice.

Often, the lattice point are chosen as the highest point of symmetry in the motif. In this case, that correspond to the center of the motif. The next step is to identify the identical point in the rest of the pattern.

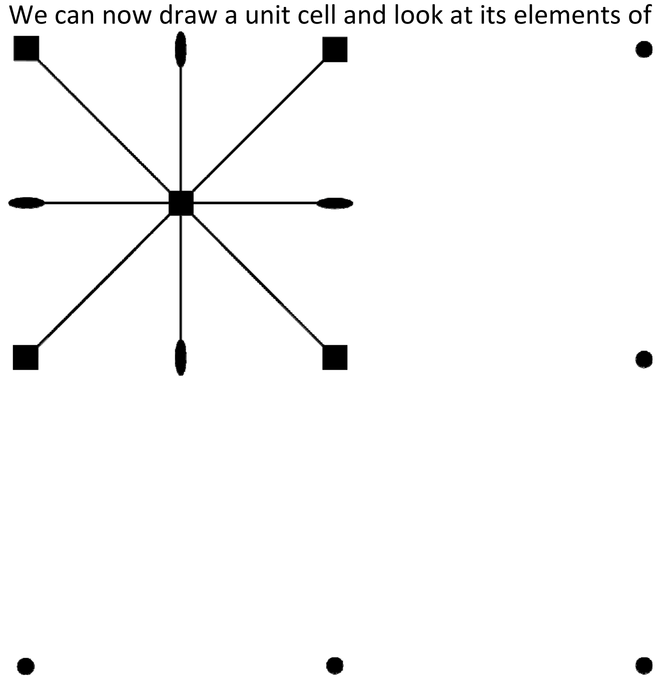


With this point of reference, only four lattice points fall inside the pattern, but remember, we assume that the pattern (and the lattice) can always extend to infinity in both directions (I represented additional lattice points that fall outside of this pattern to illustrate this point.
If we now remove the pattern and just look at the lattice, we obtain this:



The lattice is a square lattice

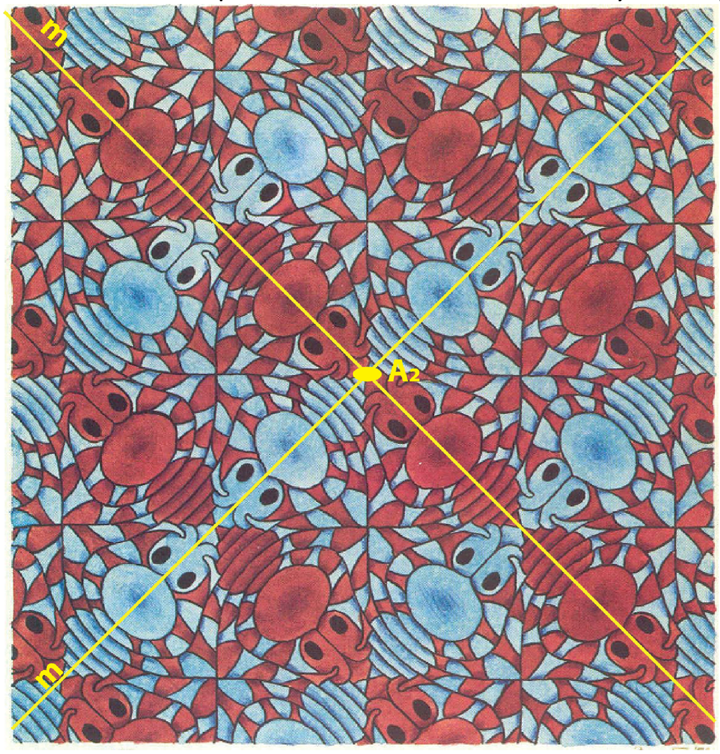
We can now draw a unit cell and look at its elements of symmetry (without the motif).



This video shows how to find the various elements of symmetry. To do this video, I used illustrator as an example. However, it is much easier to do it on paper. The best way to check for the elements of symmetry is to use **tracing paper**. You can also use your pen, placed vertically on your sheet of paper, to test for the rotation axes.

If you compare the degree of symmetry of the lattice and the degree of symmetry of the motif, in this example, the lattice present a higher symmetry than the motif.

- The last step is to look at the elements of symmetry in the full pattern.



Looking at the motif, it shows two perpendicular mirrors and one A2.

How do the elements of symmetry of the pattern compare with the element of symmetry of the motif? Of the lattice?

In this example, the pattern and the motif show the same element of symmetry, the lattice show a higher degree of symmetry.

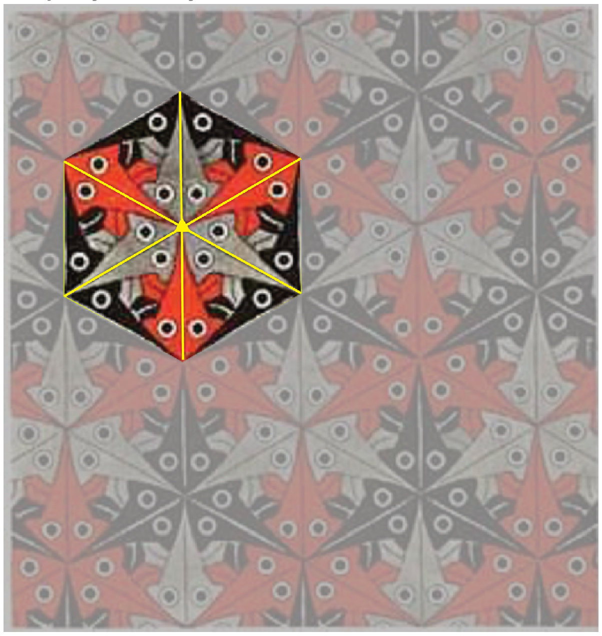
Your turn! Describe the symmetry of the motif, of the lattice and of the pattern (the solution is in the next tab).

L4: Keys practice #2

Monday, July 27, 2020   18:45

Keys of the 2D crystal lattice practice:

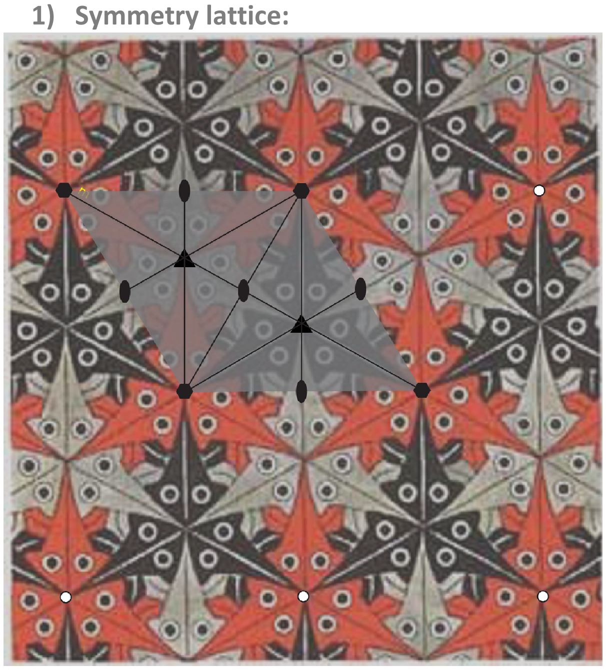
1) **Symmetry motif:**



Be sure to not get mixed up between the motif and the unit cell:
The smallest motif is not necessarily a parallelogram

The motif shows three mirrors and one A_3
A_6 at the corner of the unit cell, 2 A_3 inside the unit cell, A_2 at the middle of the faces and in the middle of the unit cell and set of three mirrors intersecting in A_3
A3 and mirrors.

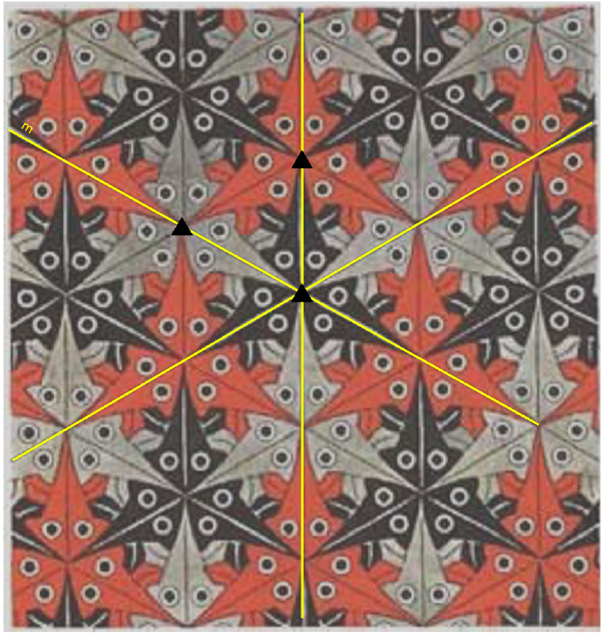
1) **Symmetry lattice:**



A_6 at the corner of the unit cell, 2 A_3 inside the unit cell, A_2 at the middle of the faces and in the middle of the unit cell and set of three mirrors intersecting in A_3

This video is an addition to the square lattice video and demonstrates the presence of the A3's in the middle of the unit cell and of the A6's at the corners of the unit cell.

3) Symmetry pattern:



A3 and mirrors.

Degree of symmetry: pattern = motif < lattice

Note: It is perfectly normal to find these exercise challenging. This particular example is probably the hardest example your will do in this lecture. In the personal assessment, I added a few examples; I strongly encourage you to look at them and attend the office hours to check your results.

In both examples presented in the lecture, the symmetry of the pattern equals the symmetry of the motif and is lower than the symmetry of the lattice.

In your problem set #2, you will try other (simpler) examples to see if this observation is always true or not.
Based on the observations you will do in your problem set, you will be able to define the relationship between the pattern (=exterior crystal structure), the lattice (=disposition of the anions in the crystal structure) and the motif (the group of ions, molecules, atoms present at each lattice point).

L4: 3D symmetry

Saturday, July 25, 2020 15:50

3. 3D symmetry

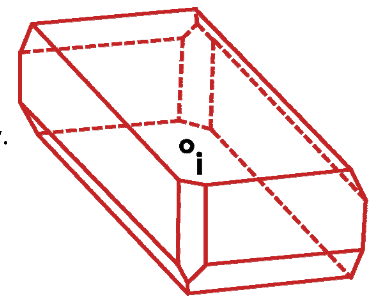
The same element of symmetry are found in 2D and 3D: center of symmetry (this time, the center of symmetry does not coincide with an A2), rotation axes (2,3,4 and 6 fold) and mirror and glide plans.

In addition, we also have:

- The rotoinversion= rotation + center of symmetry.
- The screw plan = rotation + mirror

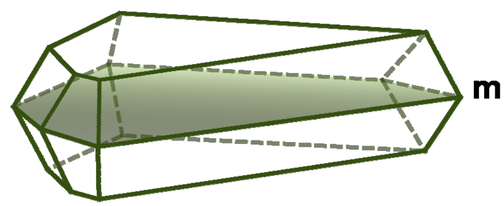
3.1 Rotoinversion

- One fold rotoinversion axis is equivalent to a center of symmetry.

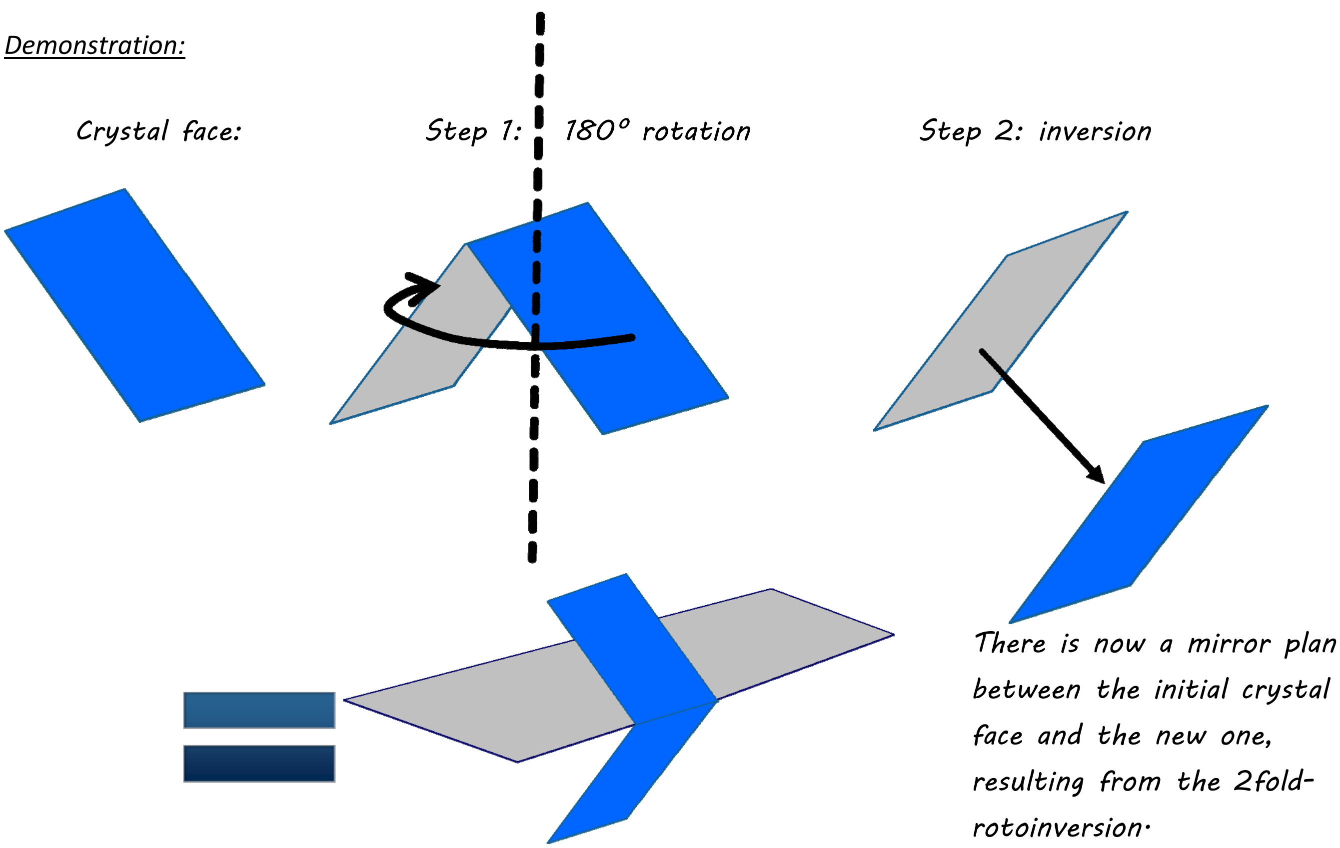


- 2-fold rotoinversion axis is equivalent to a mirror.

Step 1: 180° rotation
Step 2: center of symmetry

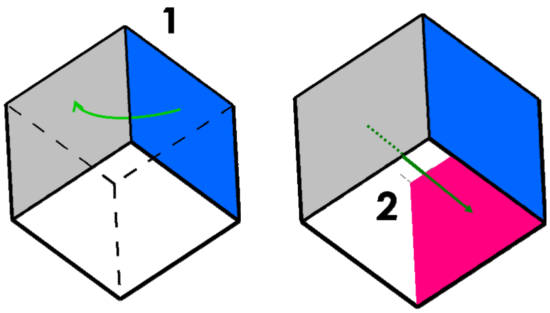


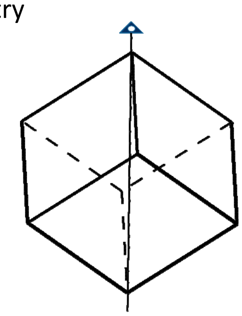
Demonstration:



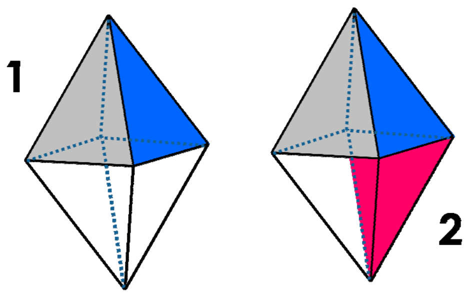
- Three-fold rotoinversion axis $(\overline{A_3})$ = (1)120° rotation (from blue to gray), 2) center of symmetry (from gray to pink).

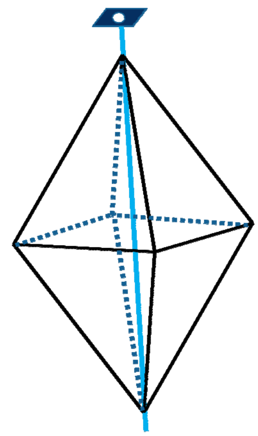
The steps below demonstrate the 3-fold rotation:



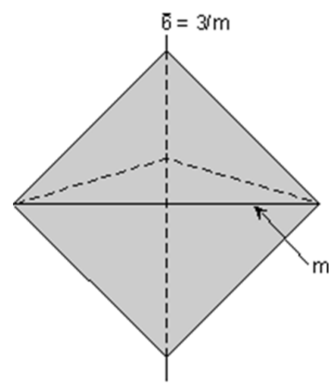


- Four-fold rotation axis $(\overline{A_4})$: (1) 90° rotation and (2) center of symmetry

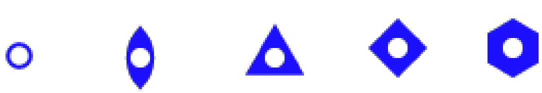




- Six-fold rotoinversion axis $(\overline{A_6})$= (1) 60° rotation, (2) center of symmetry **= A_3 + a perpendicular mirror plan.**

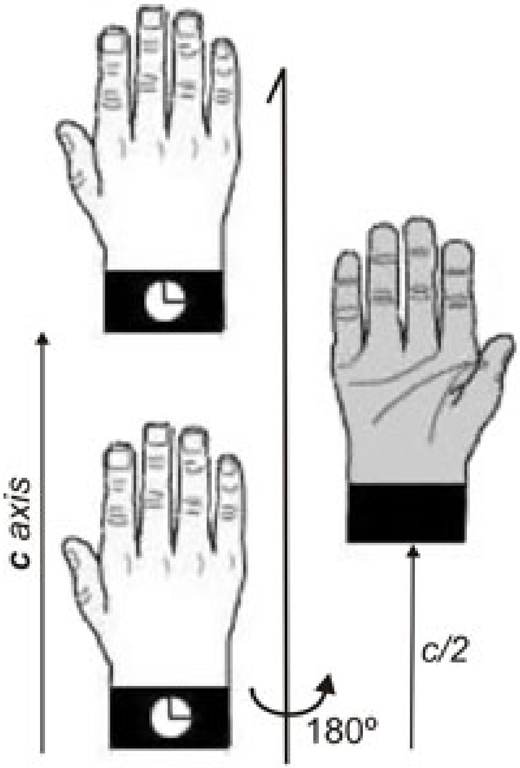


- Notation:



$\boldsymbol{i}$ $\overline{A_2}$ $\overline{A_3}$ $\overline{A_4}$ $\overline{A_6}$

3.2. Screw plan = translation + rotation.



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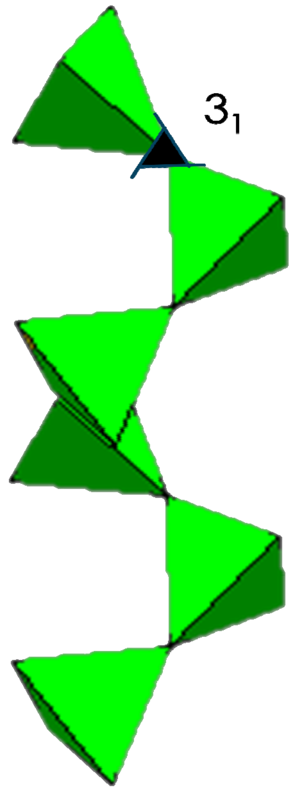


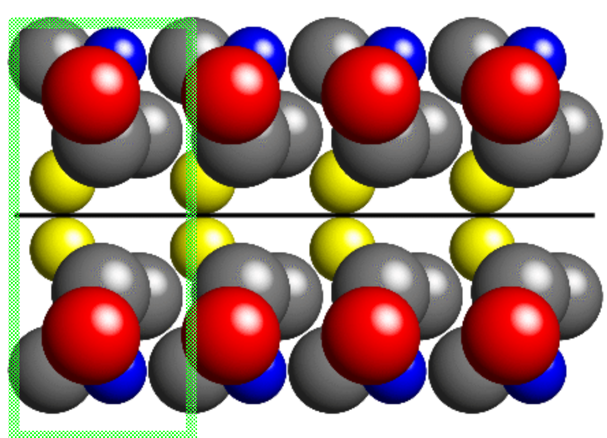
In this case, the screw axis is located at a corner of the tetrahedra. This is not always the case.

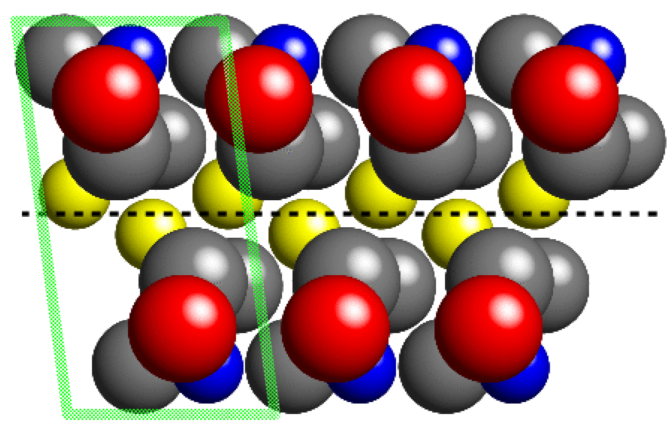
To visualize another version of a 3_1 axis in 3D, open **3D symmetry models.html** posted on Canvas with your internet browser.

This is the hardest element of symmetry to visualize.

The easiest comparison between glide and screw symmetry is to consider the case of a 2-fold screw symmetry.
For both glide and two-fold screw symmetry, the **amount of translation** along the axis is exactly one half of the length of the unit cell along the axis direction (in other words, **half of the distance between two lattice points** along the axis direction.

- **Mirror vs glide:**

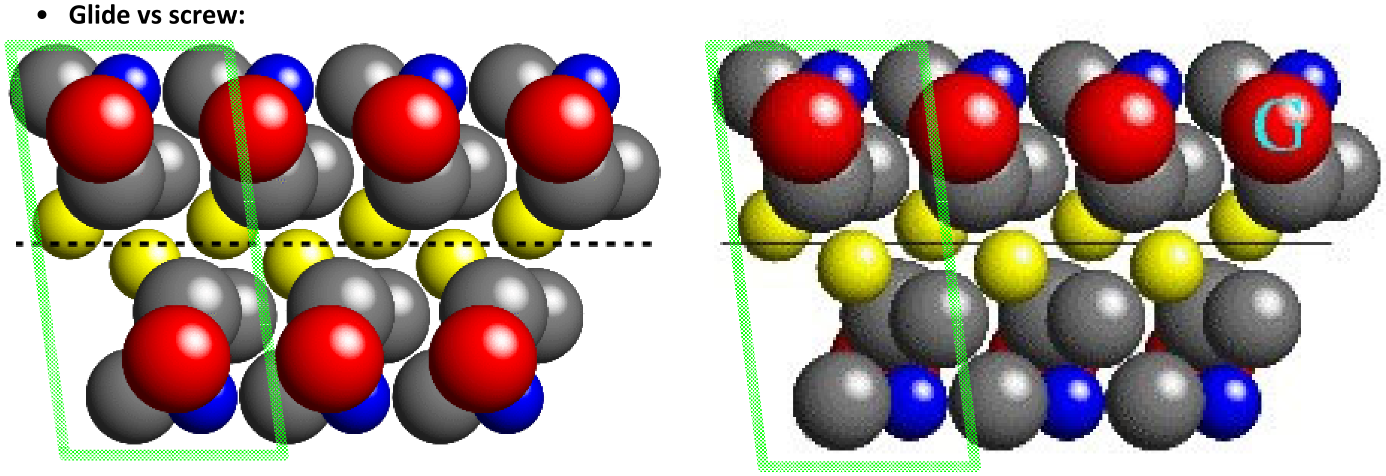




Credits: Department of Chemistry, University College London

The elements of the motif have the same orientation in both pattern, but in the first case (left), the motif shows a mirror plan, while in the second case (right), the motif show a mirror+translation plan = glide plan.

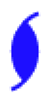
- **Glide vs screw:**



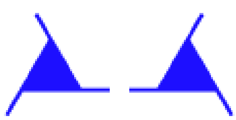
Credits: Department of Chemistry, University College London

The first case is the glide plan represented above. The motif in the second case (right) has the same translation, but the mirror plan is replaced by a 2-fold rotation axis (A_2).

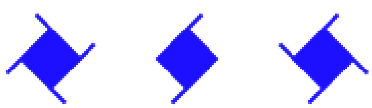
- **Notation:**



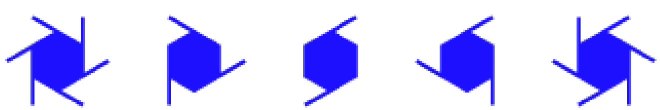
2-fold screw axis: rotation of 120° + translation of 1/2 of the distance between two lattice points (**2_1**)



3-fold screw axes: rotation of 120° + translation of either 1/3 (**3_1**) or 2/3 (**3_2**) of the distance between the two lattice points.



4-fold screw axes: rotation of 90°. The translation can be 1/4,1/2 or 3/4 (**4_1, 4_2, 4_3,** respectively)



6-fold screw axes: rotation of 60°. The translation can be 1/6, 1/3, 1/2, 2/3, or 5/6 (**6_1, 6_2, 6_3,6_4, 6_5,** respectively)

You don't need to remember all the various screw symmetry, I just want you to recognize the symbol when you see it.

L4: 32 Crystal classes

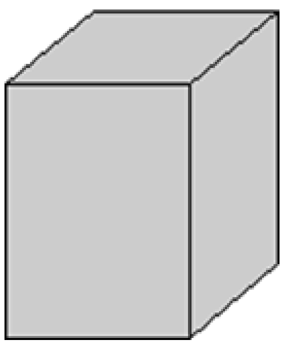
Wednesday, July 29, 2020 7:19

3.3. Combination of symmetry operations

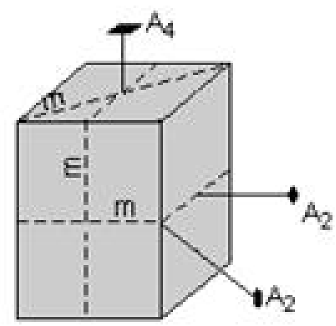
In crystals there are 32 possible combinations of symmetry elements. These 32 combinations define the **32 Crystal Classes**. Every crystal must belong to one of these 32 crystal classes.

In this section, we will go over each of these crystal classes, but the best way to be able to identify each crystal class is to pick up the plastic models you have in your kits, look at them and rotate them around. You will do that during the 3rd lab. But this lecture should help you to do this lab.

Right now, we will just look at one example. The crystal has rectangular-shaped sides with a square- shaped top and bottom. Can you tell what is is its crystal system?

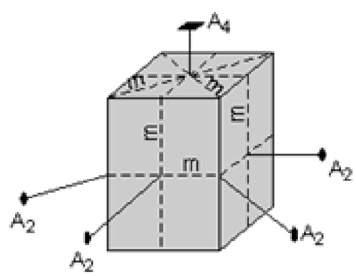


= tetragonal (or quadratic) system ($a = b \neq c$; $\alpha = \beta = \gamma = 90°$).
Let's look together at the elements of symmetry of this crystal:



- The square-shaped top indicates that there must be
  - a 4-fold rotation axis perpendicular to the square shaped face.
  - A 2-fold axis that cuts diagonally through
  - Mirror plan through the diagonal
- Rectangular faces: 2-fold rotation axis perpendicular to the rectangular face.
- Square top + rectangular sides:
  - mirror plan parallel to the 4-fold axis
  - mirror plan perpendicular to the 4-fold axis
  - One center of symmetry

The operation of the 4-fold rotation must reproduce the face and the diagonal with the perpendicular 2-fold axis on a 90° rotation.



Thus, this crystal has the following symmetry elements:
one 4-fold rotation axis (A4)
four 2-fold rotation axes (A2), 2 cutting the faces & 2 cutting the edges.
five mirror planes (m), 2 cutting across the faces, 2 cutting through the edges, and one cutting horizontally through the center.
one center of symmetry
The symmetry content of this crystal is thus: i, $1A_4$, $4A_2$, 5m

If you look at the list of the 32 classes, you should see that this crystal belongs to the ditetragonal dipyramidal class.

Crystal System		Crystal Class / Crystal Form	Symmetry of Class
Isometric System		**hexoctahedron**	i, $3A_4$, $\mathbf{4A_3}$, $6A_2$, 9m
		gyroid	$3A_4$, $\mathbf{4A_3}$, $6A_2$
		hextetrahedron	$3A_2$, $\mathbf{4A_3}$, 6m
		diploid	i, $3A_2$, $\mathbf{4A_3}$, 3m
		tetartoid	$3A_2$, $\mathbf{4A_3}$
Hexagonal System	Hexagonal Division	**dihexagonal dipyramid**	i, $\mathbf{1A_6}$, $6A_2$, 7m
		hexagonal trapezohedron	$\mathbf{1A_6}$, $6A_2$
		dihexagonal pyramid	$\mathbf{1A_6}$, 6m
		ditrigonal dipyramid	$\mathbf{1R_6}$, $3A_2$, 3m
		hexagonal dipyramid	i, $\mathbf{1A_6}$, 1m
		hexagonal pyramid	$\mathbf{1A_6}$
		trigonal dipyramid	$\mathbf{1R_6}$
	Rhombohedral Division	**hexagonal scalenohedron**	i, $\mathbf{1A_3}$, $3A_2$, 3m
		trigonal trapezohedron	$\mathbf{1A_3}$, $3A_2$
		ditrigonal pyramid	$\mathbf{1A_3}$, 3m
		rhombohedron	i, $\mathbf{1A_3}$
		trigonal pyramid	$1A_3$
Tetragonal System		**ditetragonal dipyramid**	i, $\mathbf{1A_4}$, $4A_2$, 5m
		tetragonal trapzohedron	$\mathbf{1A_4}$, $4A_2$
		ditetragonal pyramid	$\mathbf{1A_4}$, 4m
		tetragonal scalenohedron	$\mathbf{1R_4}$, $2A_2$, 2m
		tetragonal dipyramid	i, $\mathbf{1A_4}$, 1m
		tetragonal pyramid	$\mathbf{1A_4}$
		tetragonal disphenoid	$1R_4$
Orthorhombic System		**rhombic dipyramid**	i, $3A_2$, 3m
		rhombic disphenoid	$3A_2$
		rhombic pyramid	$1A_2$, 2m
Monoclinic System		**prism**	i, $1A_2$, 1m
		sphenoid	$1A_2$
		dome	1m
Triclinic System		**parallelohedron**	i
		monohedron	no symmetry

4. 32 Crystal classes

4.1. Hermann-Mauguin symbols.

Hermann-Mauguin symbols or **international symbols** are used to describe the crystal classes from the symmetry content.

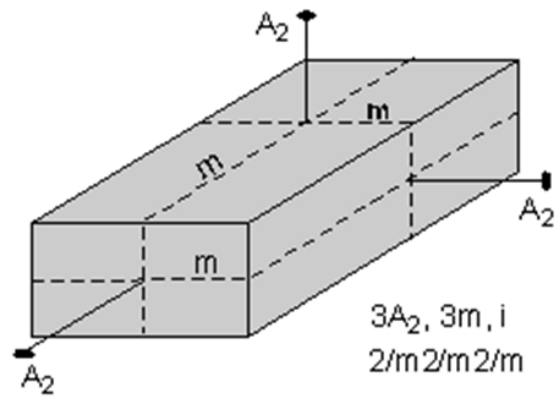
Rules:

1) Write the **number** representing **each of the unique rotation axes present**.

Unique means that the element of symmetry cannot be reproduced by another element of symmetry (i.e., intersects a face that looks different, or at another location of the face).

e.g., we have 3 unique A2, they intersect different looking faces:

2 2 2



2) Next write a "**m**" for each **unique mirror plane**

e.g., we also have 3 unique mirrors:

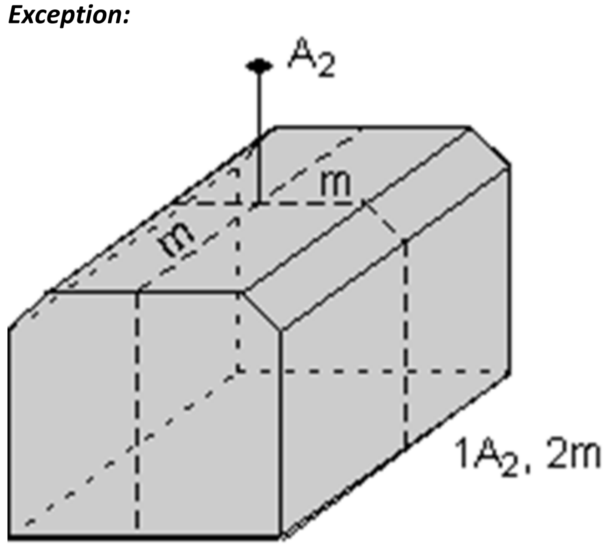
2 m 2 m 2 m

3) Then if a **rotation axis is perpendicular to a mirror plan**, put a **"/"** between the rotation axis and the mirror plane

e.g., finally, each mirror is perpendicular to one of the A_2:

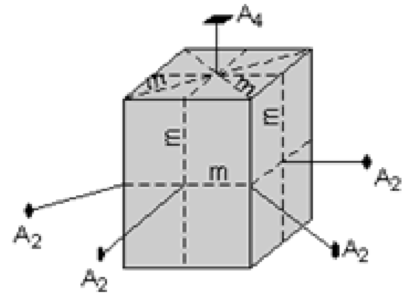
The Hermann-Mauguin symbols of this crystal are: 2/m2/m2/m and it belongs to the rhombic dipyramidal class.

Exception:



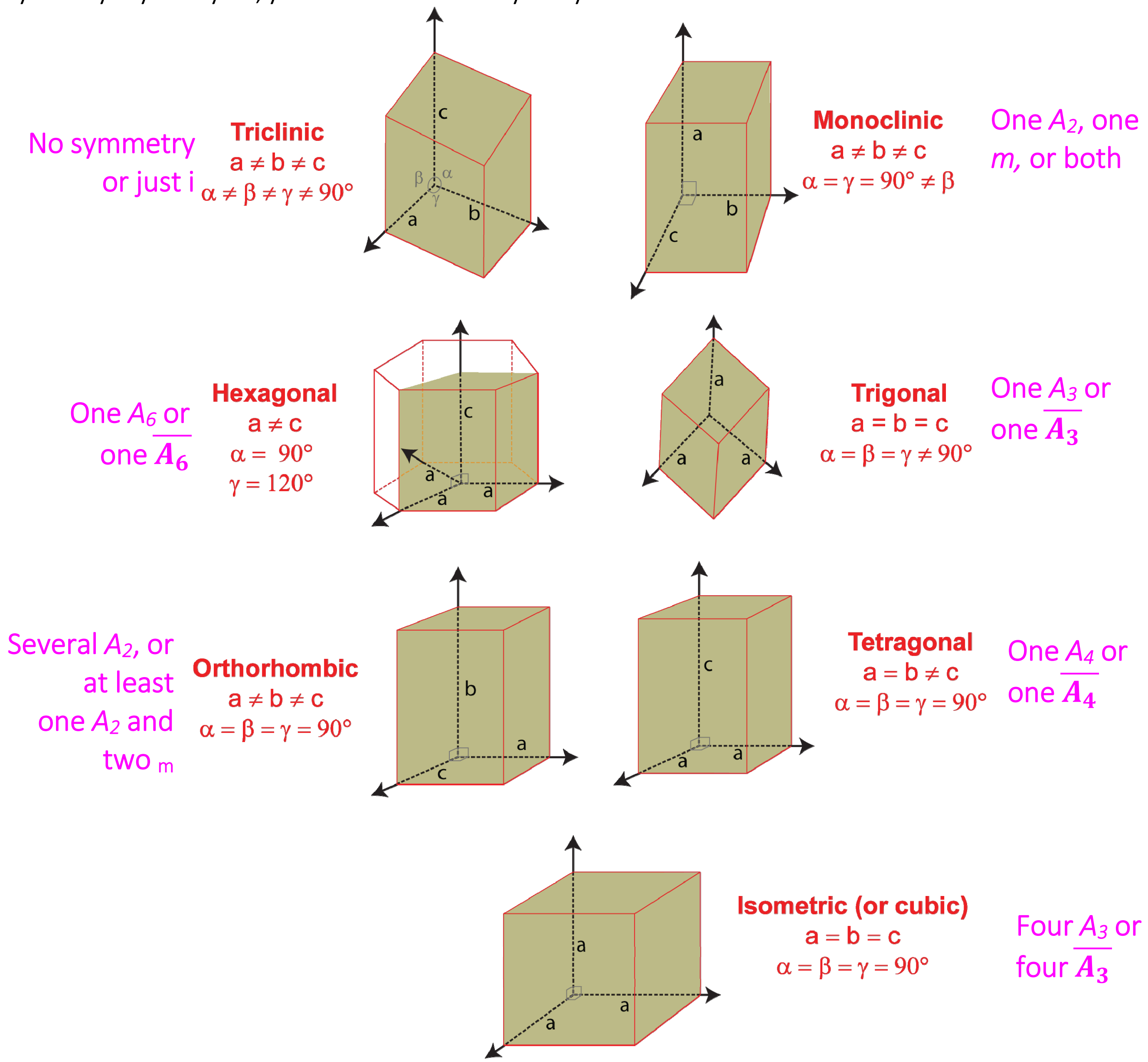
*Following these rules, the HM symbols for this crystal should be 2mm. However, we use **mm2.***

Your turn! Find the Hermann-Mauguin symbols of this crystal (answer at the end of the personal assessment)



4.2. Diagnostic symmetry

Each crystal system is characterized by one or several **diagnostic element(s) of symmetry**: if you identify these elements of symmetry in your crystal, you can determine its crystal system:



In lab 3 and 4, you will need to define the crystallographic axes in relation to the elements of symmetry in each of the crystal systems.

- **Triclinic -** Since this system has such low symmetry there are no constraints on the axes, but the most pronounced face should be taken as parallel to the c axis.
- **Monoclinic** - The A_2 is the b axis, or if only a mirror plane is present, the b-axis is perpendicular to the mirror plane.
- **Orthorhombic** - The current convention is to take the longest axis as b, the intermediate axis is c, and the shortest axis is a. The old convention was to take c has the longest axis and a as the shortest axis. You will find both in the literature.
- **Tetragonal** - The c axis is either the A_4 or the $\overline{A_4}$
- **Hexagonal** - The c axis is parallel to the 6-fold axis
- **Trigonal**- The c axis is parallel to the 3-fold axis
- **Isometric** - The equal length a axes are either parrallel to the three 3 4-fold axes, or, in cases where no 4-fold axis present, the three 2-fold axes

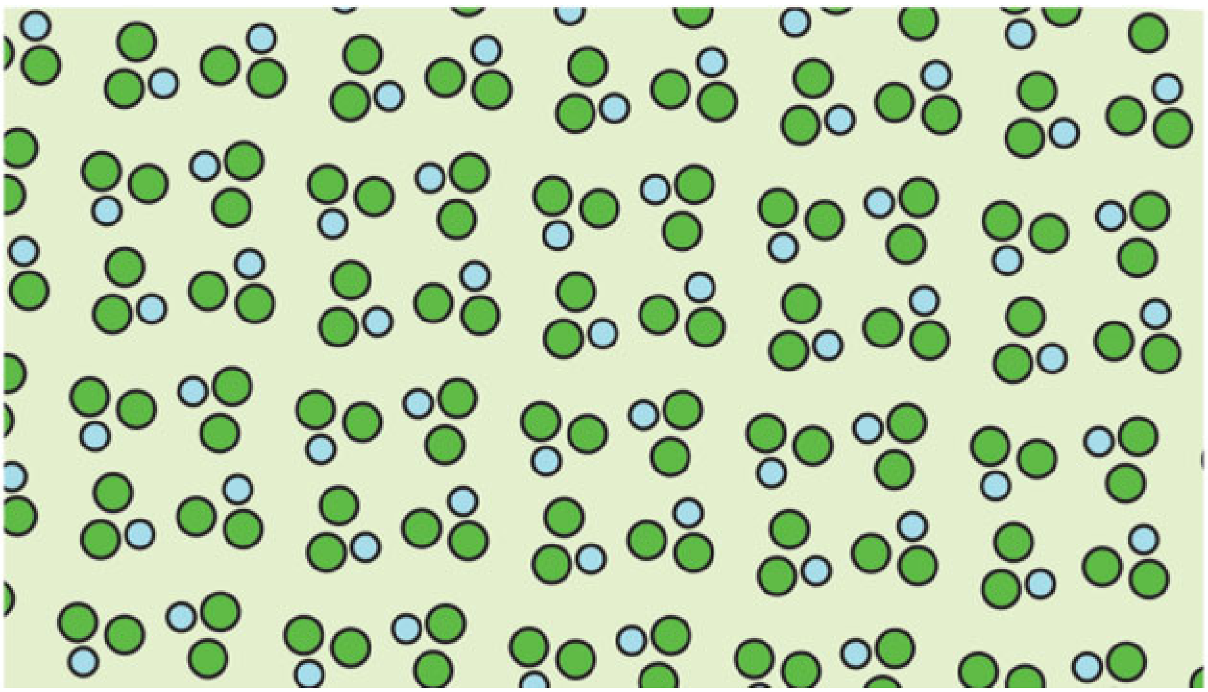
L4: Personal assessment

Monday, July 27, 2020 18:50

After reviewing the third lecture, you can try to answer these questions. Visualizing elements of symmetry is a difficult exercise, so if you can't answers all the questions on the first try, don't despair and keep practice. Our TA and myself are here to help.

****Multiple choices possible!****

1) **How many types of symmetry operation are present this pattern?**



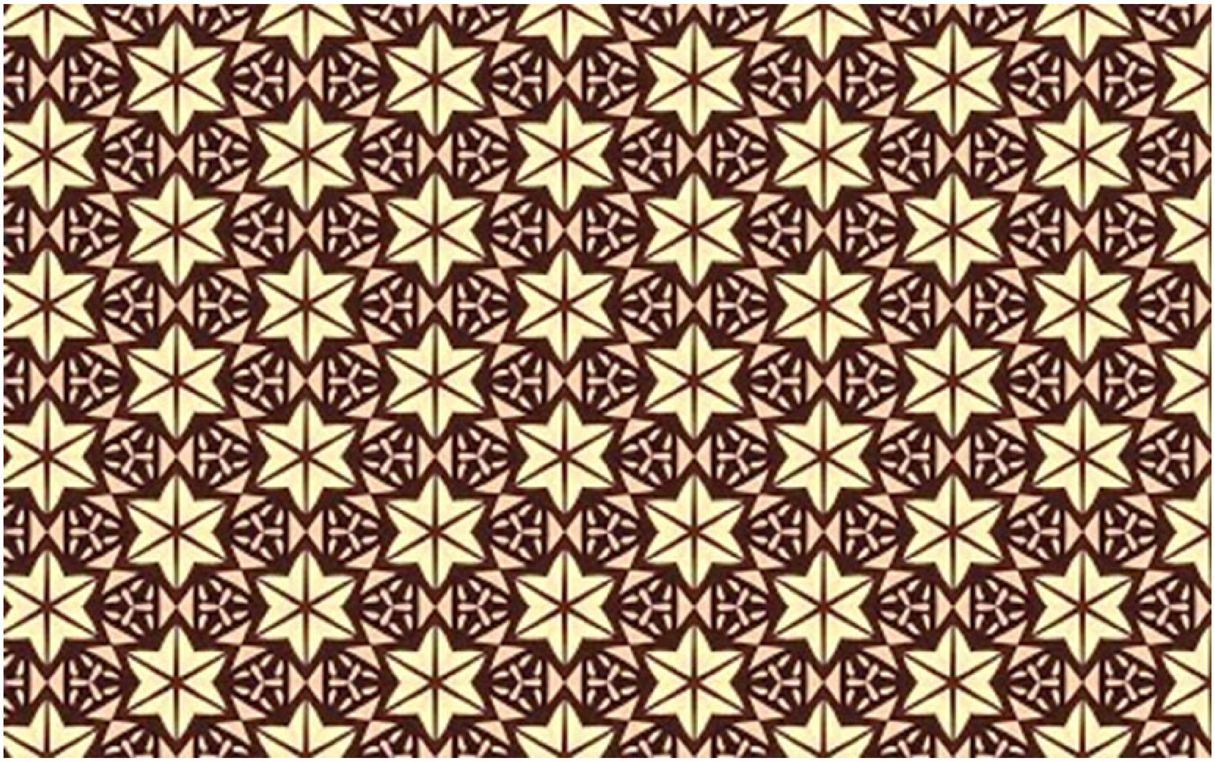
A - 1 **B - 2** **C - 3** **D - 4**

3) **The diagonal of a rectangle is a mirror.**

A - True **B - False**

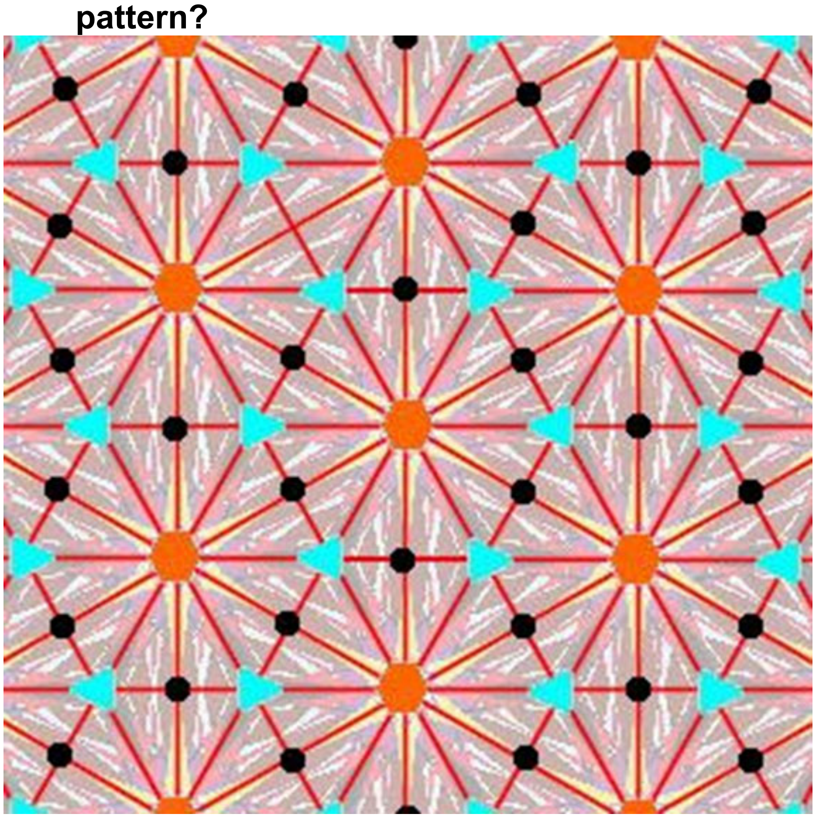
3) **Draw the element of symmetry of a rectangle (p) lattice.**

4) **This pattern contains:**



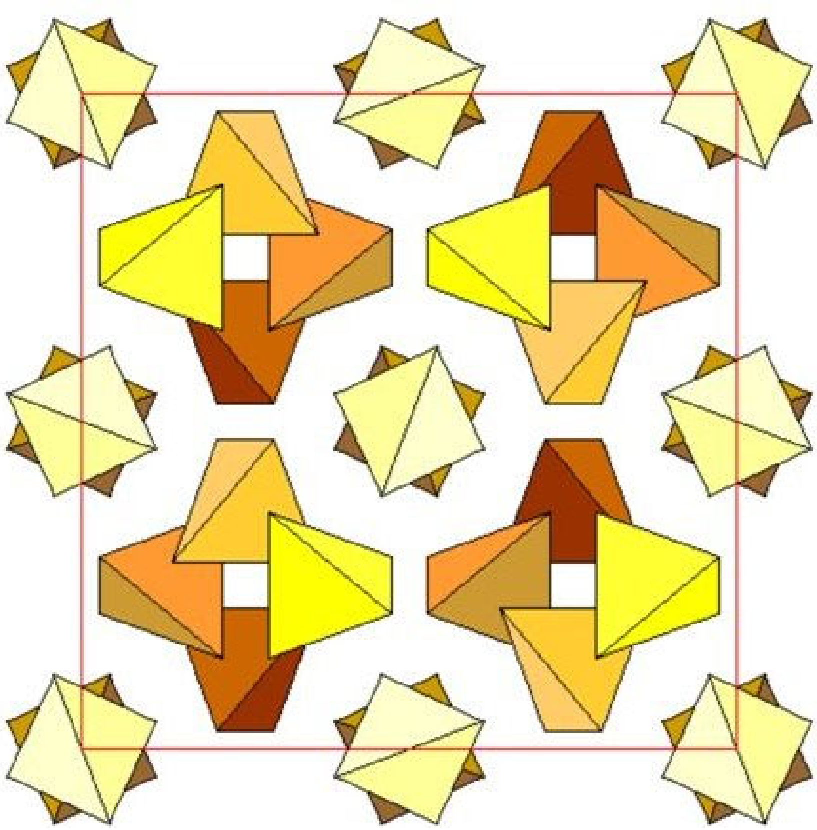
A - A6 **B - A3** **C - A2** **D - g (glide)**

4) **What are the elements of symmetry in the motif? In the lattice? In the pattern?**

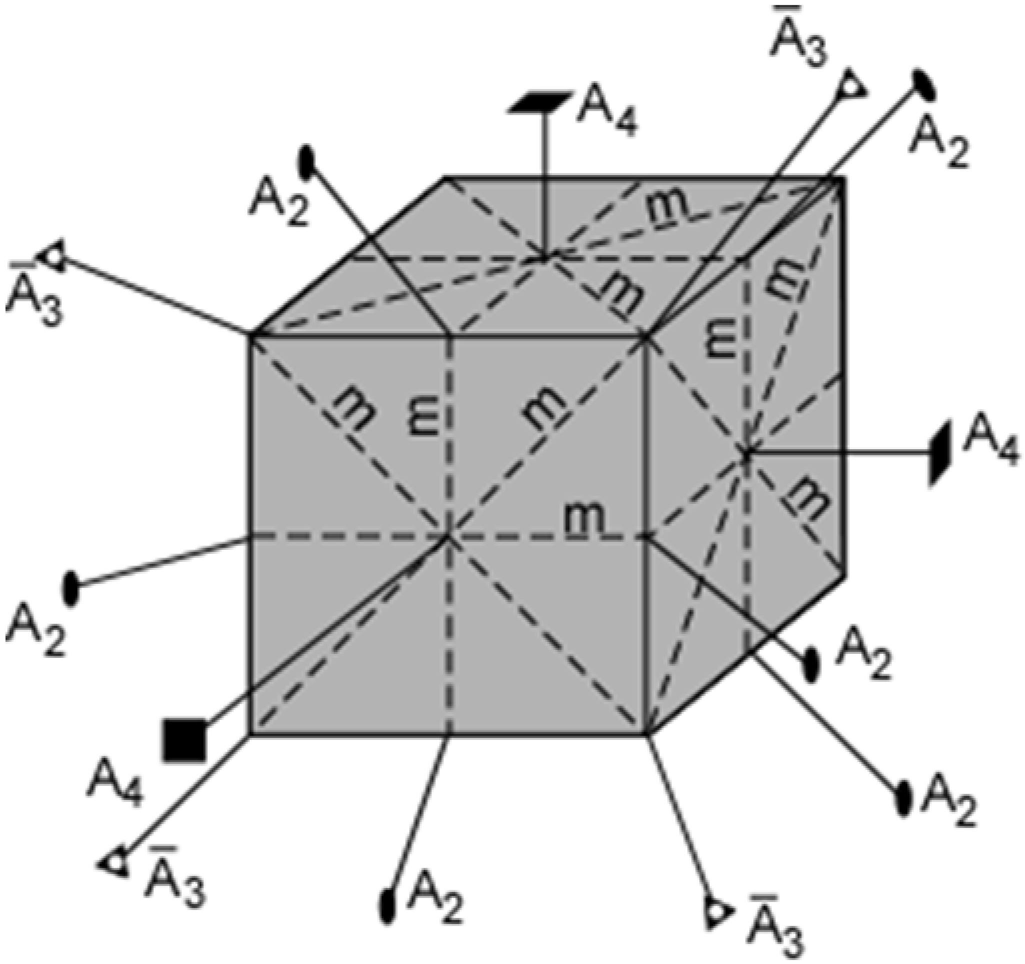


6) What is the crystal lattice represented by this pattern? What are the elements of symmetry of the pattern?

7) What is the symmetry relationship between the silica tetrahedra in this mineral structure?



8) Knowing that a cube present: 3 A_4, 4 $\overline{A_3}$, 6 A_2, 9 *m* and i, determine the Hermann-Mauguin symbols and the crystal class of a cube.



9) The Herman-Mauguin symbol of bismutite are mm2, hence this minerals belongs to:

A - the monoclinic system
B - the orthorhombic system
C - the pyramidal class
D - the dipyramidal class.

Keys for ditetragonal-dipyramidal crystal:
4/m2/m2/m