

Crystal Symmetry

The external shape of a crystal reflects the presence or absence of translation-free symmetry elements in its unit cell.

While not always immediately obvious, in most well formed crystal shapes, *axis of rotation*, *axis of rotoinversion*, *center of symmetry*, and *mirror planes* can be spotted.

All discussed operations may be combined, but the number of (i.e. unique) combinations is limited, to 32. Each of these is known as a point group, or crystal class.

The crystal classes may be sub-divided into one of 6 crystal systems.

Space groups are a combination of the 3D lattice types and the point groups (total of 65).

Each of the 32 crystal classes is unique to one of the 6 crystal systems:

Triclinic, monoclinic, orthorhombic, tetragonal, hexagonal and isometric (cubic)

Interestingly, while all mirror planes and poles of rotation must intersect at one point, this point may not be a center of symmetry (*i*).

Crystallographic Axes

The identification of specific symmetry operations enables one to orientate a crystal according to an imaginary set of reference lines known as the *crystallographic axes*.

These are distinct and different from the classic Cartesian Axes, x , y and z , used in other common day usage, such as plotting graphs.

With the exception of the hexagonal system, the axes are designated ***a***, ***b***, and ***c***.

The ends of each axes are designated **+** or **-**. This is important for the derivation of *Miller Indices*.

The angles between the positive ends of the axes are designated **α** , **β** , and **γ** .

α lies between ***b*** and ***c***.

β lies between ***a*** and ***c***.

γ lies between ***a*** and ***b***.

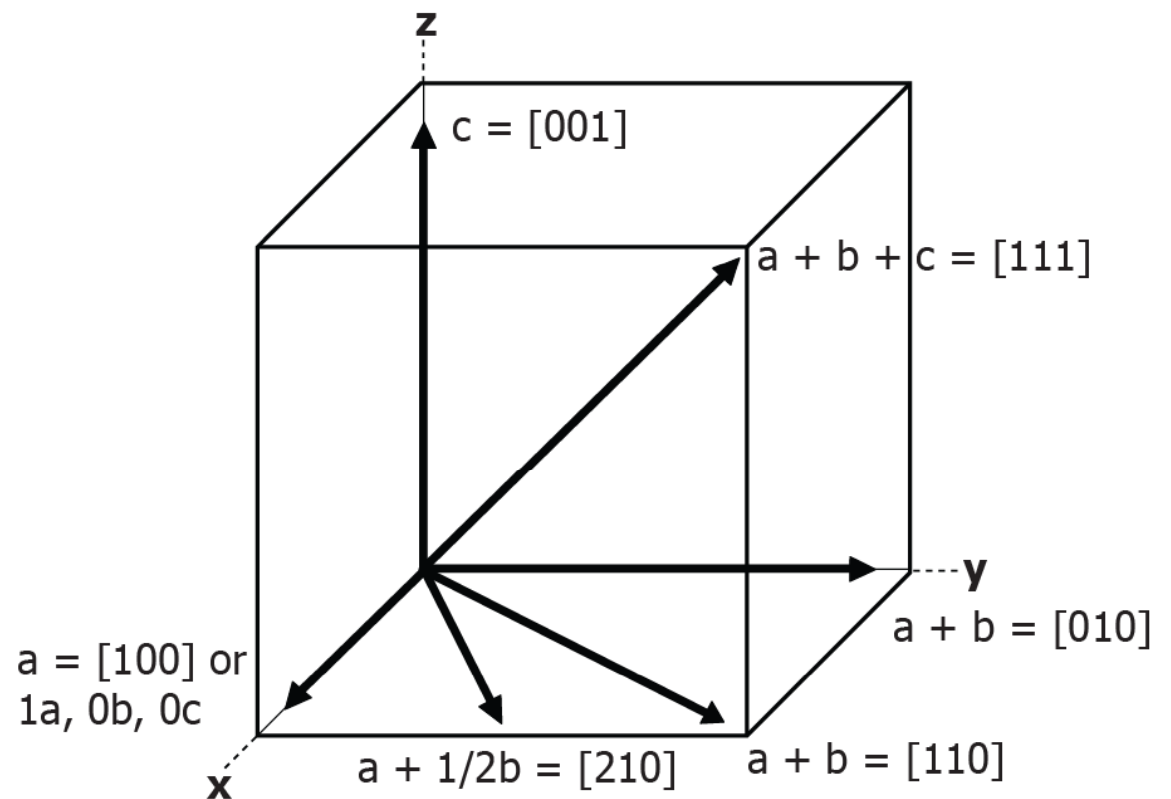
Quantities can also be applied to further describe *vectors* and planes relative to **a**, **b**, and **c**

These are **u**, **v**, **w**:

u: projection along **a**

v: projection along **b**

w: projection along **c**



Quantities can also be applied to further describe vectors and *planes* relative to **a**, **b**, and **c**

These are **h**, **k**, **l**:

h: information relative to **a axis**

v: information relative to **b axis**

w: information relative to **c axis**

[uvw] with (hkl)

(hkl) faces on a cube

Axial Ratios

With the exception of the cubic (isometric) system, there are crystallographic axes differing in length.

Imagine one single unit cell and measuring the lengths of the a , b , and c axes.

To obtain the axial ratios we normalise to the b axis.

These ratios are relative.

Unique crystallographic axes of the 6 crystal systems

Triclinic: Three unequal axes with oblique angles.

Monoclinic: Three unequal axes, two are inclined to one another, the third is perpendicular.

Orthorhombic: Three mutually perpendicular axes of different lengths.

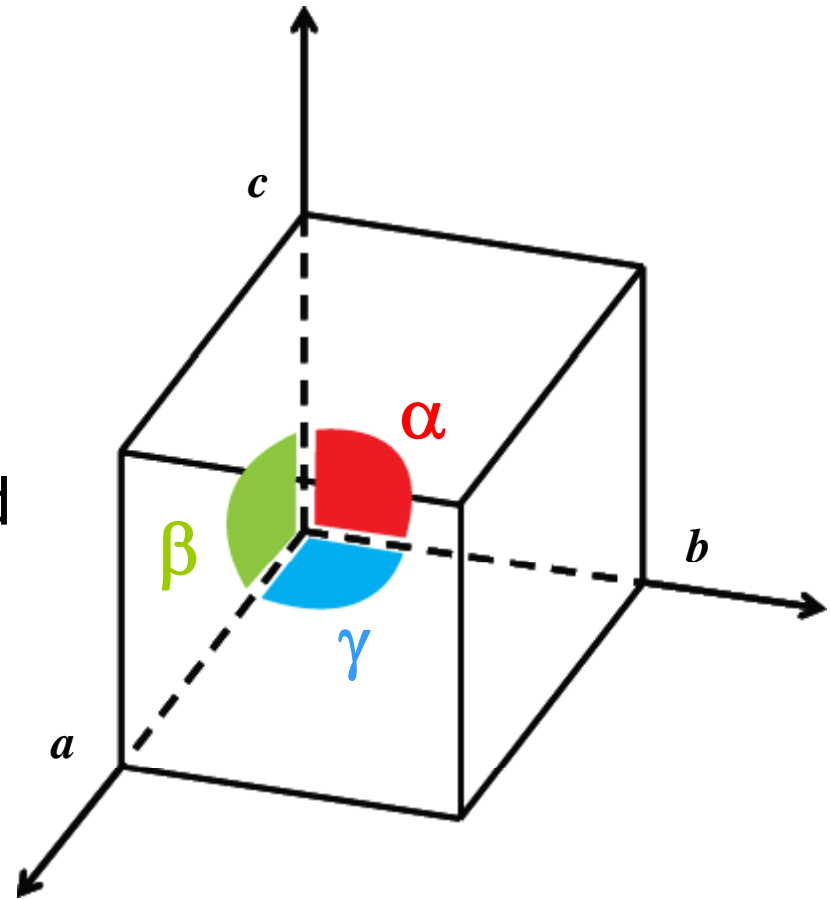
Tetragonal: Three mutually perpendicular axes, two are equal, the third (vertical) is shorter.

Hexagonal: Three equal horizontal axes (a_1, a_2, a_3) and a 4th perpendicular (vertical) of different length.

Cubic: Three perpendicular axes of equal length.

Triclinic: Three unequal axes with oblique angles.

- To orientate a triclinic crystal the most pronounced zone should be vertical.
- a and b are determined by the intersections of (010) and (100) with (001).
- The b axis should be longer than the a axis.



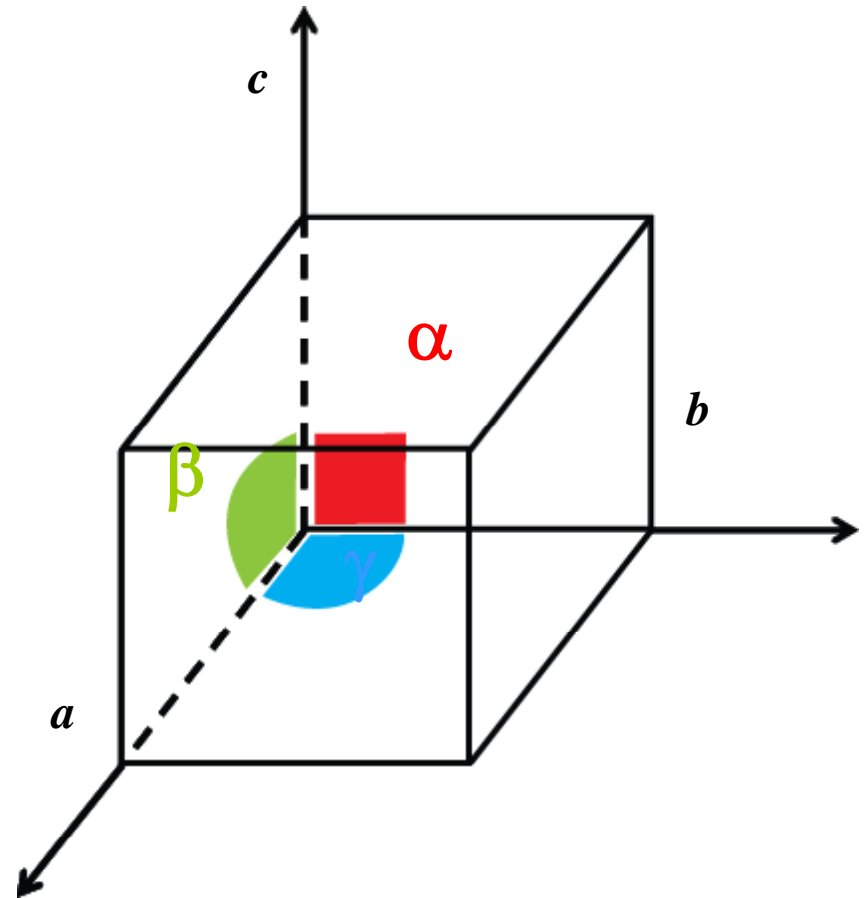
The unique symmetry operation in a triclinic system is a 1-fold axis of rotoinversion (equivalent to a center of symmetry or inversion, $\bar{1}$).

All forms are pinacoids – therefore must consist of two identical and parallel faces.

Common triclinic rock-forming minerals include microcline, some plagioclases, and wollastonite.

Monoclinic: Three unequal axes, two are inclined with oblique angles, the third is perpendicular.

- Orientation of a crystal has few constraints – b is the only axis fixed by symmetry.
- c is typically chosen on the basis of habit and cleavage.
- a and $\gamma = 90^\circ$.
- There are some very rare cases where b equals 90° giving a pseudo-orthorhombic form.



The unique symmetry operation in a monoclinic system is $2/m$ – a twofold axis of rotation with a mirror plane.

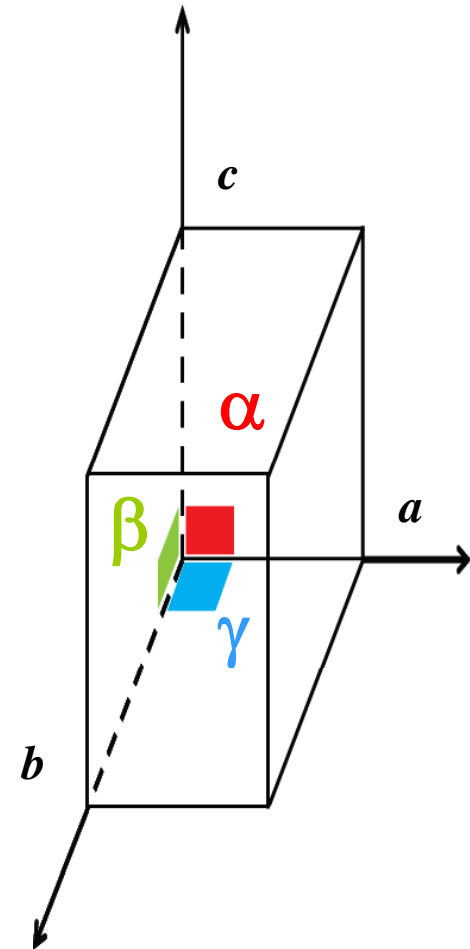
b is the rotation, while a and c lie in the mirror plane.

Monoclinic crystals have two forms: pinacoids and prisms.

Common monoclinic rock-forming minerals include clinopyroxene, mica, orthoclase and titanite.

Orthorhombic: Three mutually perpendicular axes of different lengths.

- Convention has it that a crystal is oriented such that $c > b > a$.
- Crystals are oriented so that c is parallel to crystal elongation.
- In this case the length of the b axis is taken as unity and ratios are calculated thereafter.



The unique symmetry operation in an orthorhombic system is $2/m\ 2/m\ 2/m$ – Three twofold axis of rotation coinciding with the three crystallographic axes.

Perpendicular to each of the axes is a mirror plane.

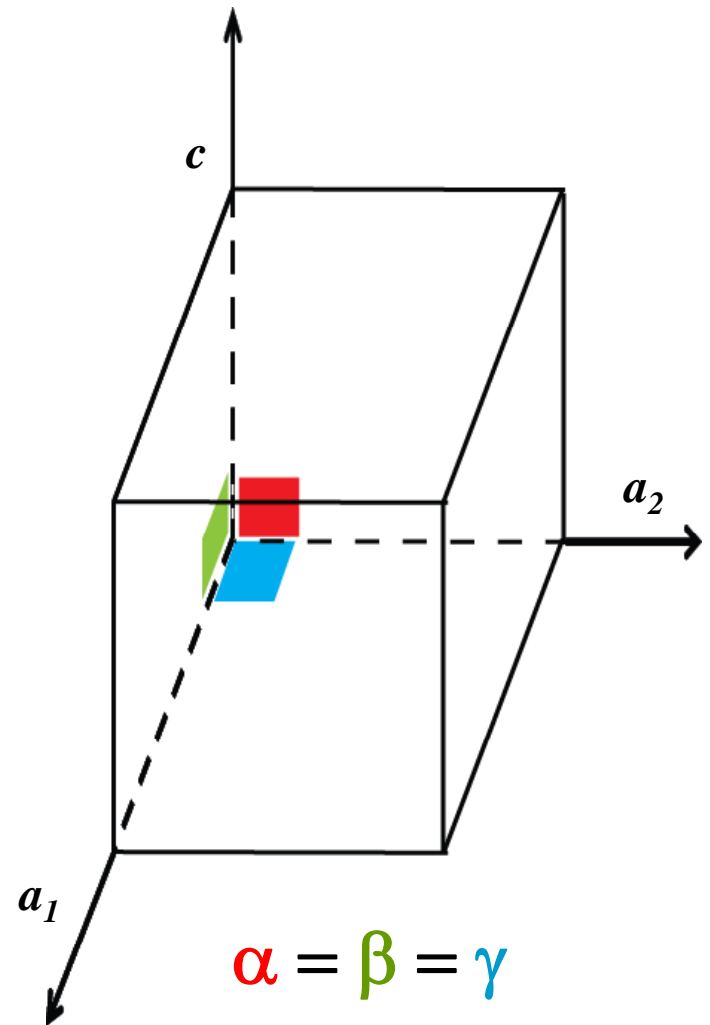
The general class for the orthorhombic system are *rhombic dipyramid* $\{hkl\}$.

There are three types of form in the class: pinacoids, prisms, and dipyramids.

Common orthorhombic rock-forming minerals include andalusite and sillimanite, orthopyroxene, olivine and topaz.

Tetragonal: Three mutually perpendicular axes, two are equal, the third (vertical) is shorter.

- The two horizontal axis in a tetragonal mineral are oriented in the plane of the horizontal. Therefore, if $a = b$, c must be in the vertical.
- There is no rule as to whether c is greater or less than a .



The unique symmetry operation in a tetragonal system is $4/m\ 2/m\ 2/m$ – The vertical axis (c) is always a fourfold axis of rotation.

There are 4 two-fold axis of rotation: 2 parallel to the crystallographic axes a and b , the others at 45° .

There are 5 mirror planes.

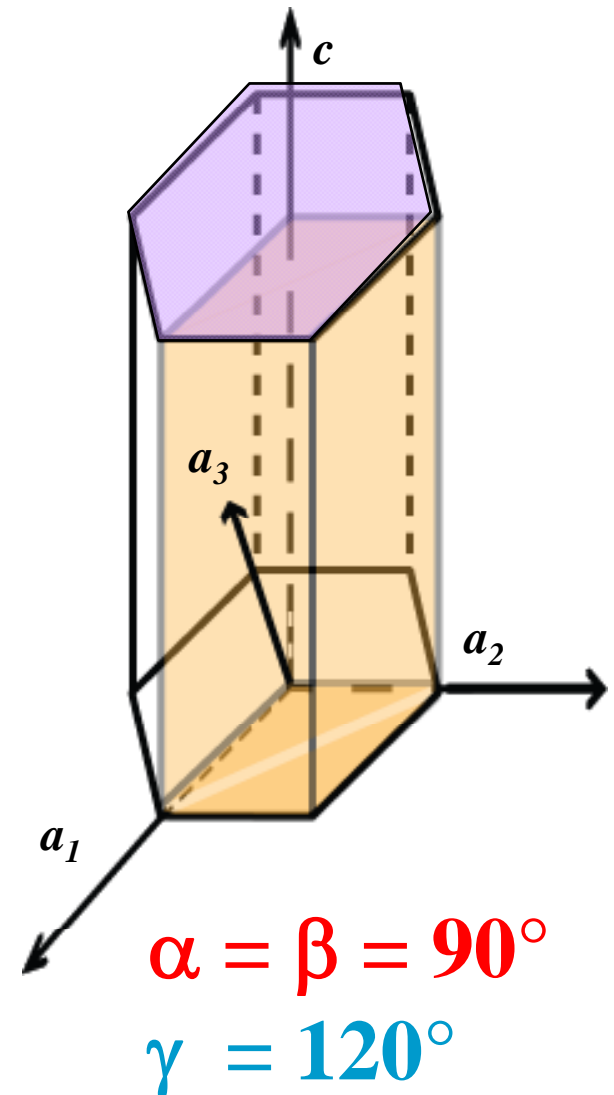
The general class for the orthorhombic system is known as the *ditetragonal-dipyramidal class*.

There are four types of form in the class: basal pinacoids, tetragonal prisms, tetragonal dipyramids, and ditetragonal prisms.

Common tetragonal rock-forming minerals include zircon, rutile and anatase, and apophyllite.

Hexagonal: Three equal horizontal axes (a_1, a_2, a_3) and a 4th perpendicular vertical axis of different length.

- The three horizontal axis of a hexagonal mineral are oriented in the plane of the horizontal, with c in the vertical.
- Unlike the other systems the Bravais-Miller nomenclature for crystal faces is given by 4 numbers (i.e. $\{0001\}$)
- The first three numbers are listed in order of a_1, a_2, a_3 .



The unique symmetry operation in the hexagonal system is a six-fold axis of rotation, and the most common space group is $6/m\ 2/m\ 2/m$.

The vertical axis is the six-fold rotational operation, while there are a further 6 two-fold axes of rotation in the horizontal plane (3 coincide with the a_n axes).

There are 7 mirror planes.

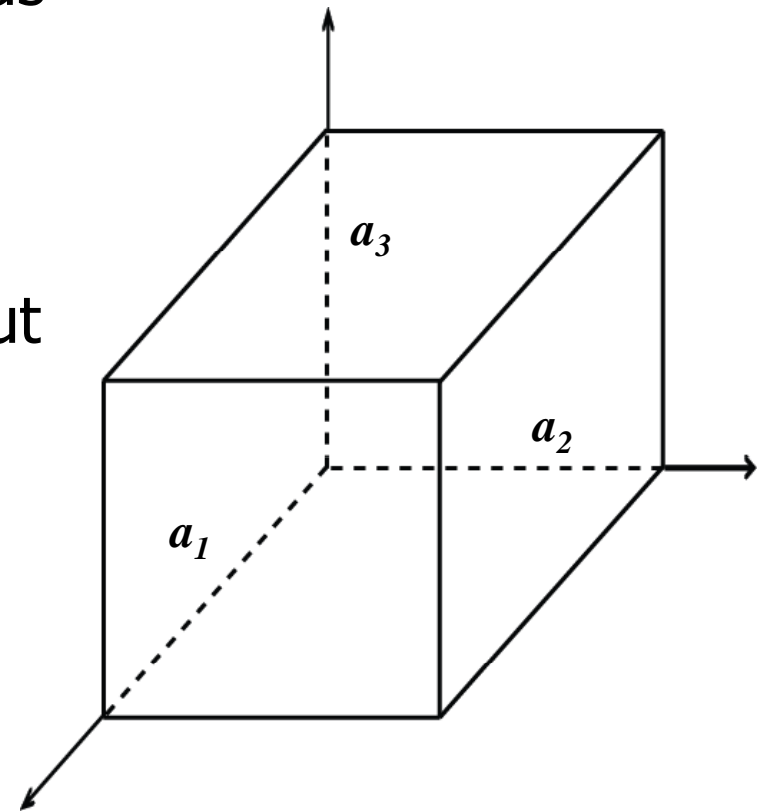
The general class for the orthorhombic system is known as the *dihexagonal-dipyramidal class*.

There are five types of form in the class: pinacoids, hexagonal prisms, hexagonal dipyramids, dihexagonal prisms, and dihexagonal dipyramids.

Common hexagonal minerals include beryl and apatite.

Isometric (cubic): Three equal length axes that intersecting at right-angles to one another.

- The axes are indistinguishable, as are the intersecting angles. As such all are interchangeable.
- There are 15 isometric forms, but the most common are:
 - Cube
 - Octahedron
 - Dodecahedron
 - Tetrahexahedron
 - Trapezohedron
 - Trisoctahedron
 - Hexoctahedron



$$\alpha = \beta = \gamma = 90^\circ$$