U3A

Introduction to Crystallography

Crystallography

Crystallography is the “study of crystals and the crystalline state”

- Crystal definition:

“ A regular polyhedron bounded by planes called crystal faces”

- in crystalline substances atoms or groups of atoms occur in a regular 3-dimensional pattern called a crystal lattice

- crystal faces develop parallel to planes of atoms in the internal crystal lattice forming a number of lattice types

- almost all minerals are crystalline

- minerals crystallise in one of seven crystal systems

Seven crystal systems

Cubic

Tetragonal

Hexagonal

Trigonal

Orthorhombic

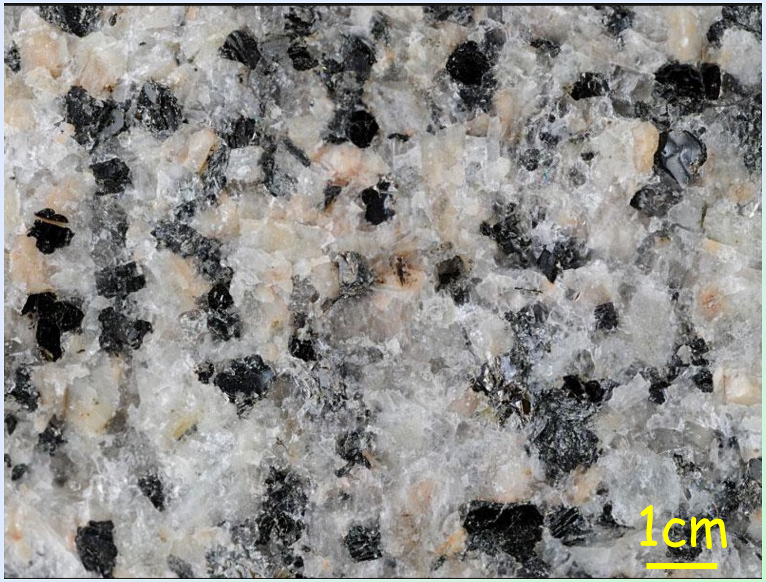
Monoclinic

Triclinic

Occurrence of quartz crystals

Smokey quartz crystals grown in a cavity in rhyolite

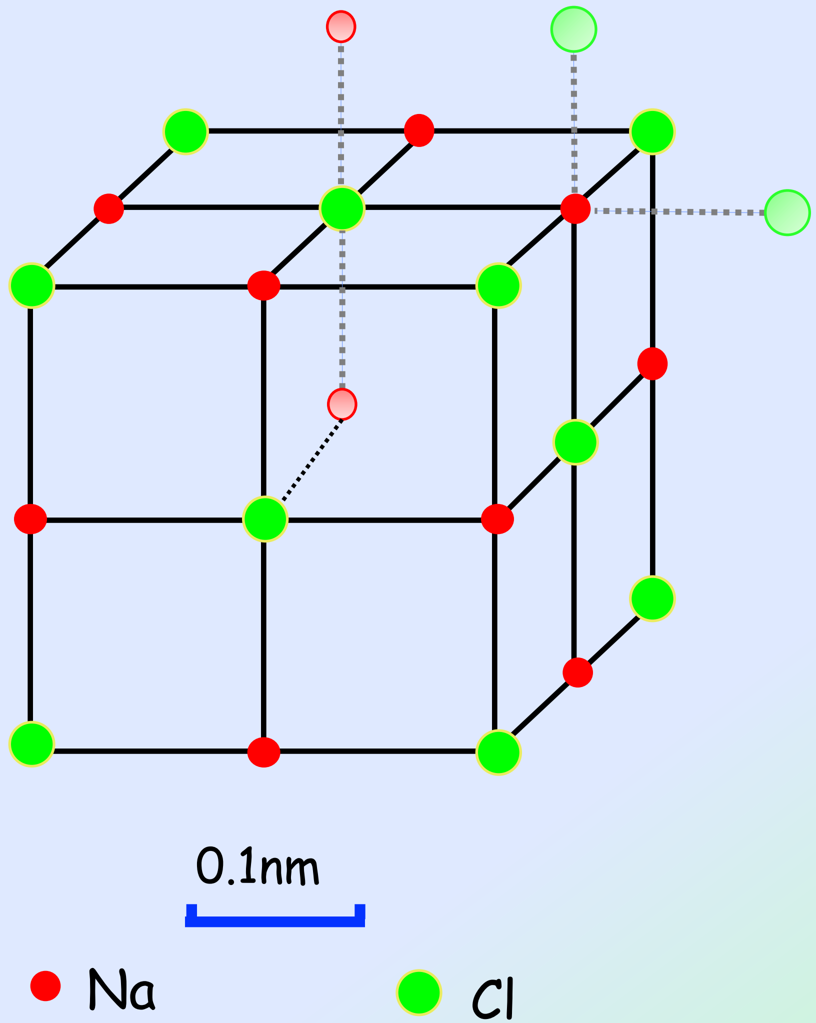
Staurolite crystal in schist



Granite

NaCl crystal lattice

Na and Cl ions are in 6-fold co-ordination in a cubic lattice



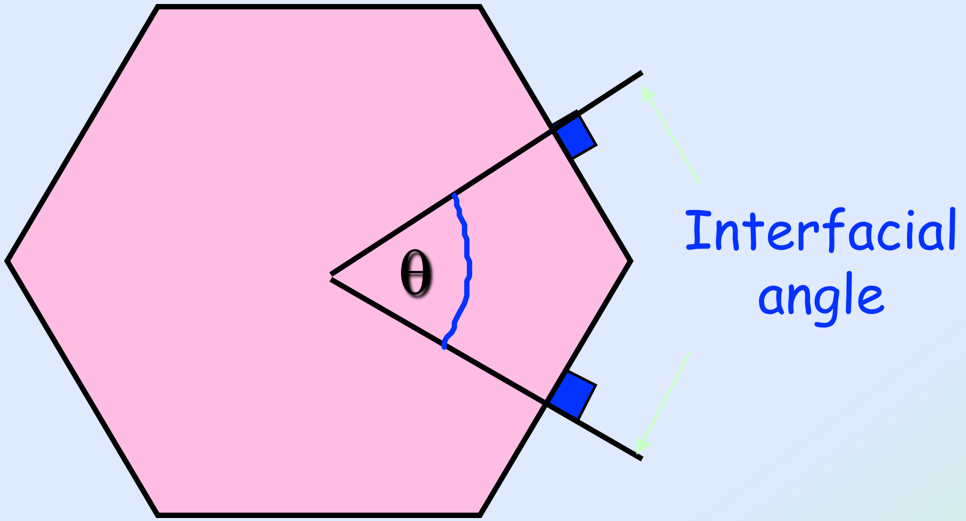
Nature of crystals (1)

- In the late 17th century, Domenica Guglielmini split larger crystals along cleavage planes into smaller crystals
- in 1784 Rene Hauy broke a calcite rhomb into smaller and smaller rhombs of constant rhombohedral shape
- Hauy proposed continue cleaving would lead to the smallest unit of which the whole crystal is built → unit cell
- faces parallel to cleavage produced by the regular packing of units
- Hauy showed that faces with other shapes could be formed by regular omitting successive rows

Nature of crystals (2)

Nicolaus Steno (1669)

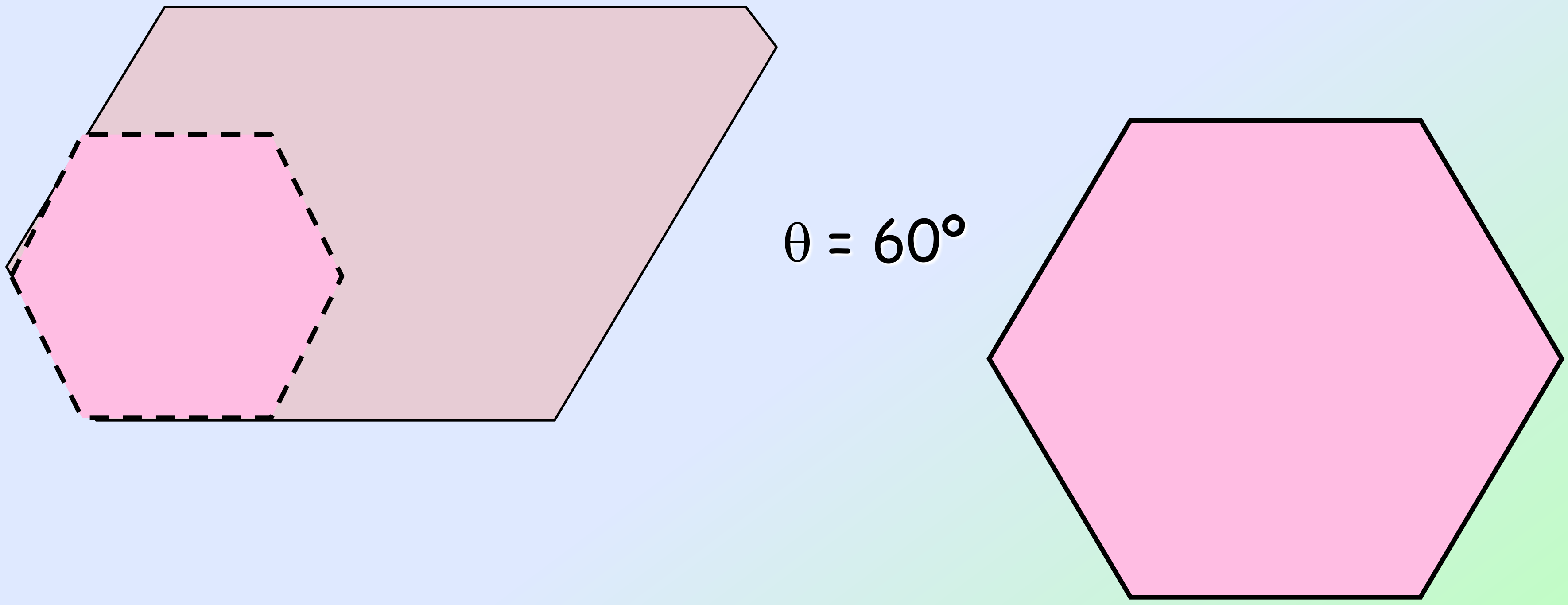
Law of constancy of interfacial angles "in all crystals of the same substance, the angles between corresponding faces are constant"



Contact goniometer

Interfacial angle

The interfacial angles of corresponding crystal faces of the same mineral are constant even when shape of crystal is different

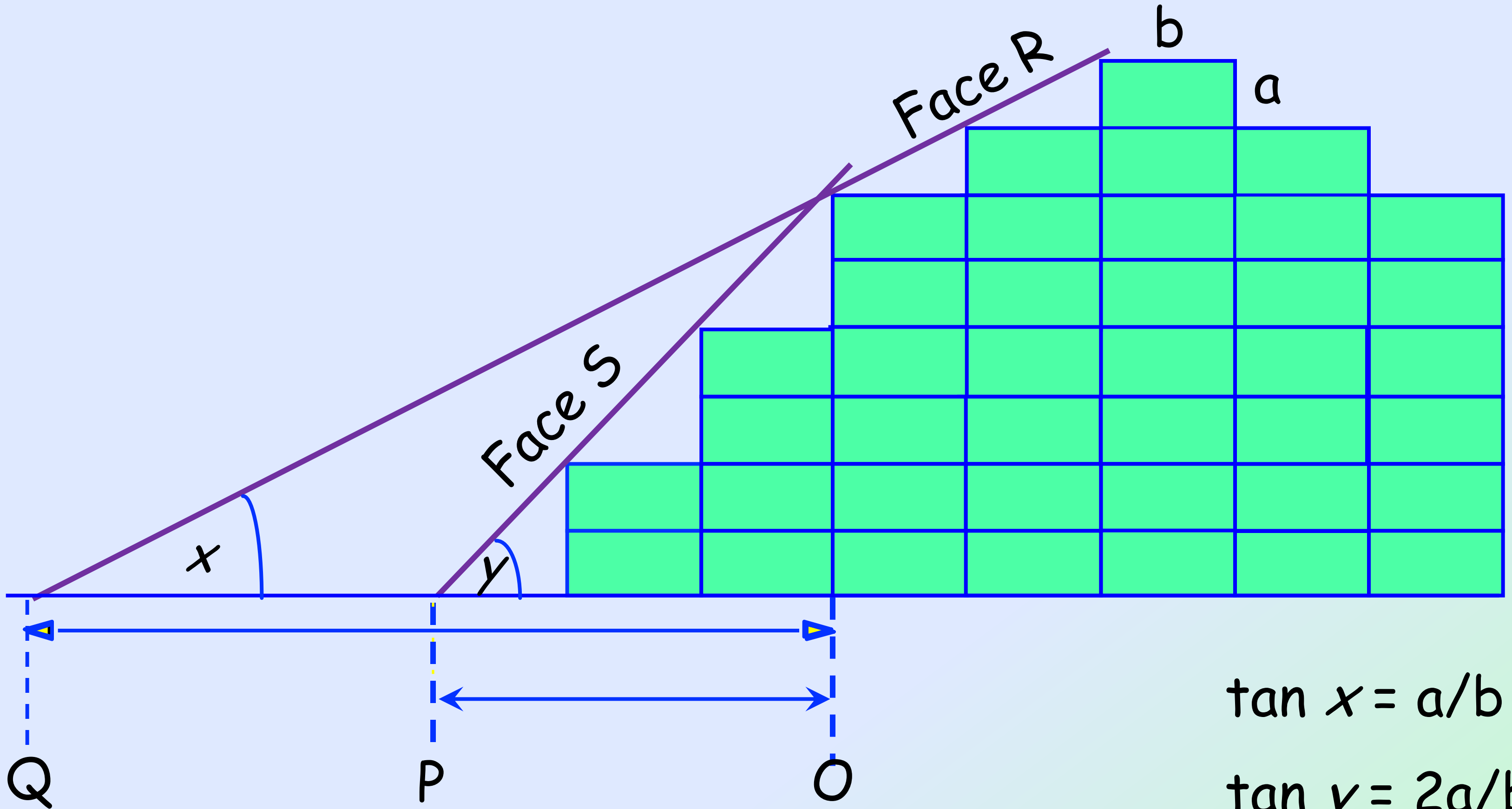


Unit cell

Rene Hauy (1784)

- Proposed that all crystals are composed of fundamental building blocks that he called unit cells
- A regular change in the packing arrangement of unit cells could account for the constancy of interfacial angles
- A unit cell is the smallest atomic arrangement that can on replication build up an entire crystal

Unit cell



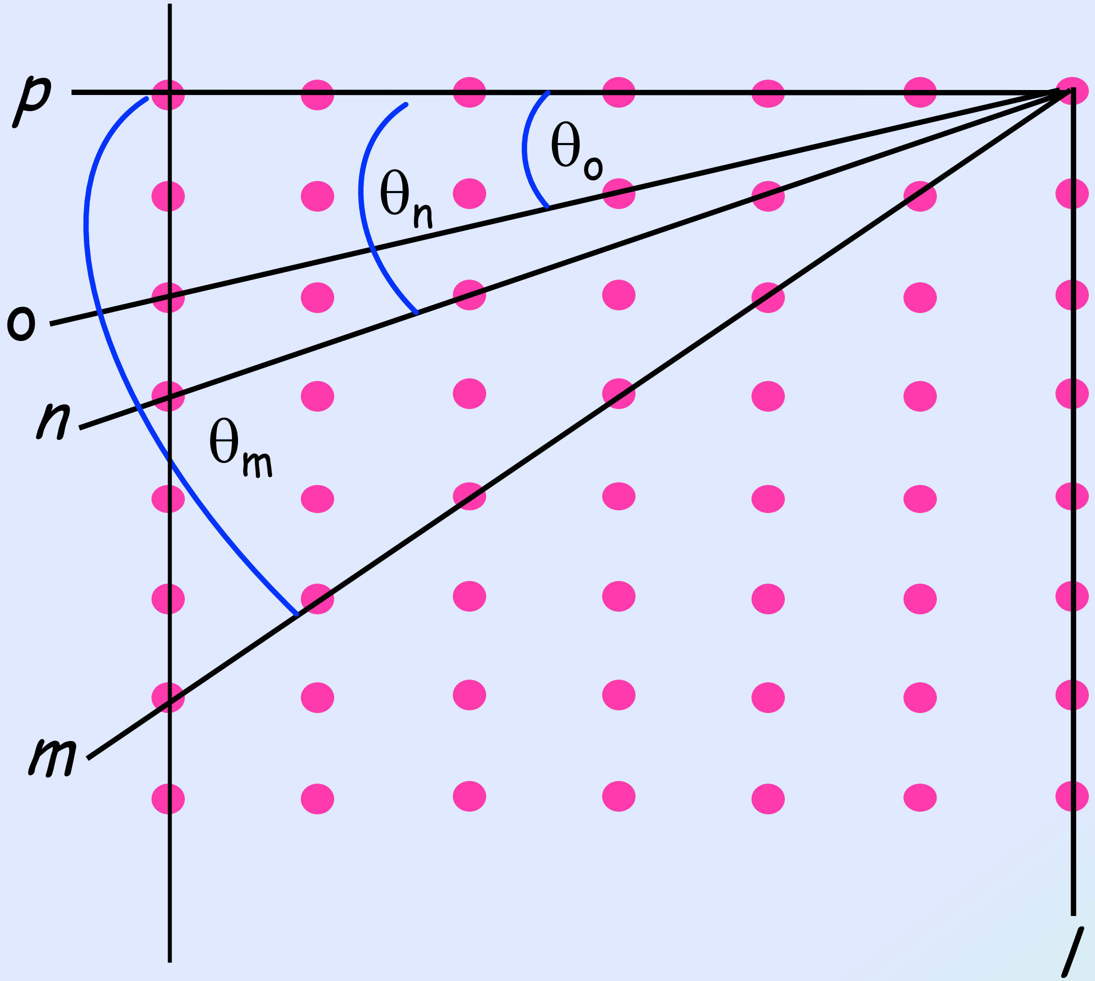
$\tan x = a/b$

$\tan y = 2a/b$

$\tan y = 2 \tan x$

NB. Intercept length OQ = 2OP

Stability of crystal faces



$\tan \theta_o = 2/6 = 1/3$

$\tan \theta_n = 3/6 = 1/2$

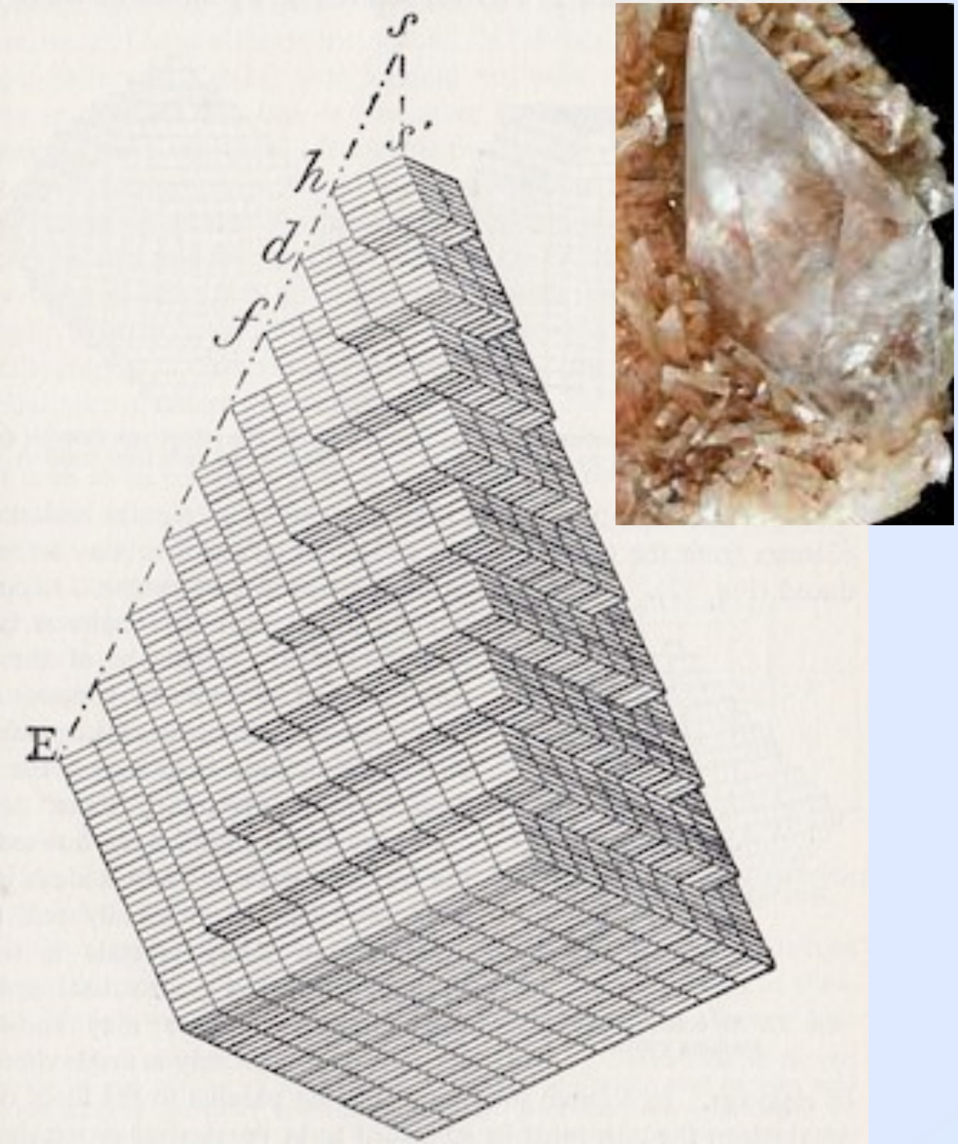
$\tan \theta_m = 6/6 = 1$

l > *m* > *n* > *o*

Law of rational ratio of intercepts

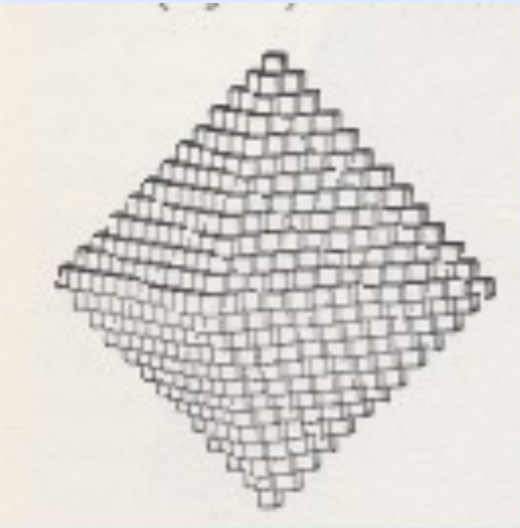
"Where two or more faces intersect an axis, the ratio of the intercepts are simple rational multiples"

Hauy's models for stacking of unit cells



Dog-tooth spar built up

from rhombohedral units



Octahedral crystal

built by stacking

cubelets

Description of symmetry

- To determine the crystal system to which a crystal belongs we need to describe its symmetry

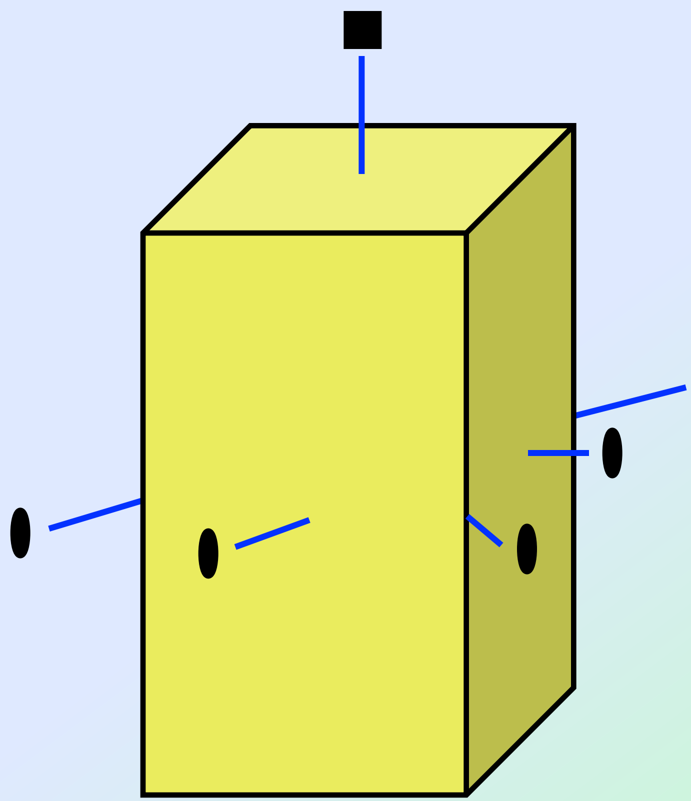
- Symmetry refers to the regular way that its component parts (crystal faces) are arranged

- Crystal lattices (and crystals) have a symmetry that can be described in terms of three types of symmetry elements:

1. rotational axes of symmetry
2. planes of symmetry (mirror planes)
3. centre of symmetry

Rotational axes of symmetry

Rotational axes of symmetry are imaginary lines through the centre of a crystal, about which the crystal may be rotated such that a particular face type occurs in the same orientation more than once in a 360° rotation



1^{iv} 4^{ii}

Location of rotational axes within a crystal

(1) Rotational axes of symmetry always pass through the centre of crystals

(2) To locate axes, imagine that they pass through:

(a) the centre of opposite faces

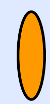
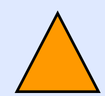
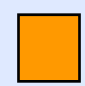
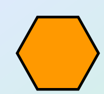
(b) the centre of opposite edges

(c) opposite corners

(3) Orient axis vertically

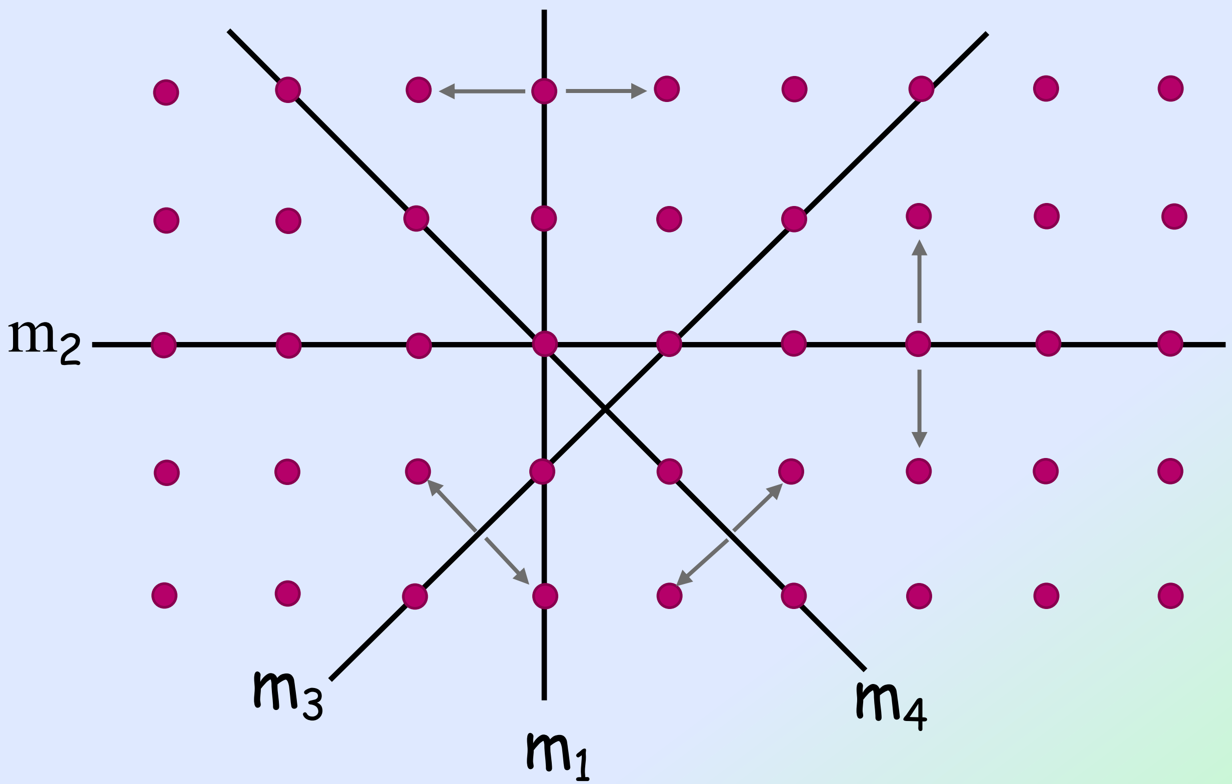
Degrees of rotational axes

If a crystal face type is repeated after a rotation of 360°/*n*, then *n* is said to constitute the degree of the axis

n = 1	identity axis		not designated
n = 2	diad		N^{ii}
n = 3	triad		N^{iii}
n = 4	tetrad		N^{iv}
n = 6	hexad		N^{vi}

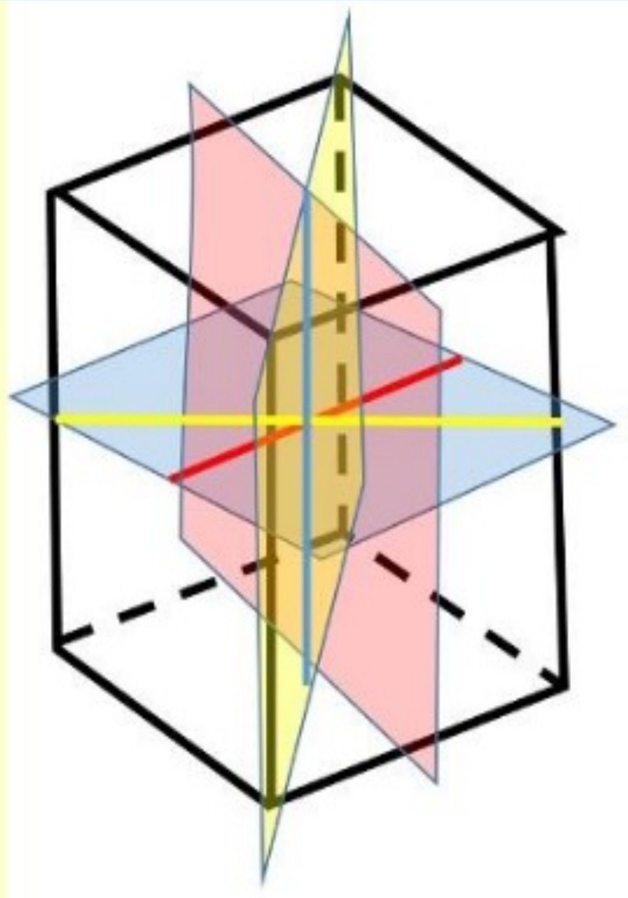
Planes of symmetry

Planes of symmetry or mirror planes are imaginary planes through a crystallographic lattice that divide the lattice into two halves such that one half is a mirror image of the other



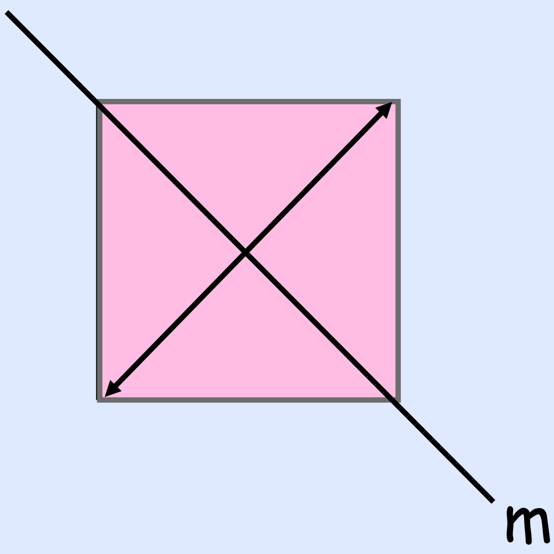
Planes of symmetry (mirror planes)

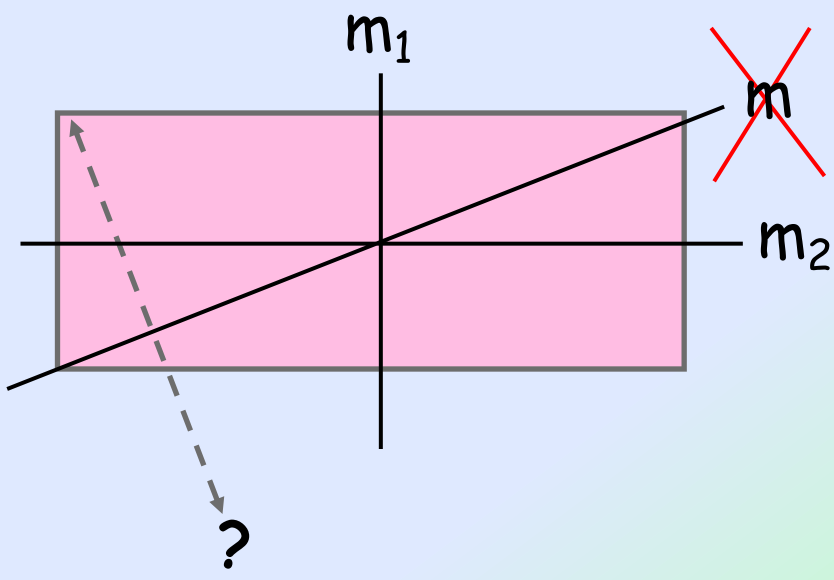
A plane of symmetry divides a crystal in half such that each half is a mirror image of the other



notation - 5m

Mirror planes must reflect all points an equal distance on the other side of the mirror plane



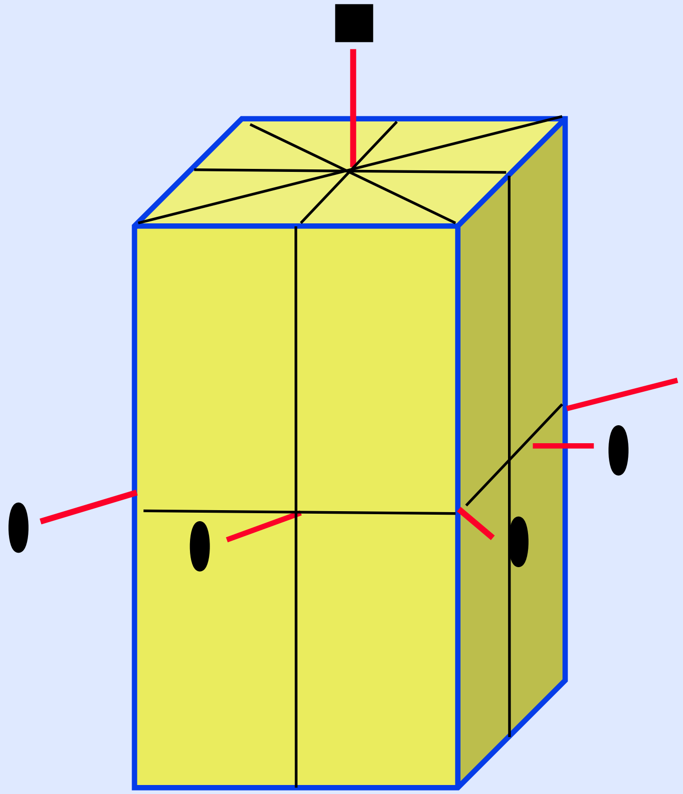


Centre of symmetry

A crystal has a centre of symmetry if an imaginary line can be passed from any point on the surface of the crystal and, the line emerges from an equivalent (but inverted) point at an equal distance beyond the centre

Notation $\bar{1}$

Listing symmetry elements

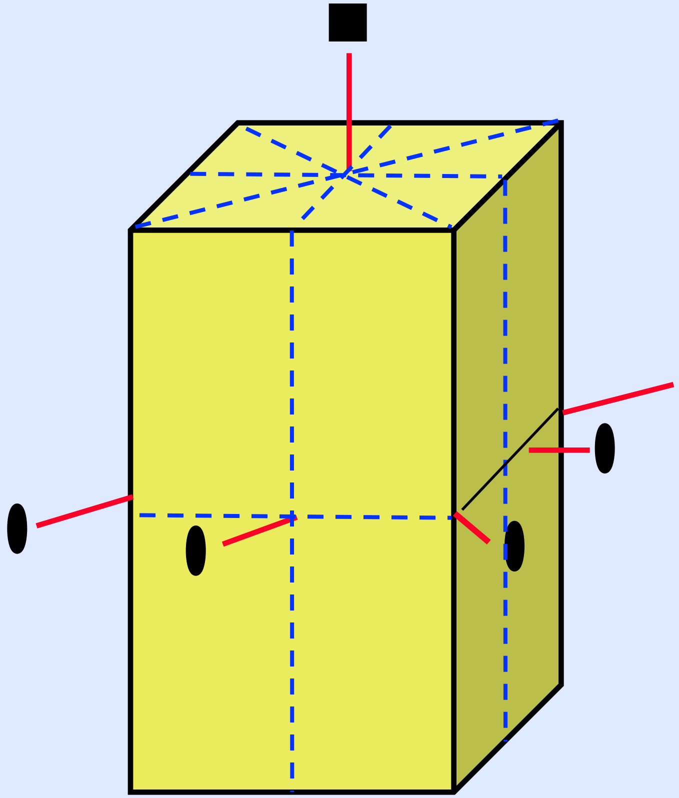


1^{iv} 4^{ii} 5m $\bar{1}$

Crystal systems and diagnostic symmetry elements

cubic	-	four triad axes
trigonal	-	a single triad axis
hexagonal	-	a single hexad axis
tetragonal	-	a single tetrad axis
orthorhombic	-	three mutually perpendicular axes or two perpendicular mirror planes and one diad axis parallel to the mirror plane intersection
monoclinic	-	a single diad axis and/or a single mirror plane (usually both but not invariably)
triclinic	-	may or may not have a centre of symmetry. No planes of symmetry and no axes of degree higher than one

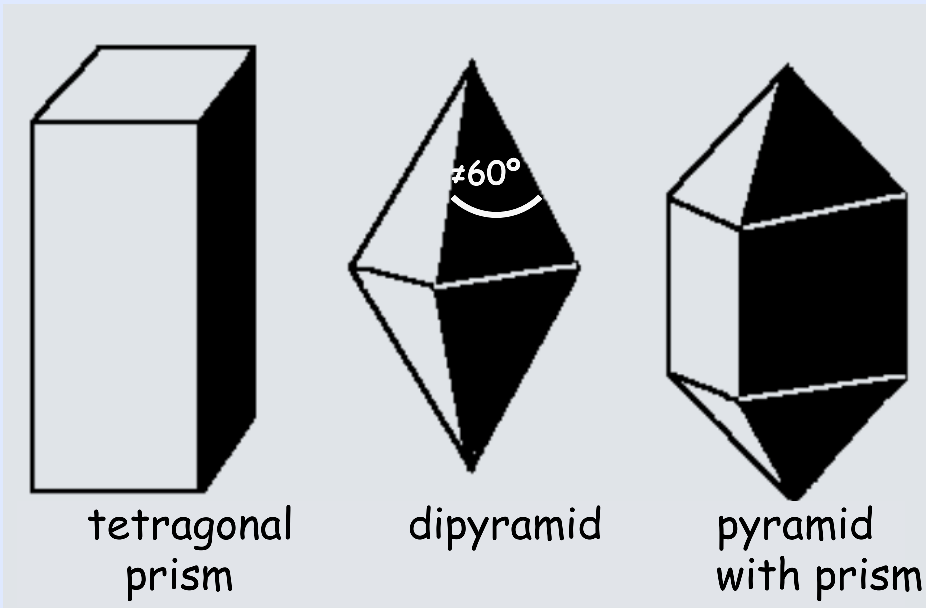
Listing symmetry elements



1^{iv} 4^{ii} 5m $\bar{1}$

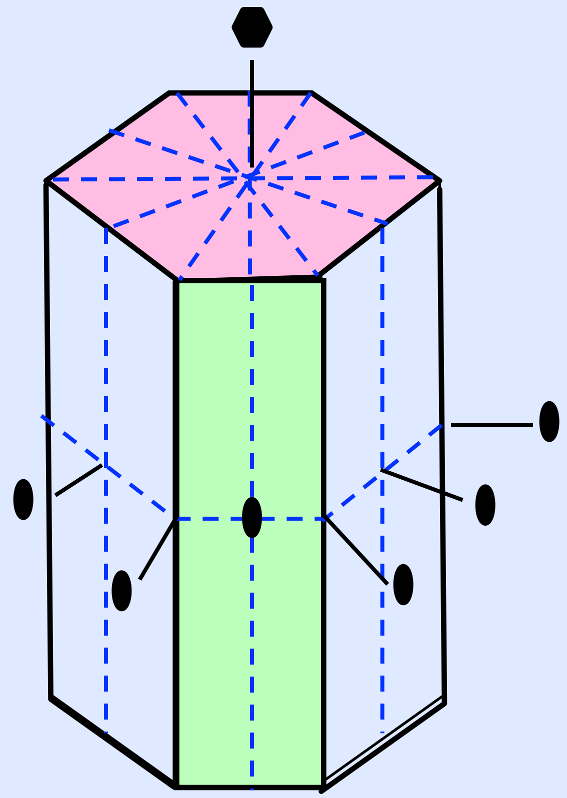
Tetragonal

Tetragonal crystal examples



zircon crystal

Symmetry – crystal AC4

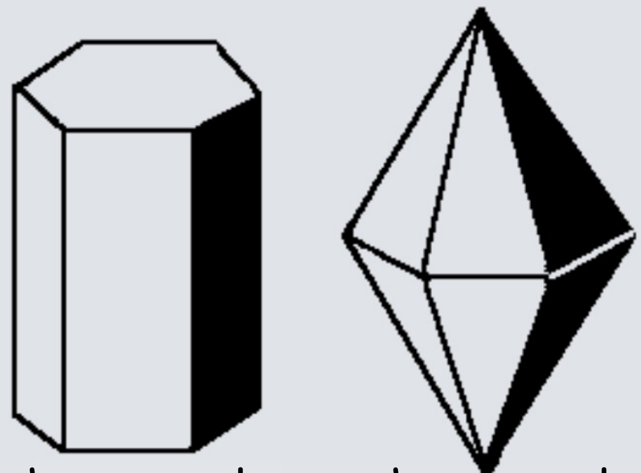


Symmetry

1^{vi} 6^{ii} 7m $\overline{1}$

Hexagonal

Hexagonal crystal examples

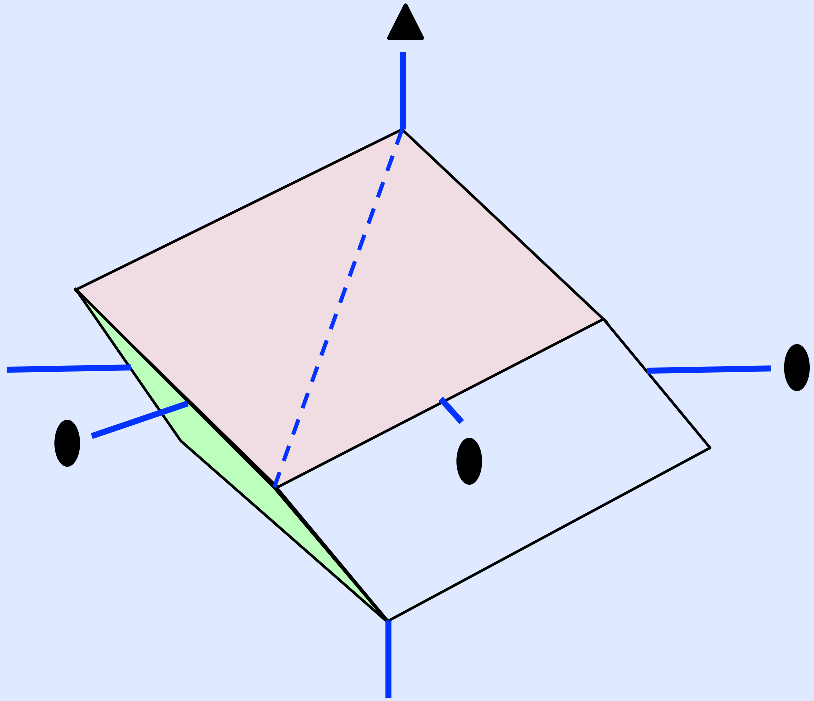


hexagonal prism

hexagonal dipyramid

red beryl crystal

Symmetry - crystal AC3

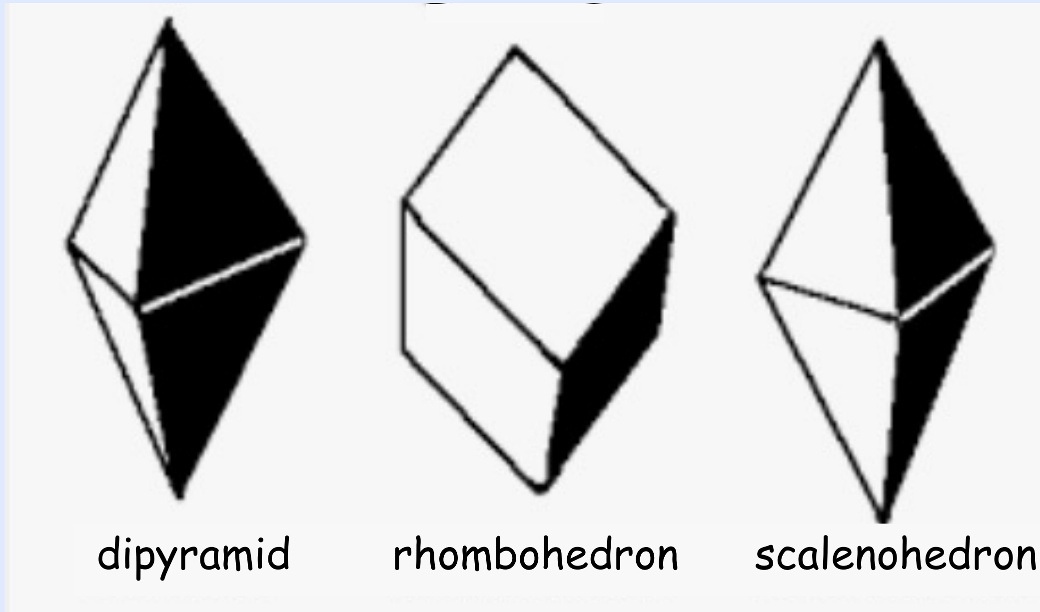


Symmetry

1^{iii} 3^{ii} 3m $\bar{1}$

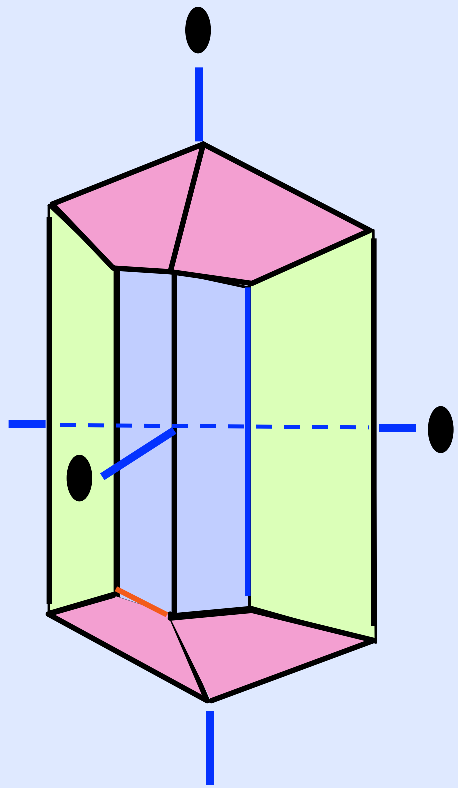
Trigonal

Trigonal crystal examples



calcite rhomb

Symmetry - crystal AC13

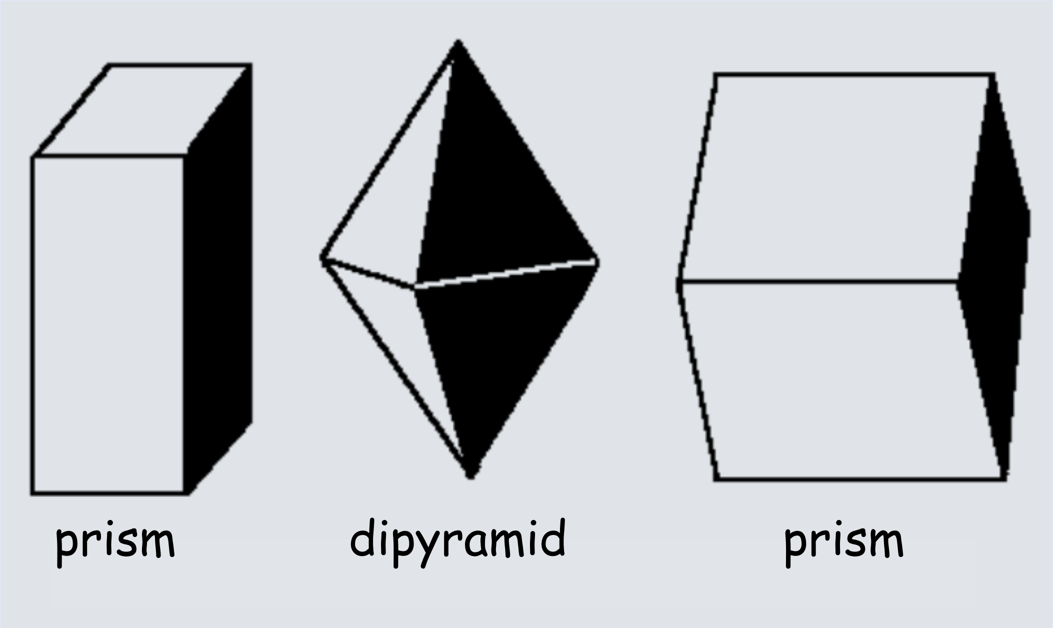


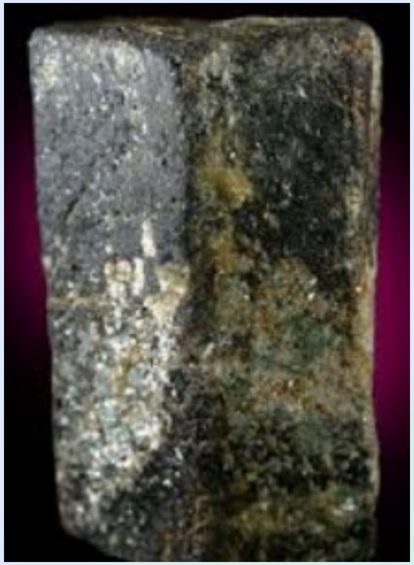
Symmetry

3ii 3m $\bar{1}$

orthorhombic

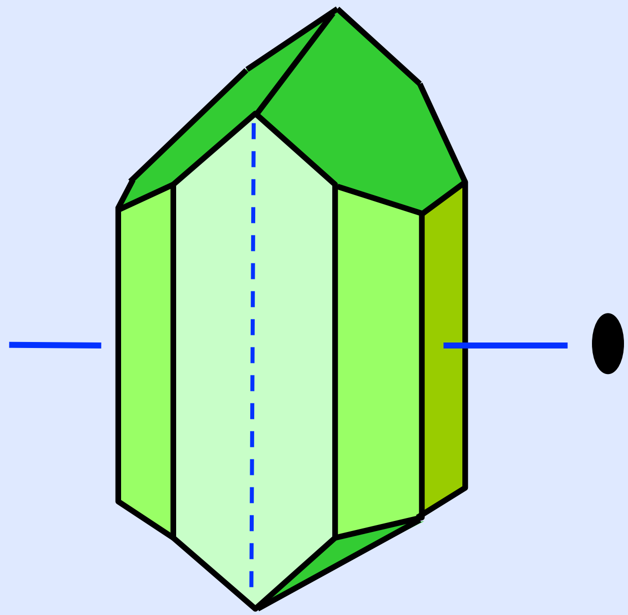
Orthorhombic crystal examples





staurolite crystal

Symmetry - crystal AC14

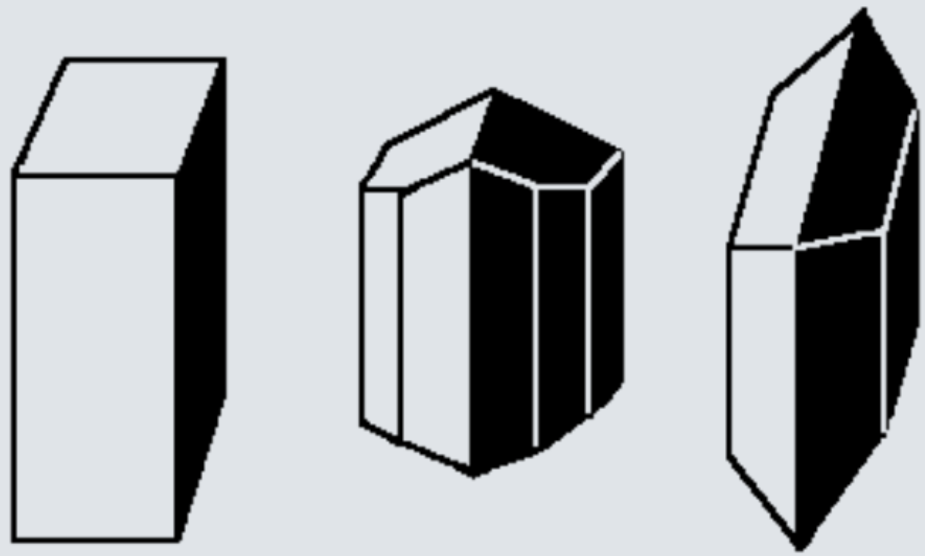


Symmetry

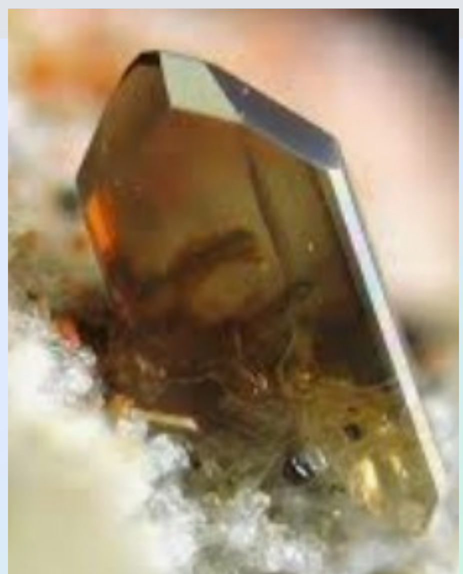
1^{ii} 1m $\bar{1}$

Monoclinic

Monoclinic crystal examples

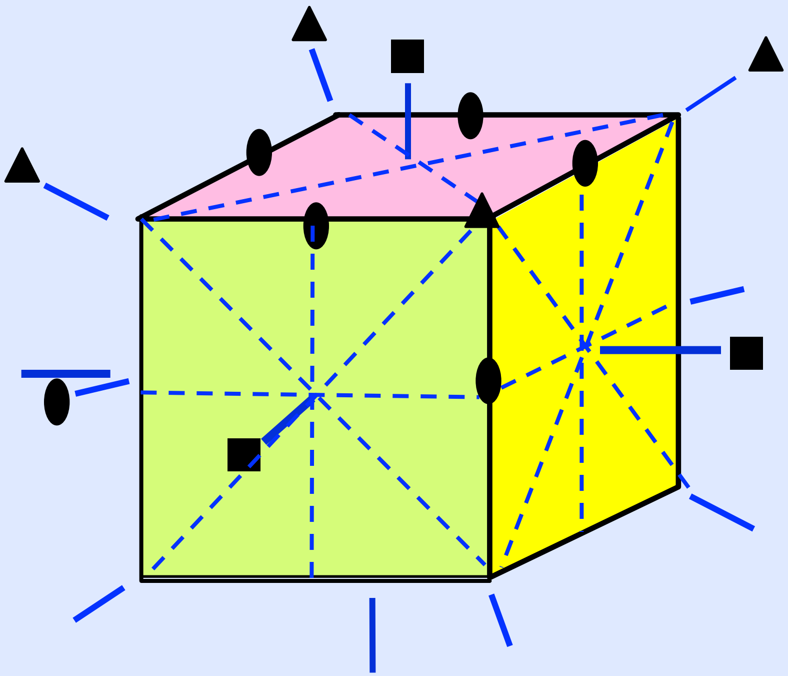


prism prism clinopinacoid



augite crystal

Symmetry - crystal AC8

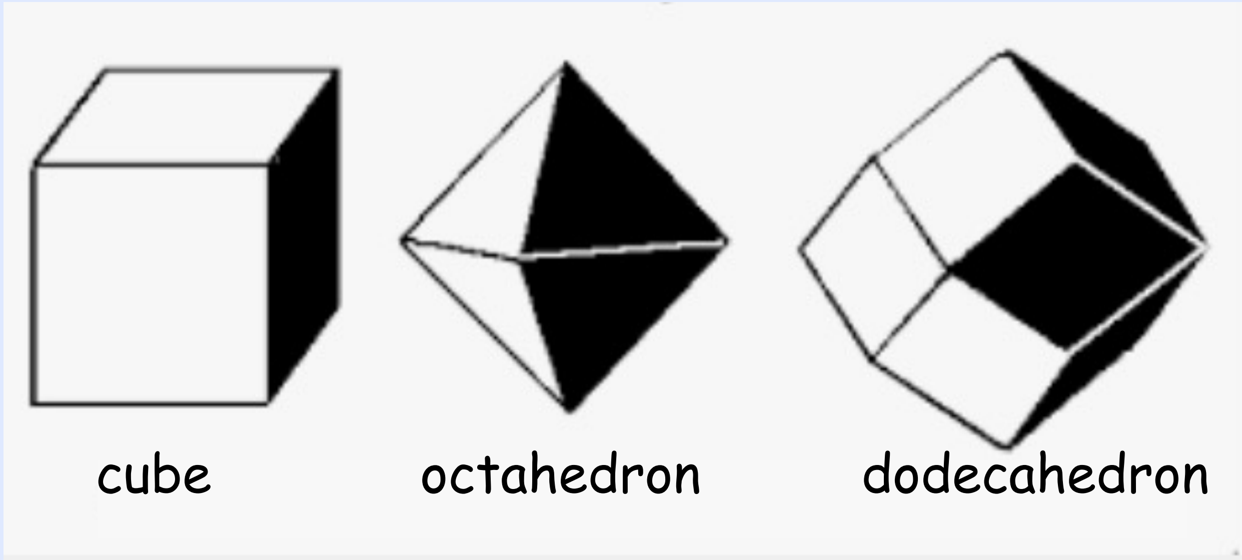


Symmetry

3^{iv} 4^{iii} 6^{ii} $9m$ $\bar{1}$

Cubic

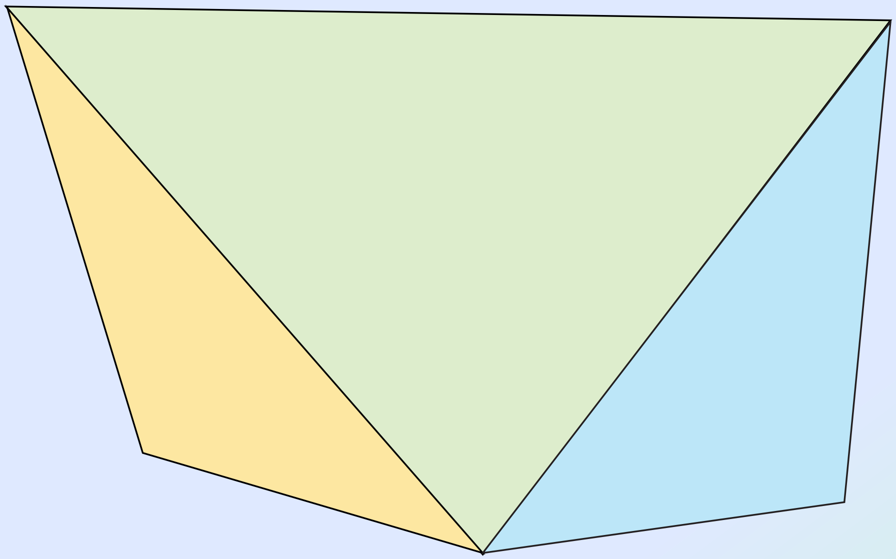
Cubic crystal examples



cubic pyrite crystal

dodecahedral garnet crystal

Symmetry - crystal AC21

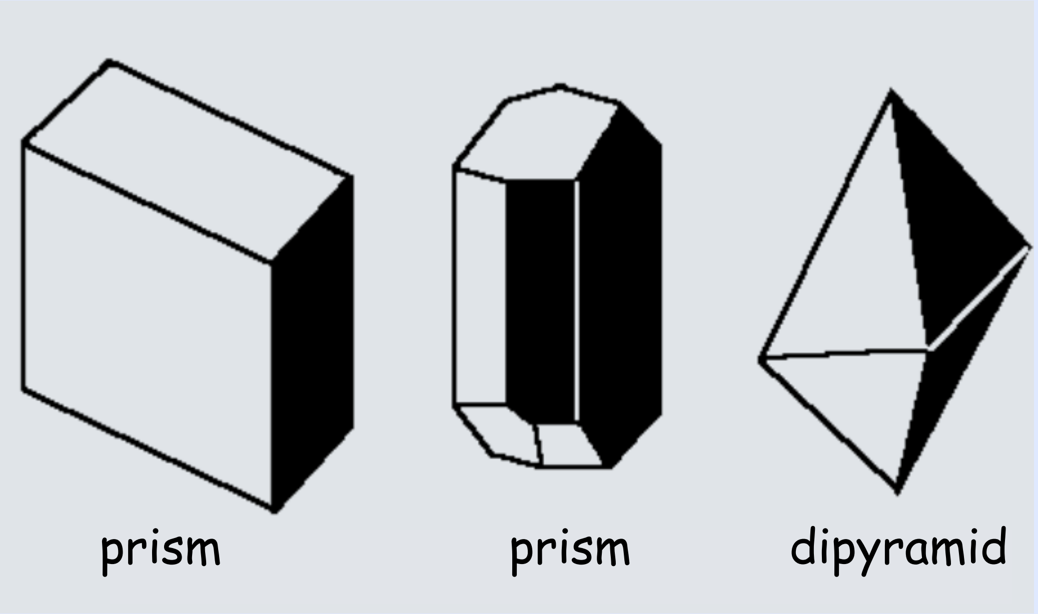


Symmetry

$\bar{1}$

triclinic

Triclinic crystal examples

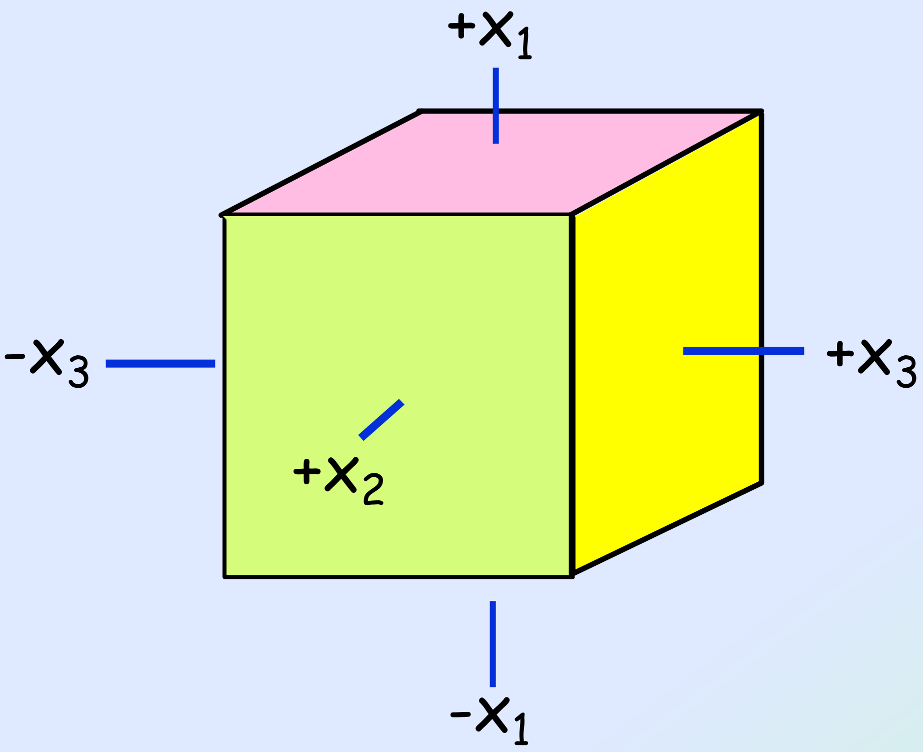


albite crystal

Assigning crystallographic axes

- To further describe and refer to planar features in crystals, we need to assign crystallographic axes to the seven crystal systems
- specific rules apply to each of the crystal systems
- when assigning axes, the z axis is always shown in vertical orientation

Cubic crystal system

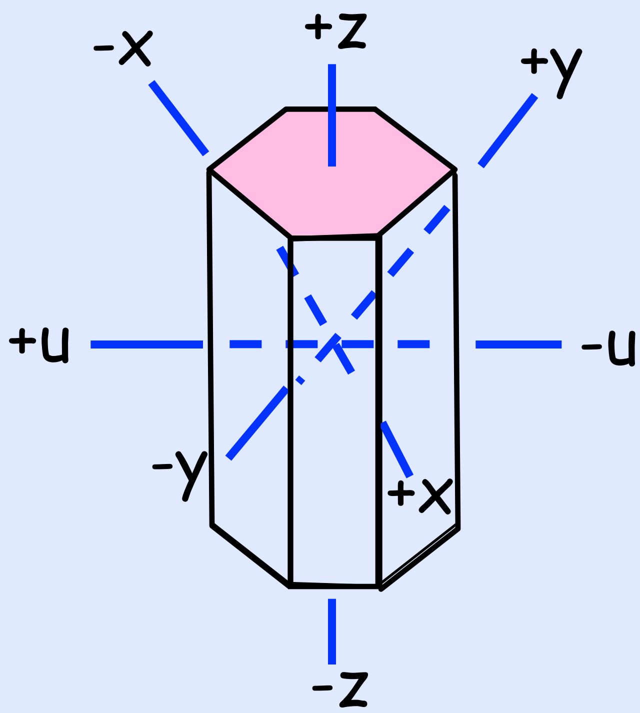


Three mutually perpendicular axes

$a_1 = a_2 = a_3$

The crystallographic axes are parallel to the three tetrads or three diads if no tetrads are present

Hexagonal crystal system



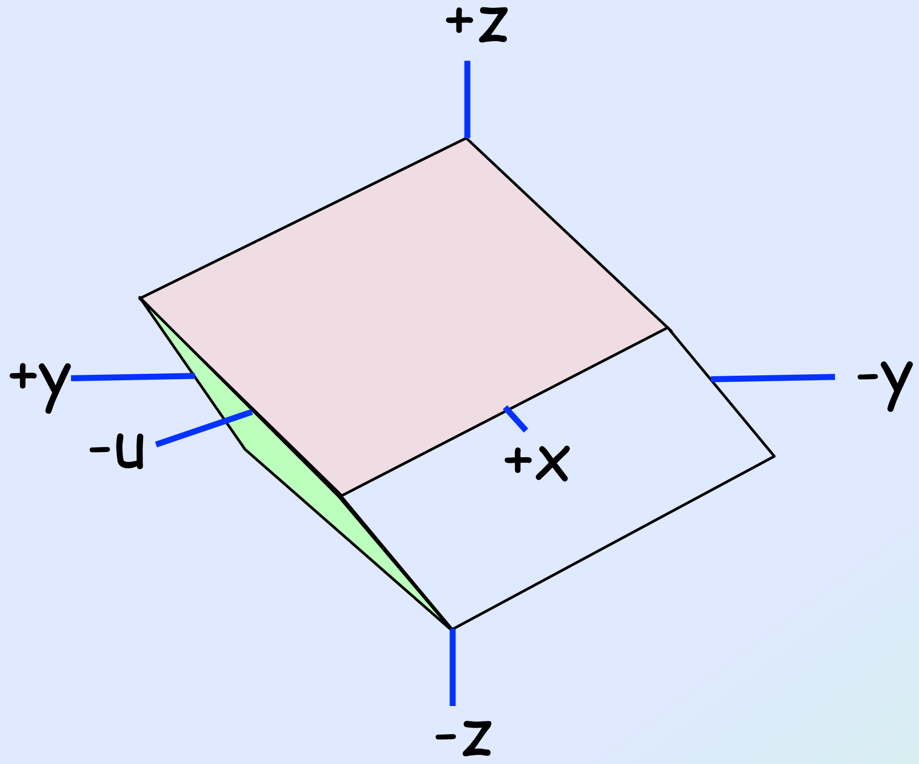
Angles between x, y and u axes = 120°

$c \neq a = b = d$

z axis is parallel to the hexad axis

x, y and u axes lie in a plane perpendicular to the z axis and are chosen to pass through the intersections of the prominent faces

Trigonal crystal system



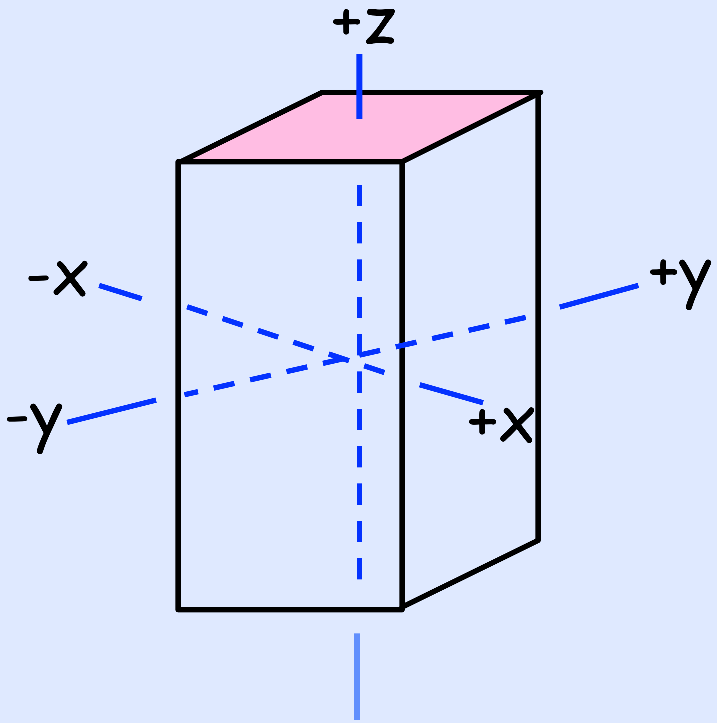
z axis is coincident with triad axis

x, y and u axes pass trough centres of opposite edges

Angles between them are 120°

Tetragonal crystal system

Three mutually perpendicular axes

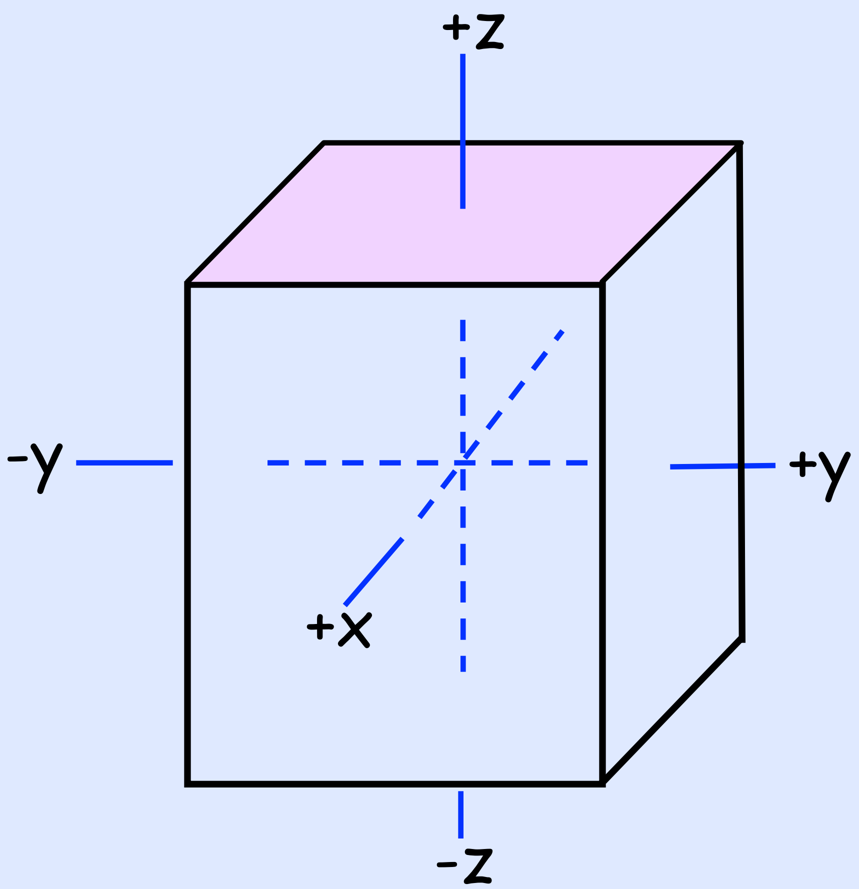


The z axis is the tetrad

$c \neq a = b$

x and y axes are chosen to pass through the intersections of prominent faces or their extensions

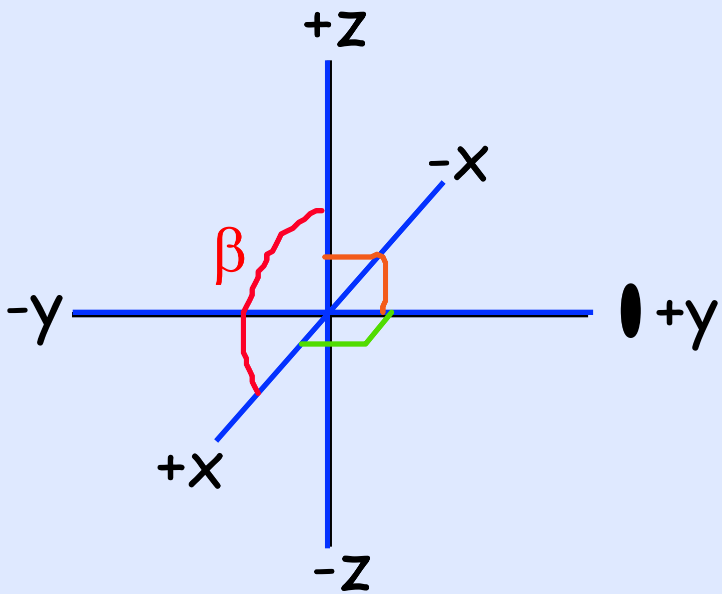
Orthorhombic crystal system



Three mutually perpendicular axes
c > b > a

The crystallographic axes are parallel to the three mutually perpendicular diad axes

Monoclinic crystal system



$\alpha = 90°$

$\beta \neq 90°$

$\gamma = 90°$

$a \neq b \neq c$

y axis is chosen parallel to the single diad

or perpendicular to the mirror plane

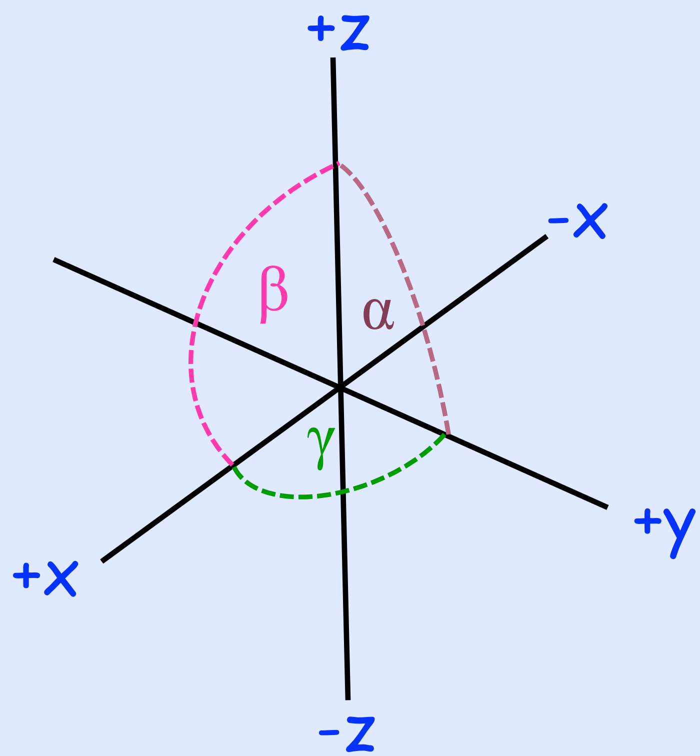
x axis is perpendicular to y axis and parallel to prominent faces

and edges

z is perpendicular to the y axis and is oriented vertical, parallel to

the elongate direction in the crystal

Triclinic crystal system



$\alpha \neq \beta \neq \gamma$

Axes are chosen parallel to prominent faces

the z axis is vertical x slopes up from front to back, y slopes upwards from right to left

a, b and c are unit intercepts on the x, y and z axes respectively

Angles between axes are α (z and y), β (z and x) and γ (x and y)

Unit intercepts are unequal

Optical properties of crystals

The crystal system of irregular shaped mineral grains can be determined under a petrographic microscope

Isotropic	cubic	
Anisotropic	tetragonal	Uniaxial
	trigonal	
	hexagonal	
	orthorhombic	Biaxial
	monoclinic	
	triclinic	