Earth and Planetary Materials

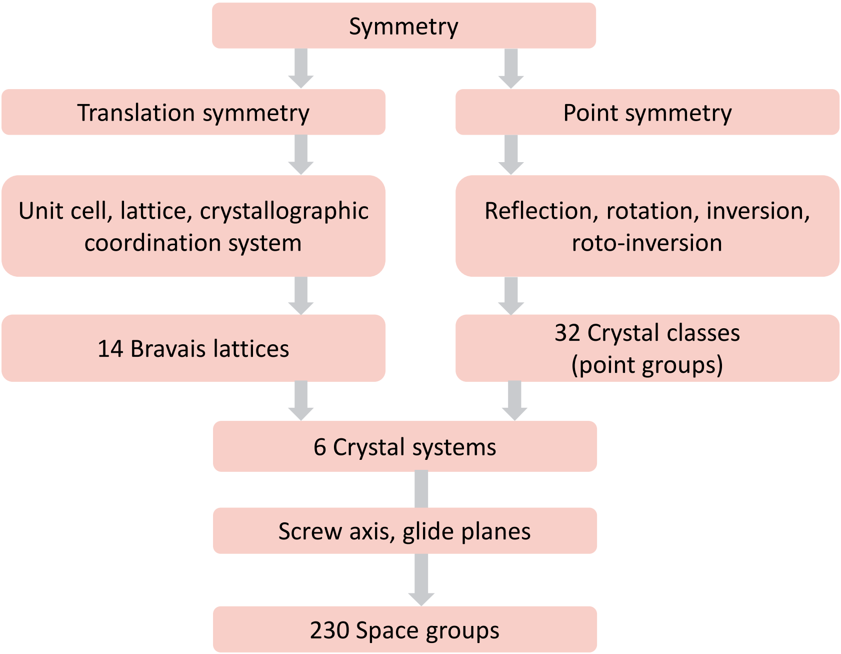
Spring 2013

Lecture 11
2013.02.13

Midterm exam

- 2/25 (Monday)
- Office hours:
  - 2/18 (M) 10-11am
  - 2/20 (W) 10-11am
  - 2/21 (Th) 11am-1pm
  - No office hour 2/25

Point symmetry



Symmetry

Translation symmetry

Point symmetry

Unit cell, lattice, crystallographic coordination system

Reflection, rotation, inversion, roto-inversion

14 Bravais lattices

32 Crystal classes (point groups)

6 Crystal systems

Screw axis, glide planes

230 Space groups

Structure (or pattern) = motif + symmetry operations

- Motif: Unit of pattern – what is repeated
- Symmetry operations – how to repeat
  - Application of the symmetry operation leaves the pattern unchanged
  - Or, starting with one motif, application of the symmetry operation generates the other motifs in the pattern

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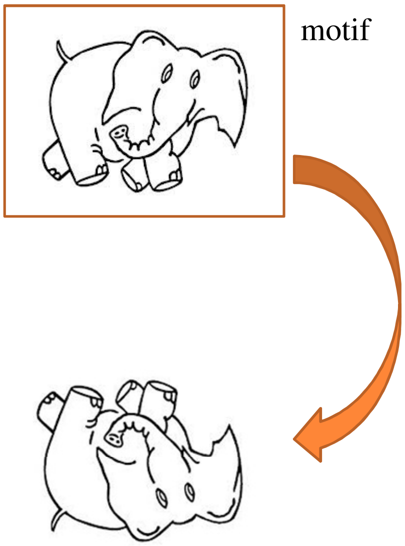


motif

Symmetry operation
(reflection)

Types of symmetry operation

- Rotation
- Reflection
- Inversion
- Roto-inversion

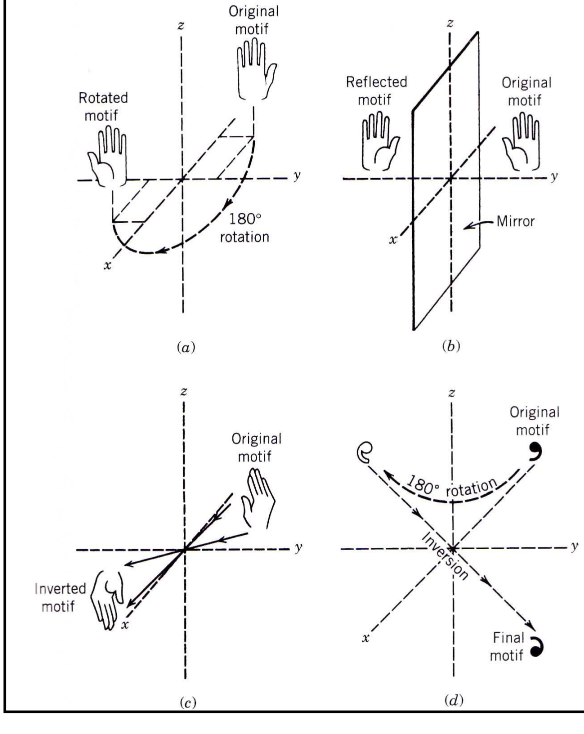


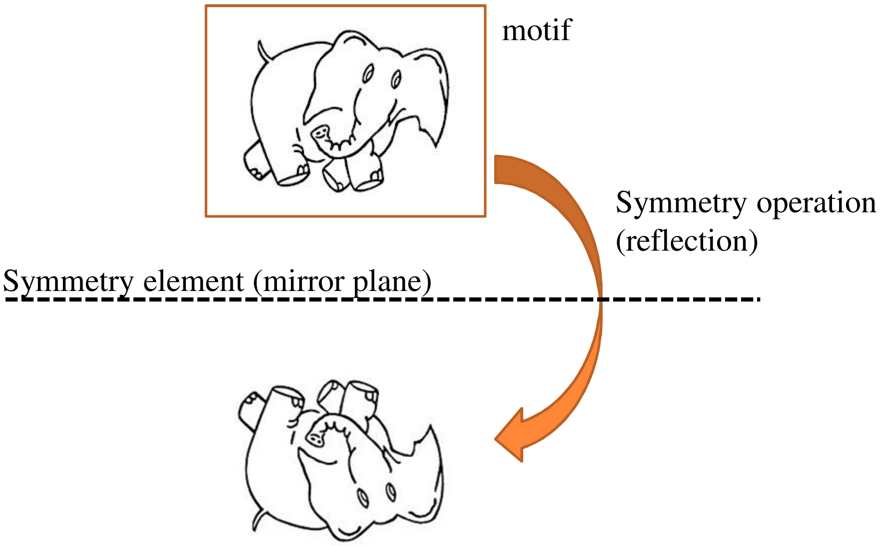
FIG. 6.9 Examples of symmetry operations. (a) Generation of a pattern by rotation of a motif through an angle of 180°. (b) Motifs as related by a mirror reflection. (c) Motifs related by inversion through a center. (d) Motifs related by 180° rotation and subsequent inversion; known as rotoinversion (see also Fig. 6.14a).

Symmetry operation

- The movement that leaves the pattern unchanged

Symmetry element

- The object about which the movement takes place



motif

Symmetry operation
(reflection)

Symmetry element (mirror plane)

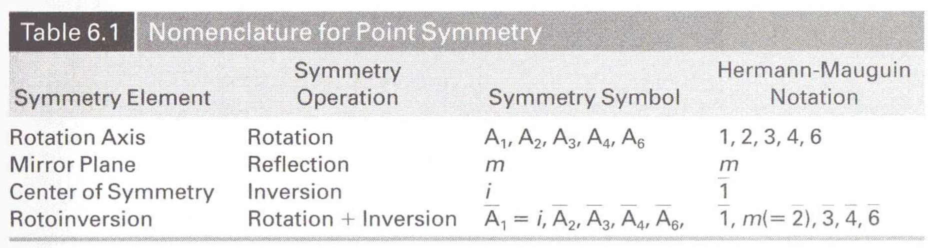


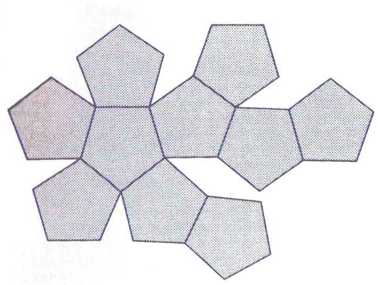
Table 6.1 Nomenclature for Point Symmetry

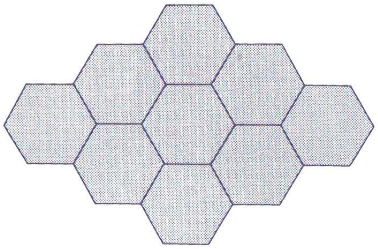
Symmetry Element	Symmetry Operation	Symmetry Symbol	Hermann-Mauguin Notation
Rotation Axis	Rotation	A_1, A_2, A_3, A_4, A_6	1, 2, 3, 4, 6
Mirror Plane	Reflection	m	m
Center of Symmetry	Inversion	i	$\bar{1}$
Rotoinversion	Rotation + Inversion	$\bar{A}_1 = i, \bar{A}_2, \bar{A}_3, \bar{A}_4, \bar{A}_6,$	$\bar{1}, m(=\bar{2}), \bar{3}, \bar{4}, \bar{6}$

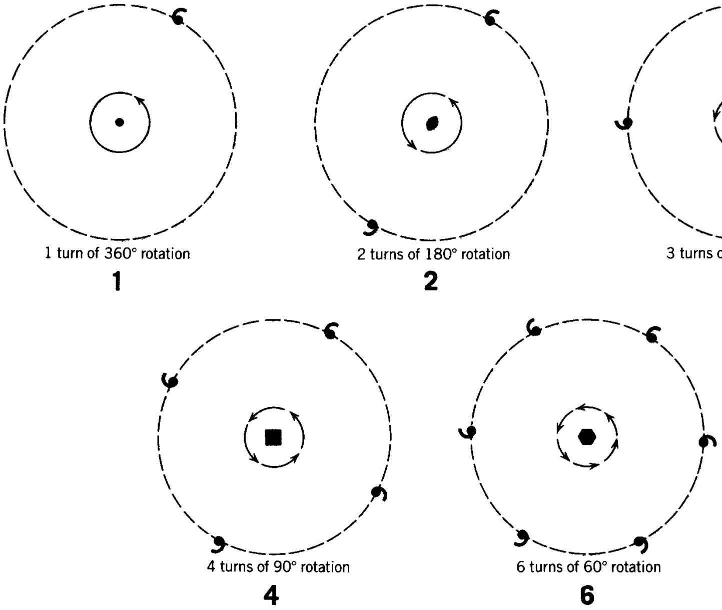
Rotation

- 2 (2-fold axis); rotation by 360°/2 = 180° leaves the pattern unchanged
- 3 (3-fold axis); rotation by 360°/3 = 120° leaves the pattern unchanged
- likewise for 4-fold and 6-fold axes

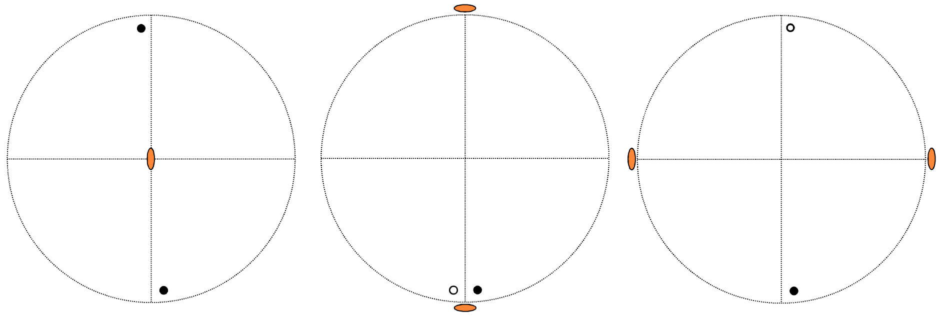
- Only need to consider 2-, 3-, 4-, and 6-fold axes
- All others (e.g., 5-fold rotation) are incompatible with translational symmetry (you can't tile a floor with pentagons!)


(*a*)


(*b*)



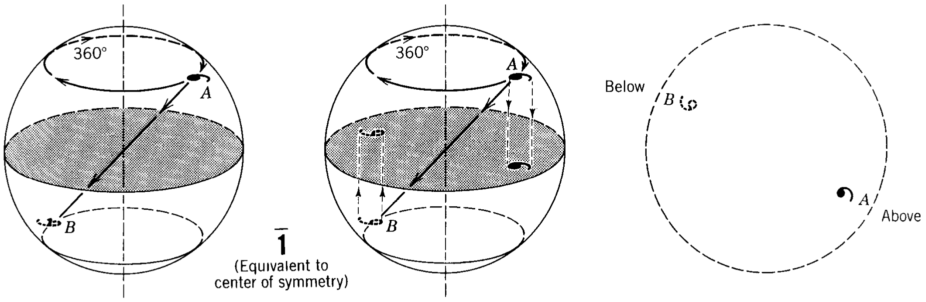
Example: Stereograms showing patterns with a 2-fold symmetry, with different orientations for the rotation axis (from left to right, parallel to *c*, *a*, and *b* axes)



Roto-inversion

- Rotation followed by inversion through the origin
- Inversion creates a point (-x,-y,-z) for each point (x,y,z)

- $\bar{1}$: same as an inversion center, often denoted as "*i*"
- $\bar{2}$: same as a mirror plane, often denoted as "*m*" and shown as a heavy solid line
- $\bar{3}$: same as a 3-fold axis with an inversion center
- $\bar{4}$: high-symmetry axis of a tetrahedron (edge to edge)
- $\bar{6}$: same as 3-fold axis with a perpendicular mirror

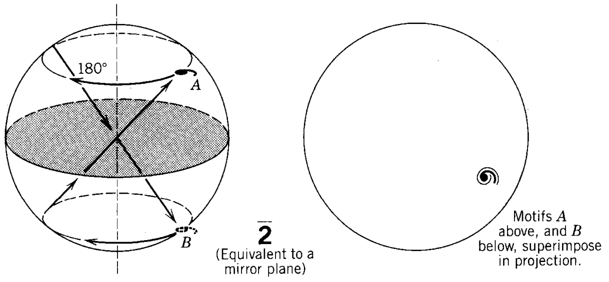


(*a*) **Rotoinversion**

(*b*) Projection of motifs on equatorial plane

(*c*) Equatorial plane with projected motifs

(a)

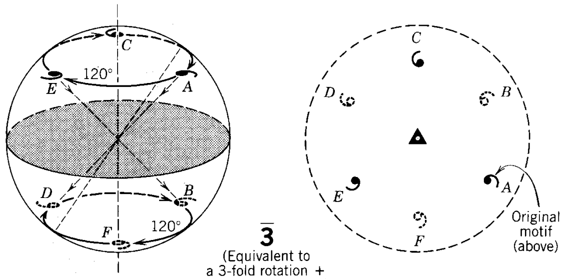


$\bar{2}$

(Equivalent to a mirror plane)

Motifs *A* above, and *B* below, superimpose in projection.

(b)

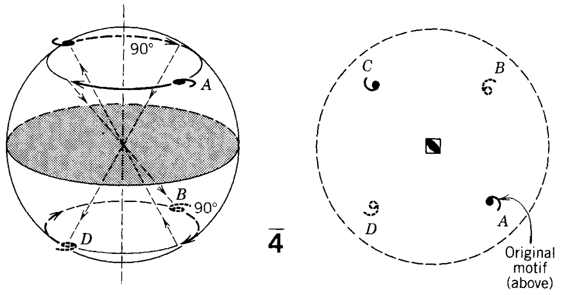


$\bar{3}$

(Equivalent to a 3-fold rotation + center of symmetry)

Original motif (above)

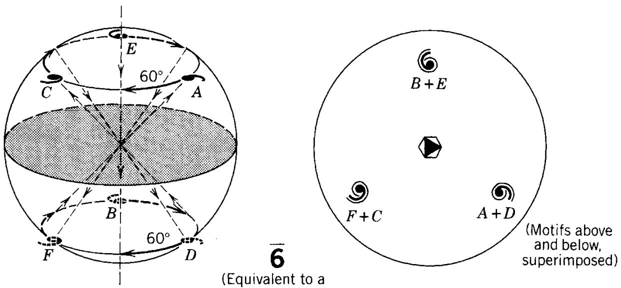
(c)



$\bar{4}$

Original motif (above)

(d)

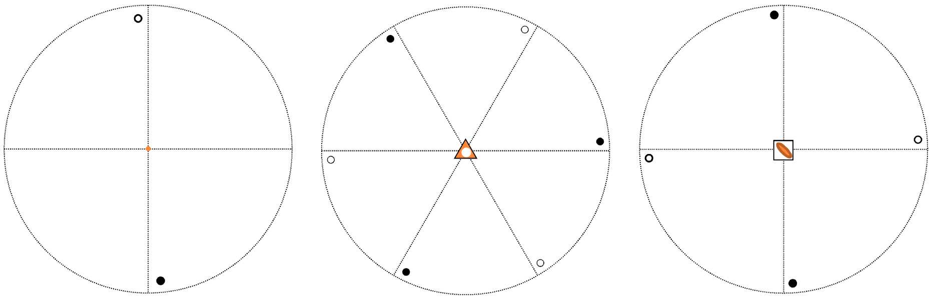


$\bar{6}$

(Equivalent to a 3-fold rotation axis with a mirror plane ⊥ to axis)

(Motifs above and below, superimposed)

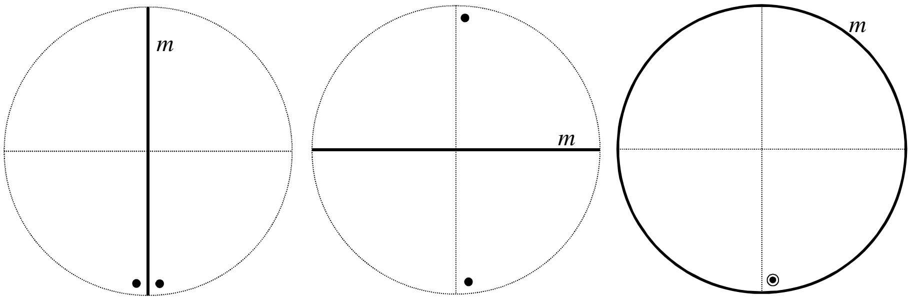
- Example: Roto-inversion axes and the resulting patterns



$\bar{1}\ (= i)$ $\bar{3}\ (= 3 + i)$ $\bar{4}$

Example: Reflection ($\bar{2}$, or *m*) symmetry – mirror plane

- From left to right, the $\bar{2}$ axes are perpendicular to **b** (left), **a** (center), and **c** (right) axes



Combination of symmetry operations

Example – combination of rotations

- If there is a 4-fold axis parallel to ***c*** and a 2-fold axis parallel to ***a***, then there must also be a 2-fold axis parallel to ***b***
- More examples: Klein p121-128

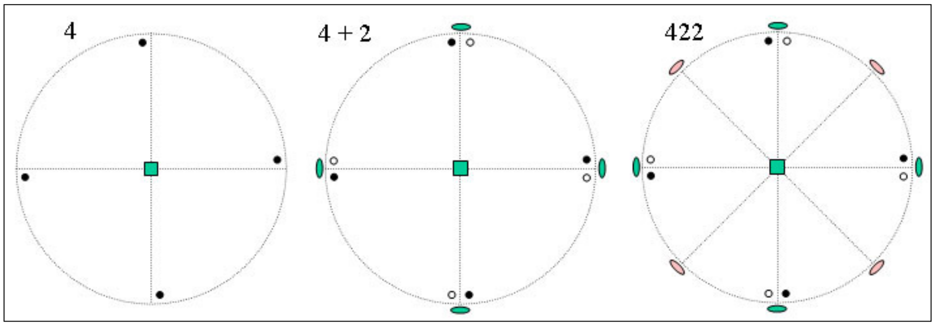
Point Groups

self-consistent set of point symmetry operations

- Only certain combinations of point symmetry elements are compatible
- 32 point groups

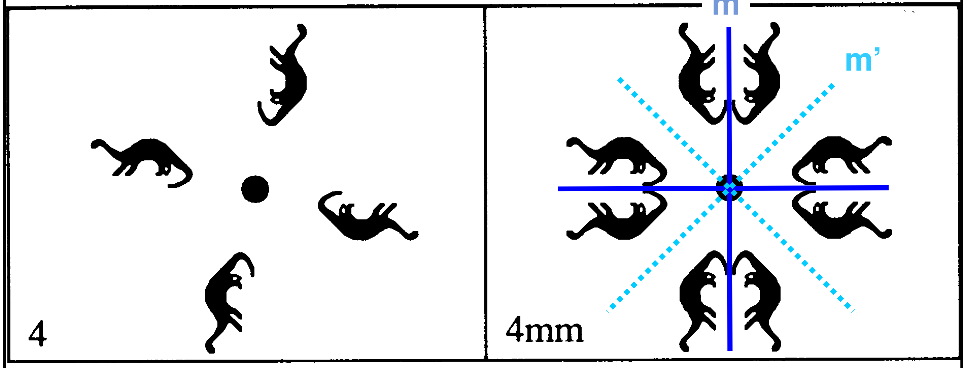
Example

- Point group 4
- Addition of one 2-fold axis that is parallel to the $\boldsymbol{a_1}$ and $\boldsymbol{a_2}$ axes
- This automatically gives another 2-fold axis between the $\boldsymbol{a_1}$ and $\boldsymbol{a_2}$ axes

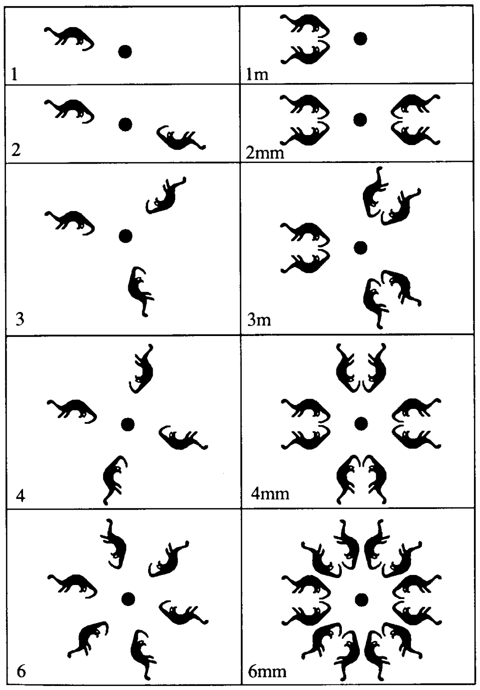


Naming point groups

- Highest symmetry axis is listed first
- Mirror planes perpendicular to an n-fold rotation axes are shown as n/m:
  - Example: 4/m (“four over m”) = mirror perpendicular to 4-fold axis
- Mirror planes that are parallel to the main rotation axes are shown as just m
  - Example: 4mm



mirror “**m’**” is generated automatically by the combination of mirror “m” and the rotation axis “4”. “**m’**” is different from “m” in how it related the dinosaurs.



Cubic systems

- Contain intersecting 3-fold or 4-fold axes
- The cube, octahedron, and tetrahedron are objects with a lot of intersecting point symmetry

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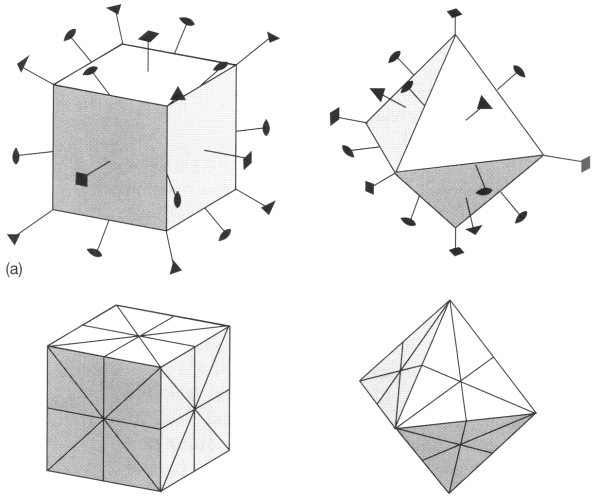
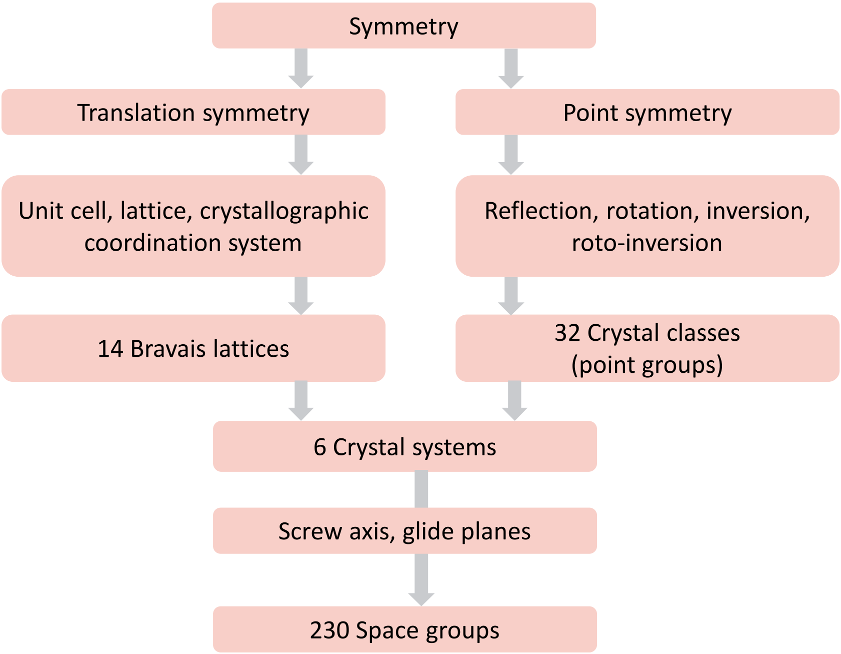
▶FIGURE 9.8
Cube and octahedron: (a) The rotation axis in a cube and an octahedron have identical orientations. Lenses, triangles and squares show 2-fold, 3-fold and 4-fold axes of symmetry. (b) The mirror planes in a cube and octahedron are also oriented identically.



Crystal systems



Symmetry

Translation symmetry

Point symmetry

Unit cell, lattice, crystallographic coordination system

Reflection, rotation, inversion, roto-inversion

14 Bravais lattices

32 Crystal classes (point groups)

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Screw axis, glide planes

230 Space groups

- Point symmetry and translational symmetry must be compatible, so that each of the types of unit cell (Bravais Lattice) has a corresponding compatible point symmetry

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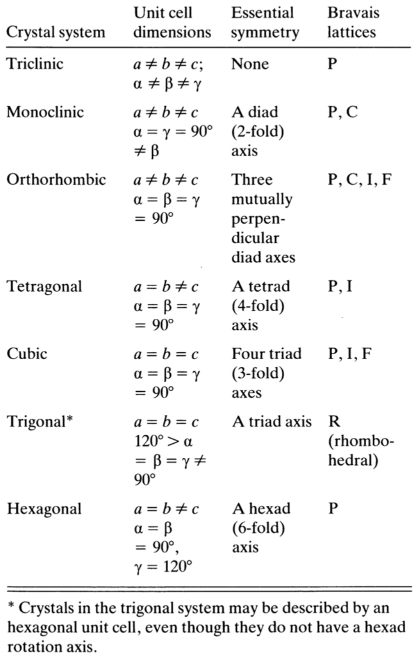
- Example 1: if there is a 4-fold axis parallel to ***c***, then the ***a*** and ***b*** unit cell dimensions must be the same, because a 90° rotation of ***a*** makes it equal to ***b***. So, the tetragonal system is characterized by a tetragonal unit cell ($\boldsymbol{a} = \boldsymbol{b} \neq \boldsymbol{c}$; $\alpha = \beta = \gamma = 90°$), and a single 4-fold rotation or roto-inversion axis (4 or $\bar{4}$). The ***c***-axis parallels the unique (4-fold) axis.

- Example 2: The monoclinic system contains either a 2-fold axis parallel to ***b*** or a mirror plane perpendicular to ***b***. This symmetry forces the ***a***-***c*** plane to be perpendicular to ***b***; so that the angles $\alpha = \gamma = 90°$. You should be able to prove to yourself that a 2-fold axis parallel to ***b*** only works if the angle between ***a*** and ***b*** is 90°. There is no constraint on the angle between ***a*** and ***c*** ($\beta \neq 90°$), and all the cell edge lengths can be different and still compatible with point symmetry.

The **six crystal systems**

You should be able to describe the types of unit cell and essential point symmetry.



Crystal system	Unit cell dimensions	Essential symmetry	Bravais lattices
Triclinic	$a \neq b \neq c$; $\alpha \neq \beta \neq \gamma$	None	P
Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90° \neq \beta$	A diad (2-fold) axis	P, C
Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	Three mutually perpendicular diad axes	P, C, I, F
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	A tetrad (4-fold) axis	P, I
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90°$	Four triad (3-fold) axes	P, I, F
Trigonal*	$a = b = c$ $120° > \alpha = \beta = \gamma \neq 90°$	A triad axis	R (rhombohedral)
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90°$, $\gamma = 120°$	A hexad (6-fold) axis	P

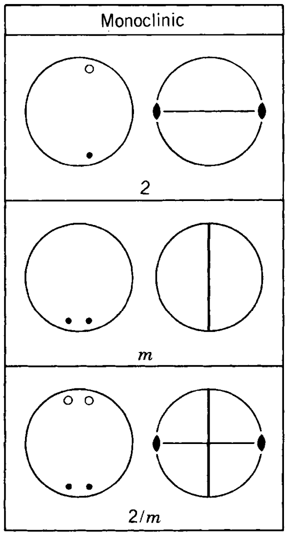
* Crystals in the trigonal system may be described by an hexagonal unit cell, even though they do not have a hexad rotation axis.

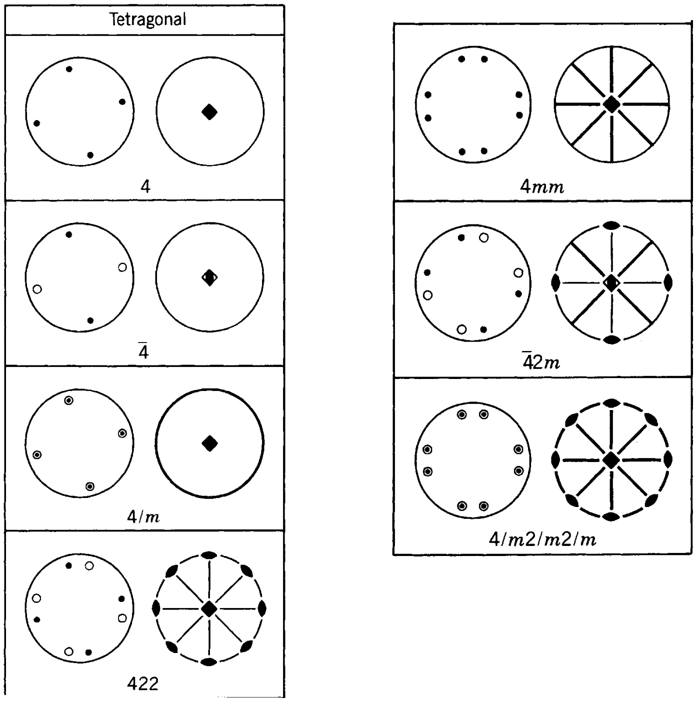
Trigonal/Hexagonal

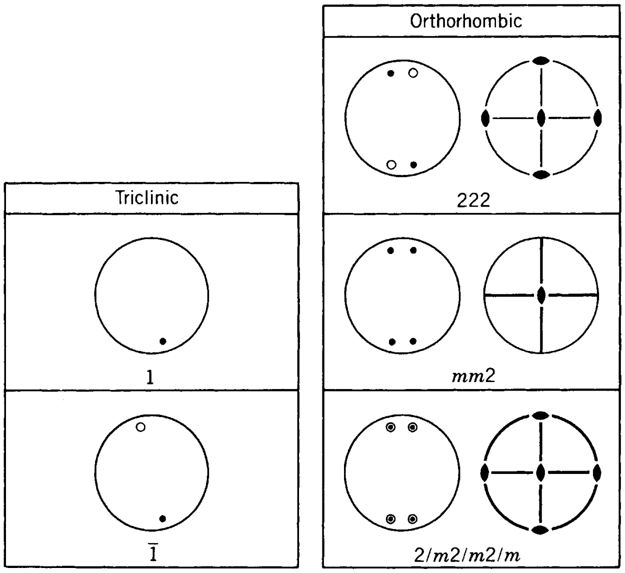
Written symbols	Graphical symbols
1	None
2	⬮
3	▲
4	◆
6	⬢
m	—
$\bar{1}$ (≡center)	*See caption
$\bar{2}$ (≡*m*)	
$\bar{3}$ (≡3 plus center)	◬
$\bar{4}$	◈
$\bar{6}$ (≡3/*m*)	⬢

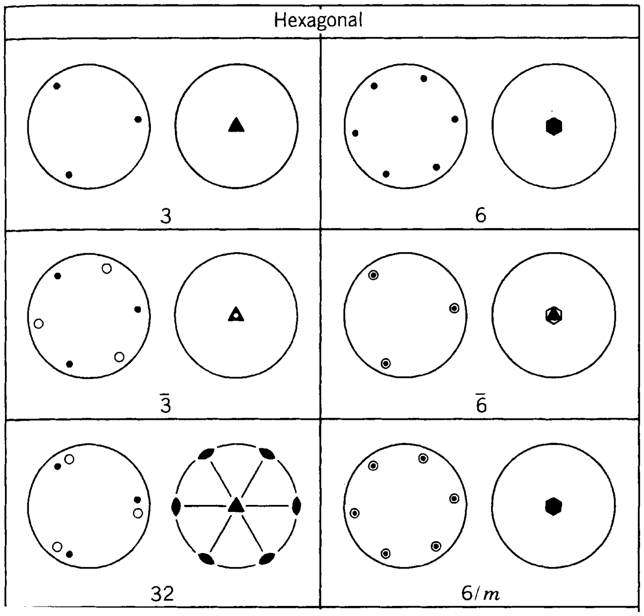
Motif above page •

Motif below page ○

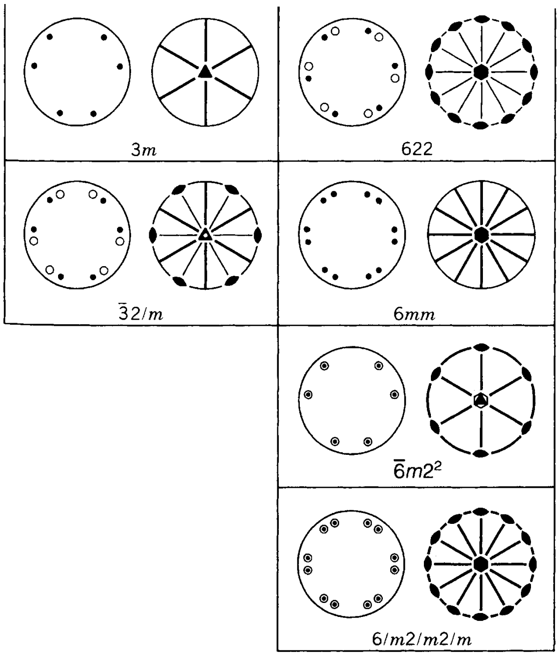


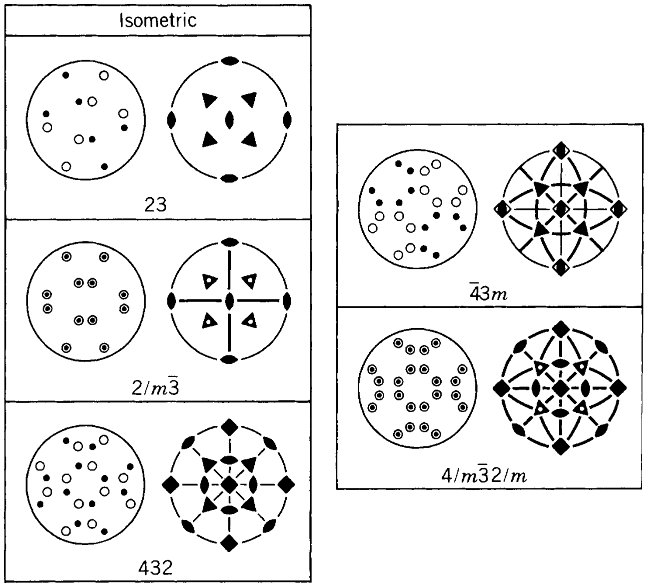



Triclinic
1
$\bar{1}$
Orthorhombic
222
*mm*2
2/*m*2/*m*2/*m*

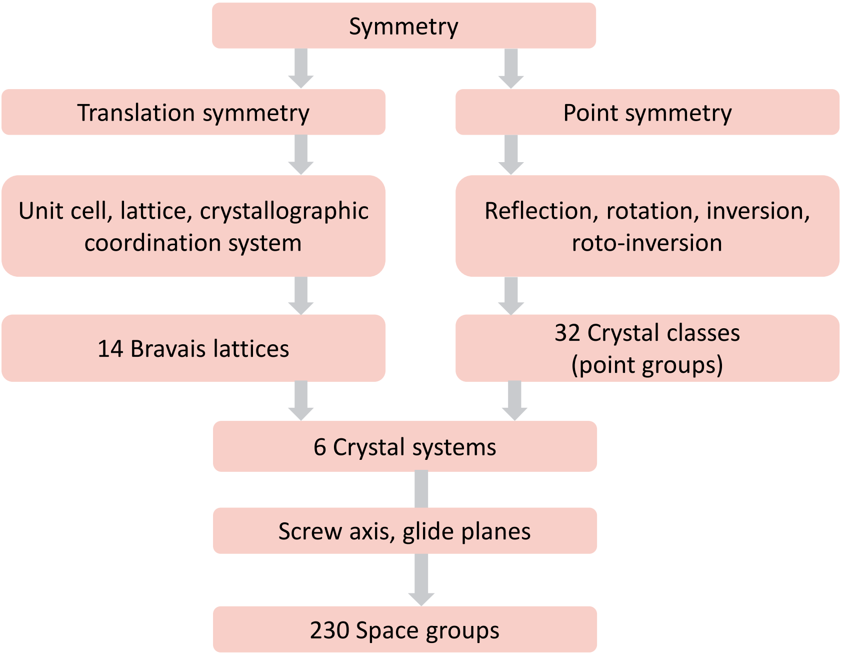

Hexagonal
3
6
$\bar{3}$
$\bar{6}$
32
6/*m*

More hexagonal





Space groups



Symmetry

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Point symmetry

Unit cell, lattice, crystallographic coordination system

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Screw axis, glide planes

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Space groups

Point symmetry plus translational symmetry

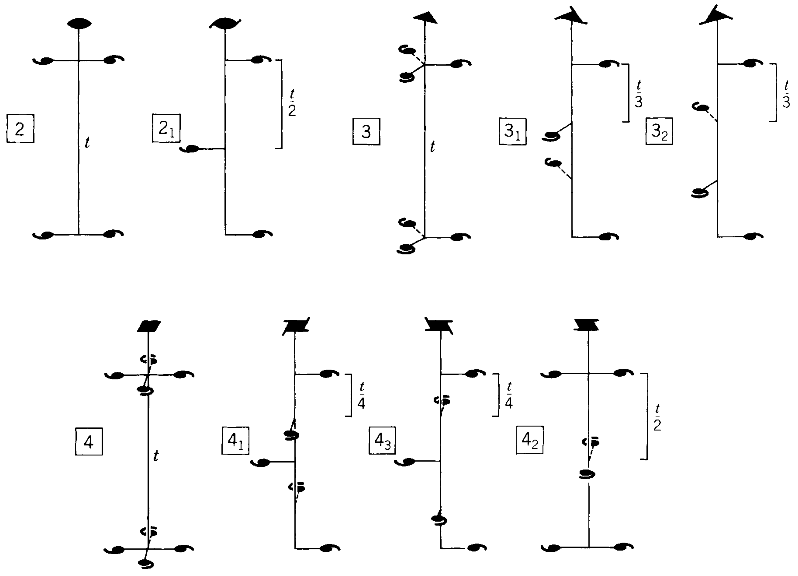
→ 230 space groups

Screw axis

Rotation plus a translation of a fraction of a unit cell

- Example: 2_1 is a rotation of 180 followed by translation of 1/2 unit cell.

Screw axes: rotation + translation

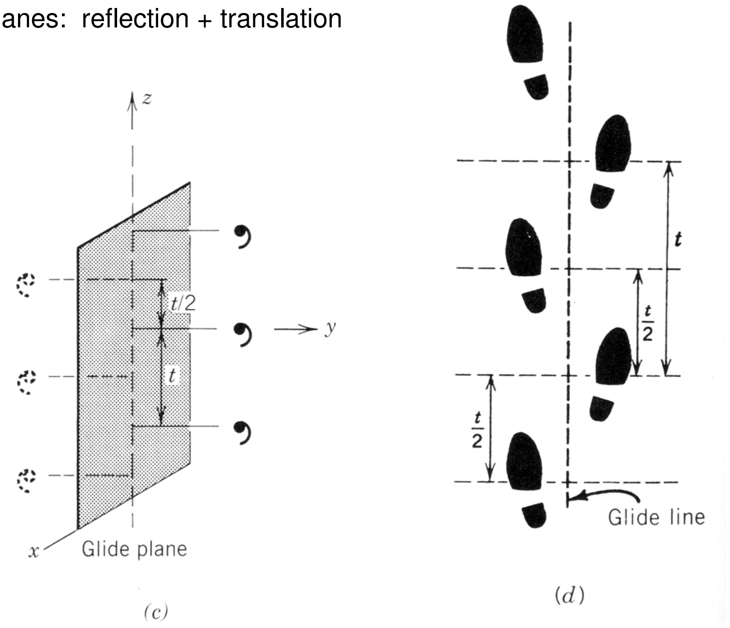


Glide plane

Reflection plus a translation of a fraction of a unit cell

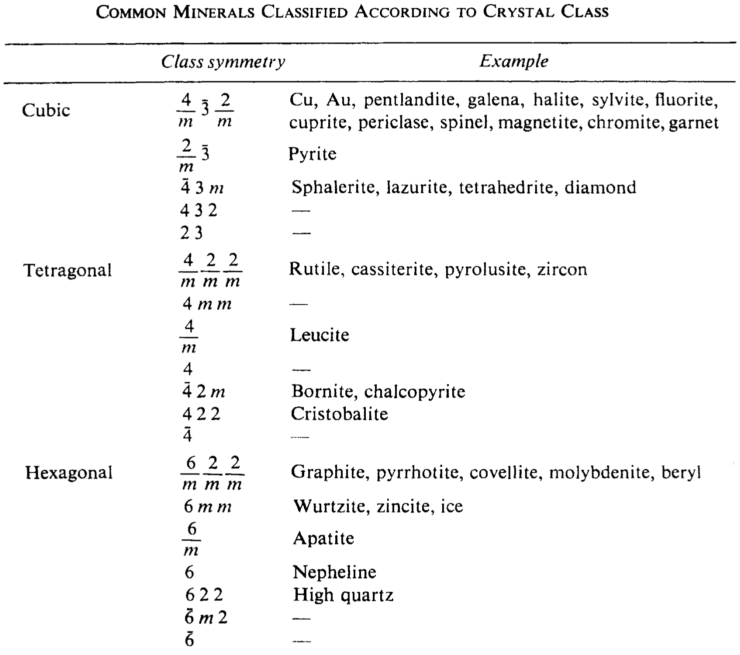
- Example: foot prints of someone walking

Glide planes: reflection + translation



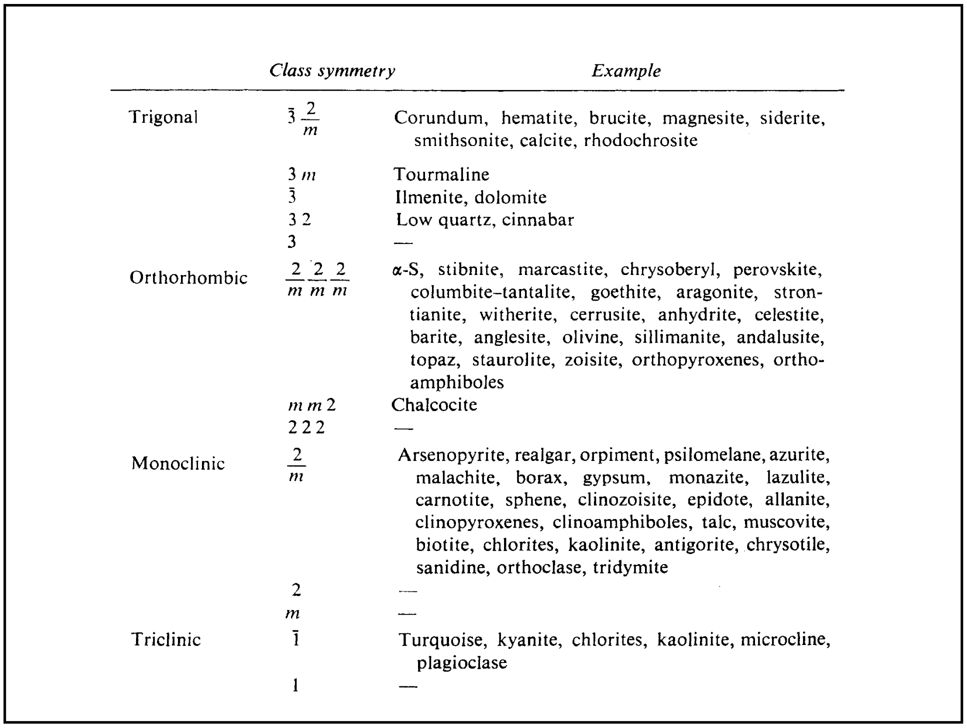
(c)

(d)



COMMON MINERALS CLASSIFIED ACCORDING TO CRYSTAL CLASS

	Class symmetry	*Example*
Cubic	$\frac{4}{m}\bar{3}\frac{2}{m}$	Cu, Au, pentlandite, galena, halite, sylvite, fluorite, cuprite, periclase, spinel, magnetite, chromite, garnet
	$\frac{2}{m}\bar{3}$	Pyrite
	$\bar{4}3m$	Sphalerite, lazurite, tetrahedrite, diamond
	432	—
	23	—
Tetragonal	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	Rutile, cassiterite, pyrolusite, zircon
	$4mm$	—
	$\frac{4}{m}$	Leucite
	4	—
	$\bar{4}2m$	Bornite, chalcopyrite
	422	Cristobalite
	$\bar{4}$	—
Hexagonal	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	Graphite, pyrrhotite, covellite, molybdenite, beryl
	$6mm$	Wurtzite, zincite, ice
	$\frac{6}{m}$	Apatite
	6	Nepheline
	622	High quartz
	$\bar{6}m2$	—
	$\bar{6}$	—



	Class symmetry	*Example*
Trigonal	$\bar{3}\frac{2}{m}$	Corundum, hematite, brucite, magnesite, siderite, smithsonite, calcite, rhodochrosite
	$3m$	Tourmaline
	$\bar{3}$	Ilmenite, dolomite
	32	Low quartz, cinnabar
	3	—
Orthorhombic	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	α-S, stibnite, marcastite, chrysoberyl, perovskite, columbite–tantalite, goethite, aragonite, strontianite, witherite, cerrusite, anhydrite, celestite, barite, anglesite, olivine, sillimanite, andalusite, topaz, staurolite, zoisite, orthopyroxenes, orthoamphiboles
	$mm2$	Chalcocite
	222	—
Monoclinic	$\frac{2}{m}$	Arsenopyrite, realgar, orpiment, psilomelane, azurite, malachite, borax, gypsum, monazite, lazulite, carnotite, sphene, clinozoisite, epidote, allanite, clinopyroxenes, clinoamphiboles, talc, muscovite, biotite, chlorites, kaolinite, antigorite, chrysotile, sanidine, orthoclase, tridymite
	2	—
	m	—
Triclinic	$\bar{1}$	Turquoise, kyanite, chlorites, kaolinite, microcline, plagioclase
	1	—