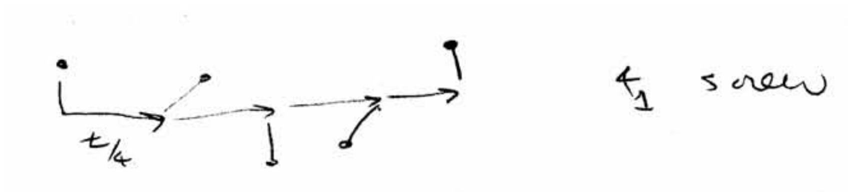
Lecture 3: Symmetry in 3D—Point Groups and Space Groups

3D Symmetry Operations

Stereographic projections are used to represent 3D symmetry elements like mirror planes and rotation axes in two dimensions. For a review, see:
Klein and Hurlbut, Jr. Manual of Mineralogy. New York: John Wiley and Sons, Inc., 1993. p. 52

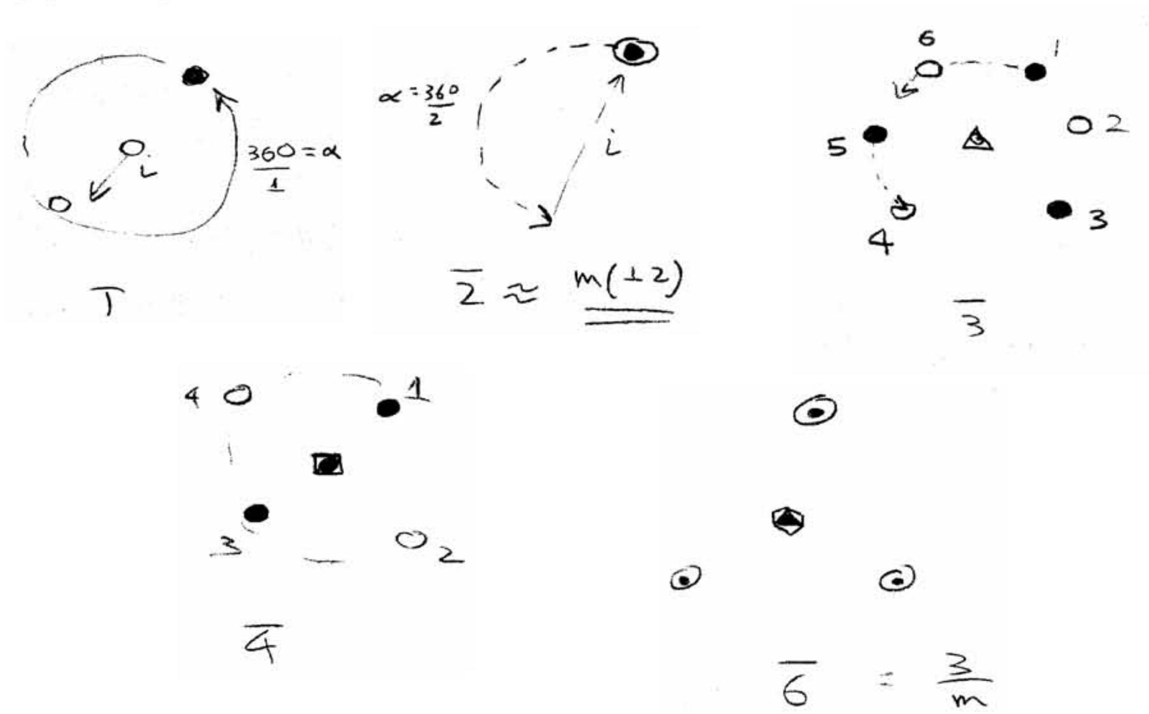
Screw Axes

Combining translation and rotation in three dimensions produces a new symmetry operation. The element is a screw axis.



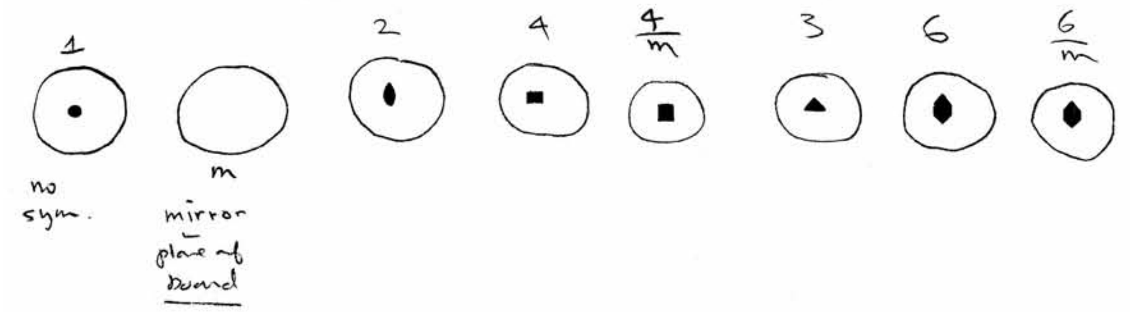
Rotoinversion

Combining rotation and inversion in three dimensions produces a new symmetry operation called rotoinversion. The diagram below gives examples of the operation. Open points are below the plane of the page; closed points are above.

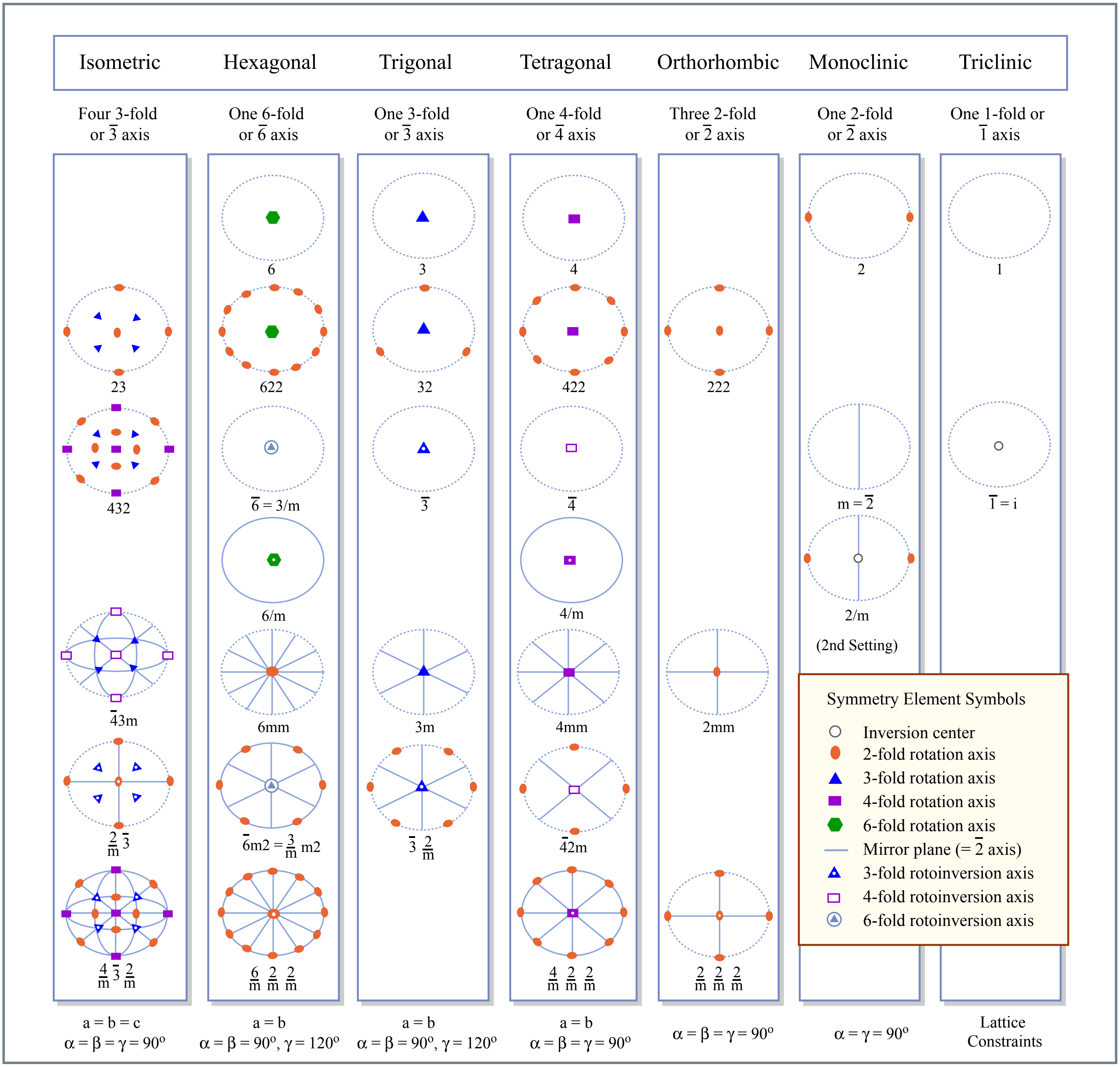


Space Point Groups

The examples of rotoinversion represent five of the thirty-two space point groups. These five belong to a group of thirteen monoaxial space groups that have a single symmetry axis. The other eight are:



The remaining point groups are multiaxial point groups—they have more than one axis of symmetry. All the space point groups are shown below. The columns are explained in the next section.



(Adapted from Klein and Hurlbut, Jr. Manual of Mineralogy. New York: John Wiley and Sons, Inc., 1993. p.)

Organizing the Point Groups

Some of the thirty-two point groups have symmetry elements in common. These common elements allow the point groups to be organized into one of six crystal systems.

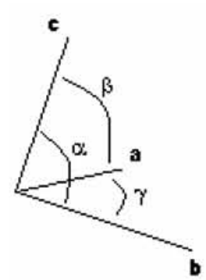
Crystal System	Characteristic Symmetry Elements
Triclinic	Onefold rotation or an inversion center
Monoclinic	One twofold rotation axis, one mirror plane, or both
Orthorhombic	Twofold rotation axes, or twofold rotation axes and mirror planes
Trigonal	Threefold rotation
Tetragonal	Fourfold rotation
Hexagonal	Sixfold rotation
Isometric	Four threefold axes

Classifying Crystals

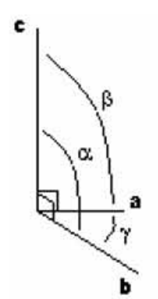
Under favorable growth conditions, the crystals of a mineral develop smooth faces. The geometry of these faces expresses the mineral's internal atomic order, and is classified according to the crystal's point symmetry. For example, crystals of salt are cubes that have 4/m 3 2/m symmetry and fall into the isometric system.

A lot of crystals have shapes that are not as straightforward as cubes. To aid in the classification of these crystals, mineralogists ascribe imaginary axes to them called crystallographic axes. The lengths of these axes and the angles between them provide a first-order approach to grouping a crystal in one of the six crystal systems.

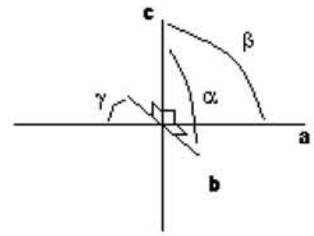
<u>System</u>	<u>Constraints</u>
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$



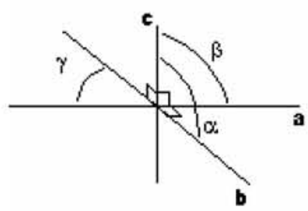
Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90°$; $\beta > 90°$



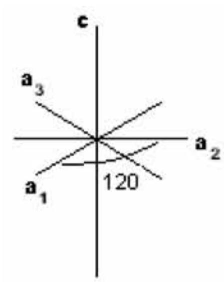
Orthorhombic $a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$



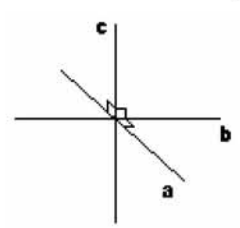
Tetragonal $a = b \neq c$
$\alpha = \beta = \gamma = 90°$



Hexagonal In the hexagonal system, there are three axes perpendicular to c called a_1, a_2, and a_3.
$a_1 = a_2 = a_3 \neq c$
a_1, a_2, and a_3 intersect at 120°



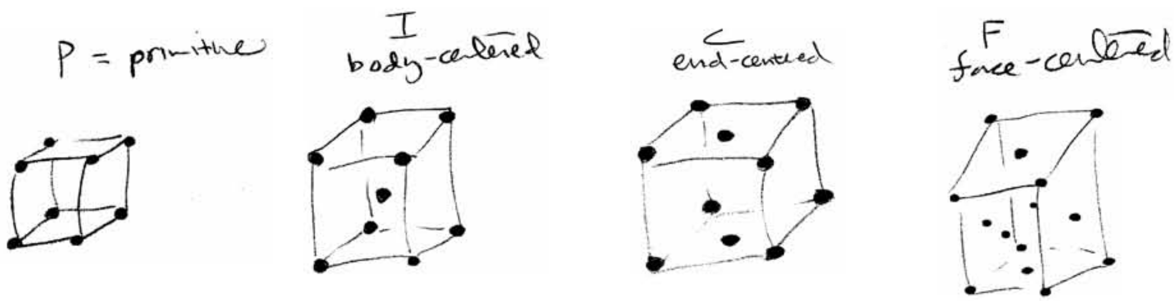
Isometric $a = b = c$
$\alpha = \beta = \gamma = 90°$



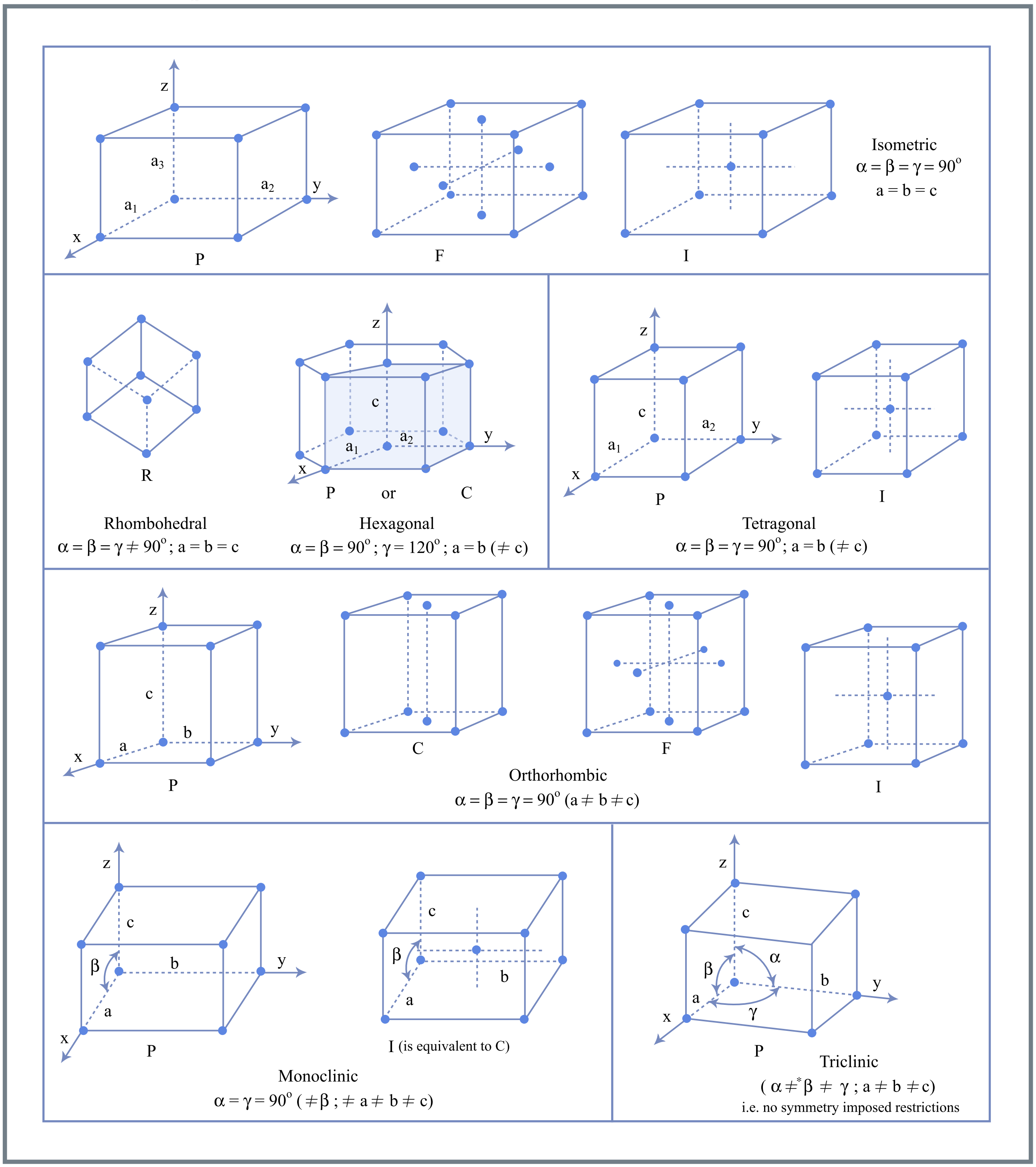
Onward to Space Groups: 3D Lattices

In the previous lecture, combining 2D point groups with 2D lattices yielded seventeen plane groups that expressed all the possible symmetry combinations in a plane. Similarly, combining 3D point groups with 3D lattices yields a number of space groups.

3D lattices have unit cells that are parallelepipeds. Depending on the location of the lattice points, the unit cells can be primitive, body-centered, end-centered, or face-centered.



Just as there are only five distinct lattices in two dimensions, there are only fourteen distinct lattices in three dimensions. They are called Bravais lattices.



(Adapted from Klein, Cornelis. Mineral Science. New York: Wiley and Sons, Inc, 2002. p. 232)

Space Groups

A particular Bravais lattice is compatible with only certain space point groups. In general, the symmetry of a lattice must be greater than or equal to the point symmetry of the motif it repeats. When the fourteen Bravais lattices are combined with space point groups having the appropriate symmetry, one arrives at 230 space groups. These space groups are like the plane groups discussed in the previous lecture: they represent the different ways in which motifs can be arranged in space. These motifs may be abstract patterns or the atoms in a crystal.

Summary of Symmetry Groups

Symmetry Group	Example	Translation?	Rotation?	Reflection?	Inversion?	Number in Group
2D point	Roadkill	no	yes	yes	n.a.	10
2D plane	Floor tiles	yes	yes	yes	yes	17
3D point	Natural objects	no	yes	yes	yes	32
3D space	crystals	yes	yes	yes	yes	230