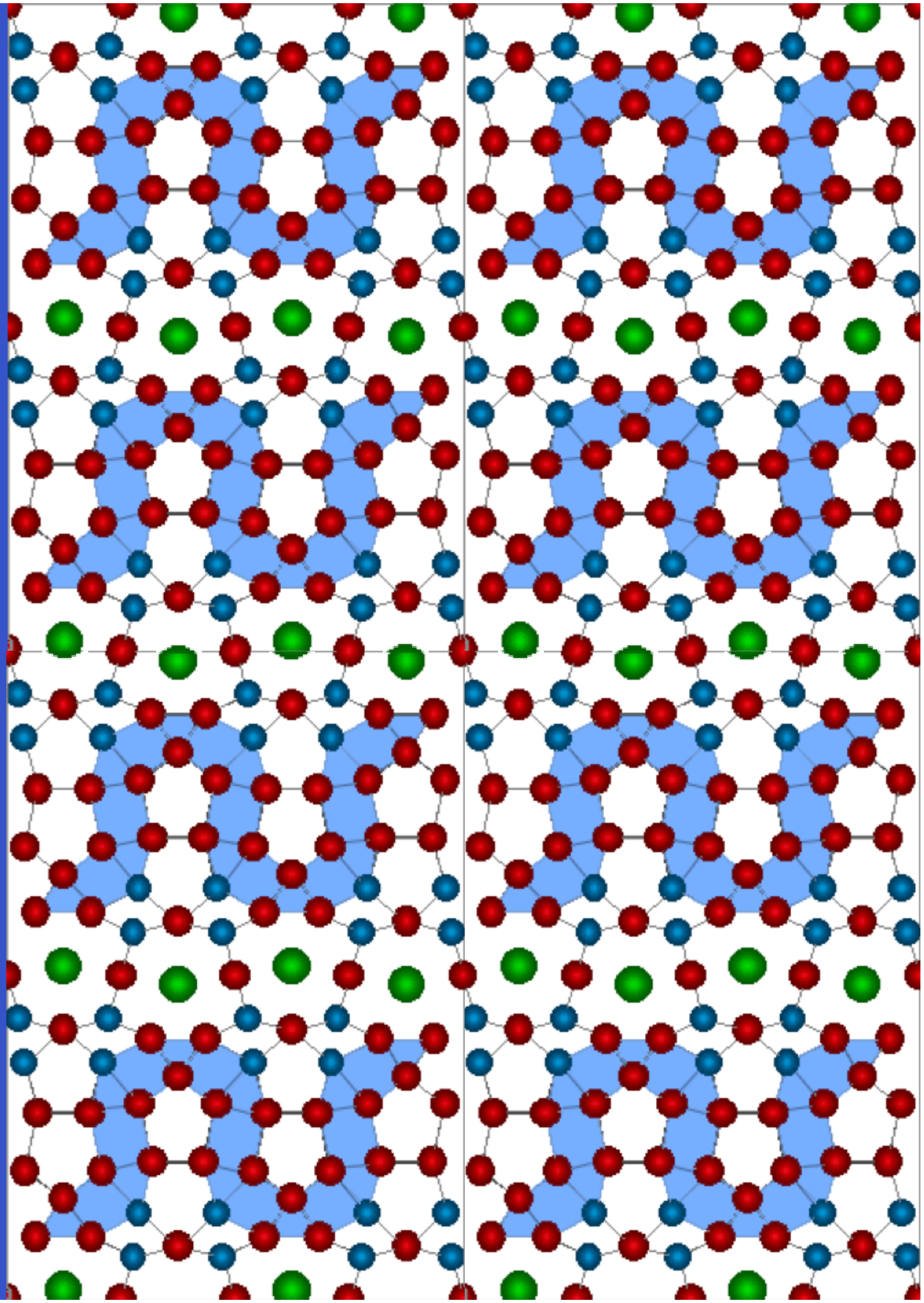
crystallography II

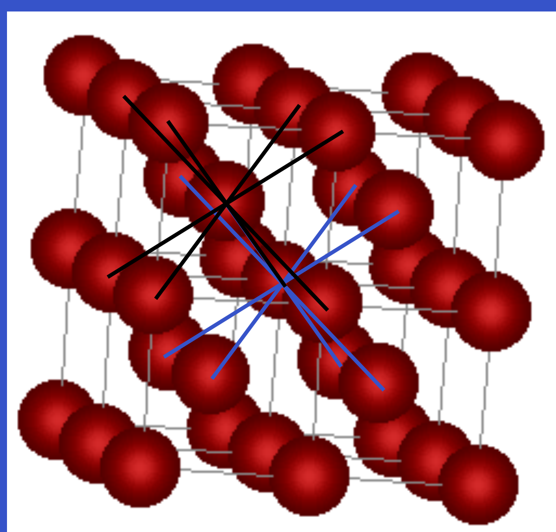


Lattice

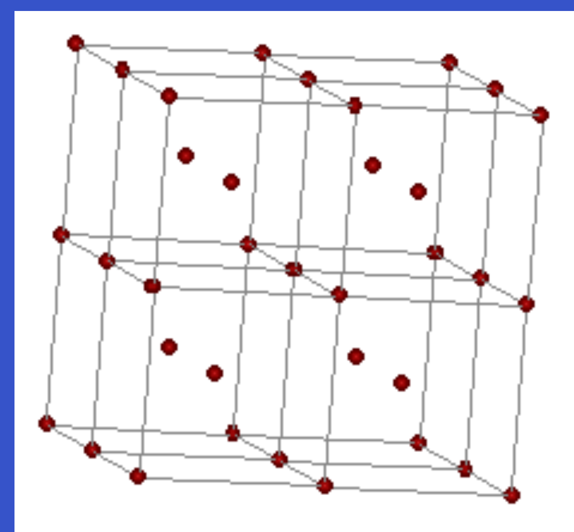
n-dimensional, infinite, periodic array of **points**,

each of which has identical surroundings.

use this as test for lattice points



A2 ("bcc") structure



lattice points

Lattice

n-dimensional, infinite, periodic array of **points**,

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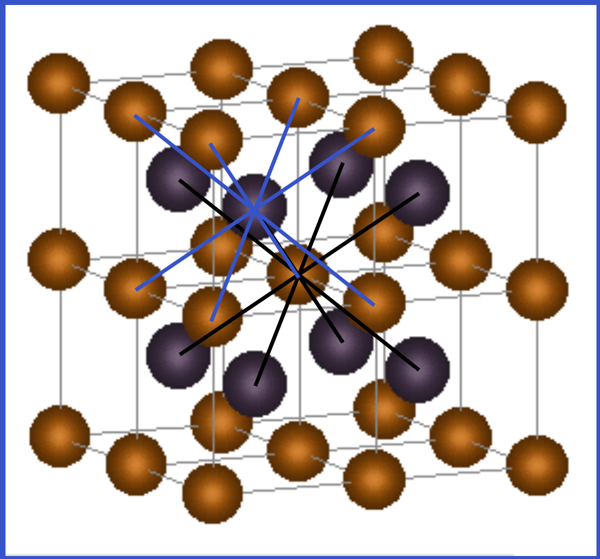
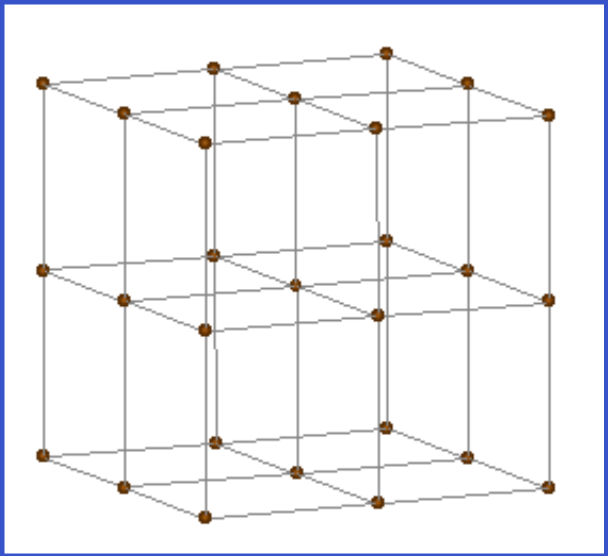
use this as test for lattice points



CsCl structure



lattice points

Choosing unit cells in a lattice

Want very small unit cell - least complicated, fewer atoms

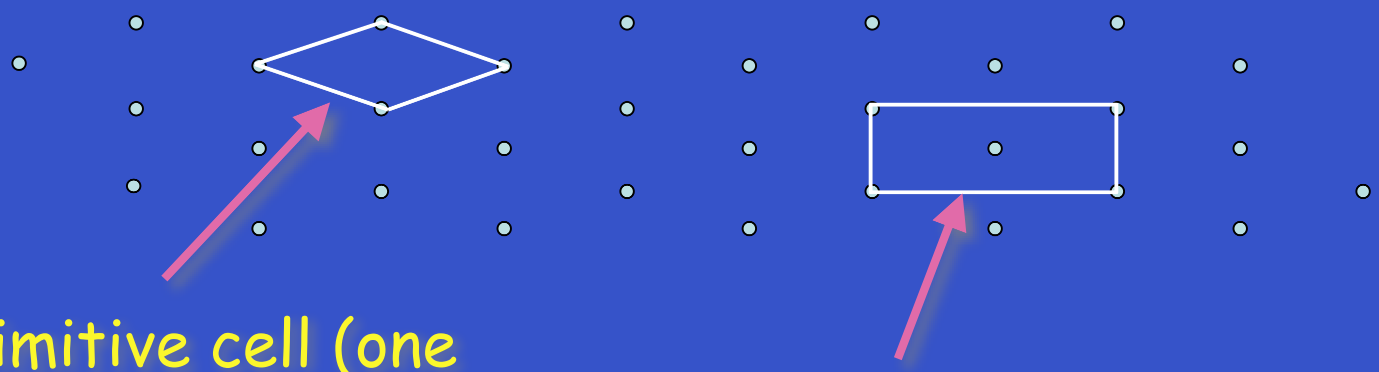
Prefer cell with 90° or 120°angles - visualization & geometrical calculations easier

Choose cell which reflects symmetry of lattice & crystal structure

Choosing unit cells in a lattice

Sometimes, a good unit cell has more than one lattice point

2-D example:



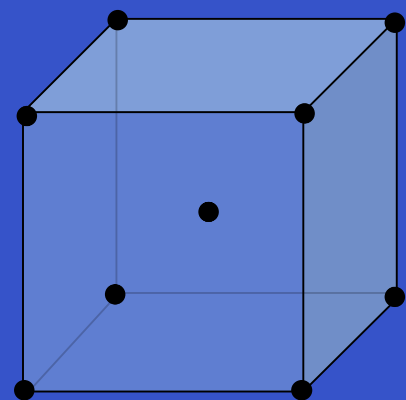
Primitive cell (one lattice pt./cell) has strange angle

End-centered cell (two lattice pts./cell) has 90° angle

Choosing unit cells in a lattice

Sometimes, a good unit cell has more than one lattice point

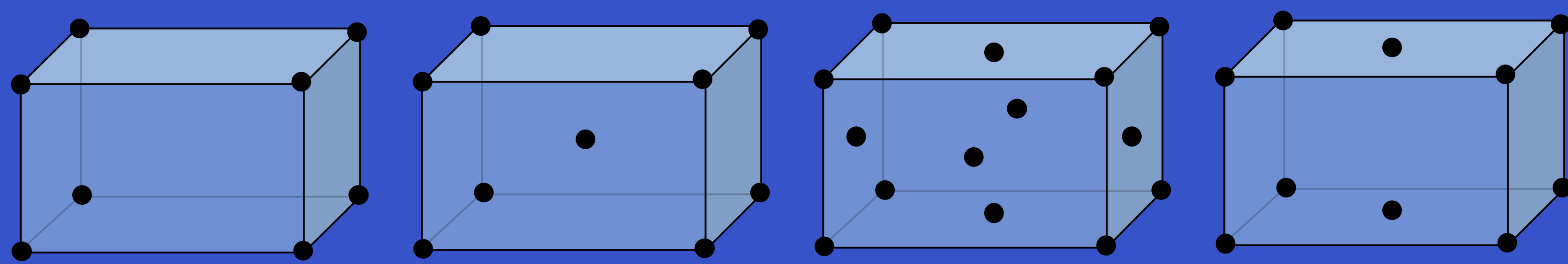
3-D example:



body-centered cubic (bcc, or I cubic)
(two lattice pts./cell)
The primitive unit cell is not a cube

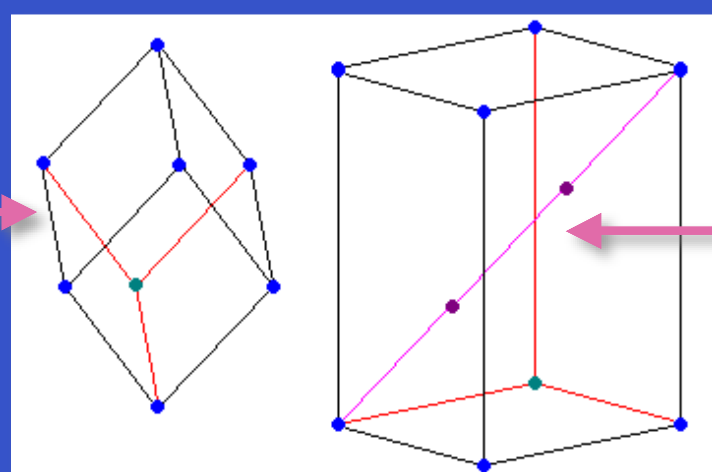
14 Bravais lattices

Allowed centering types:



P primitive | I body-centered | F face-centered | C C end-centered

Primitive rhombohedral cell (trigonal)



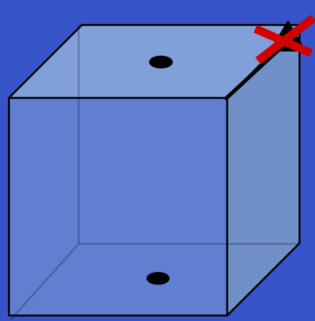
R - rhombohedral centering of trigonal cell

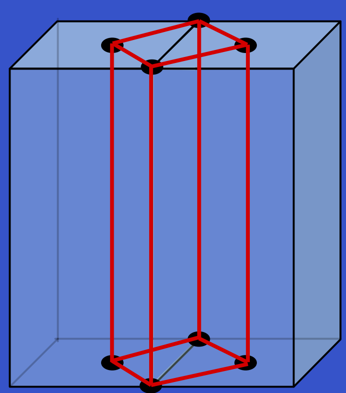
14 Bravais lattices

Combine P , I, F, C (A, B), R centering with 7 crystal systems

Some combinations don't work, some don't give new lattices -

C-centering destroys cubic symmetry





C tetragonal

= P tetragonal

14 Bravais lattices

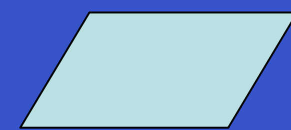
Only 14 possible (Bravais, 1848)

System	Allowed centering
Triclinic	P (primitive)
Monoclinic	P, I (innerzentiert)
Orthorhombic	P, I, F (flächenzentiert), A (end centered)
Tetragonal	P, I
Cubic	P, I, F
Hexagonal	P
Trigonal	P, R (rhombohedral centered)

Choosing unit cells in a lattice

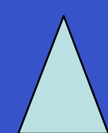
Unit cell shape must be:

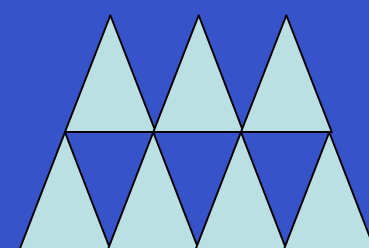
2-D - parallelogram
(4 sides)



3-D - parallelepiped
(6 faces)

Not a unit cell:





Choosing unit cells in a lattice

Unit cell shape must be:

2-D - parallelogram
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3-D - parallelepiped
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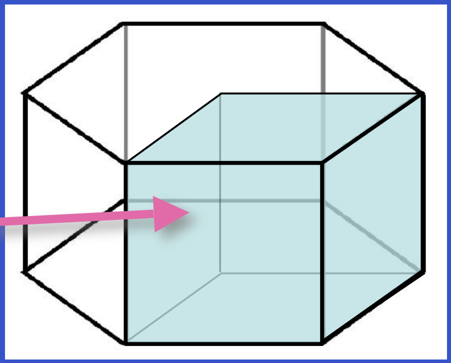
Not a unit cell:



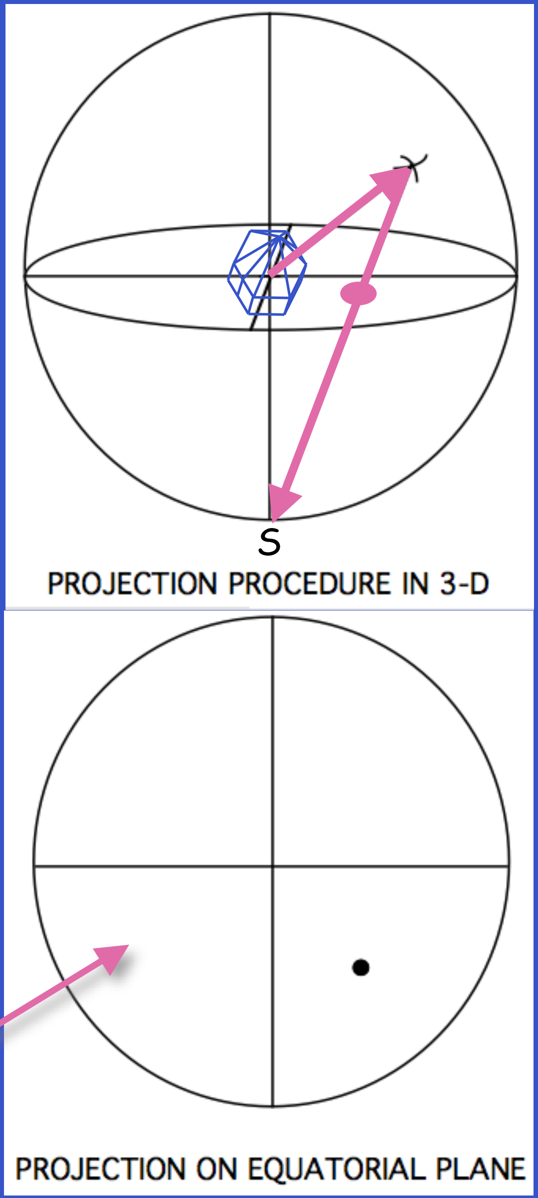
correct cell

Stereographic projections

Show or represent 3-D object in 2-D

Procedure:

1. Place object at center of sphere
2. From sphere center, draw line representing some feature of object out to intersect sphere
3. Connect point to N or S pole of sphere. Where sphere passes through equatorial plane, mark projected point
4. Show equatorial plane in 2-D – this is stereographic projection



PROJECTION PROCEDURE IN 3-D

PROJECTION ON EQUATORIAL PLANE

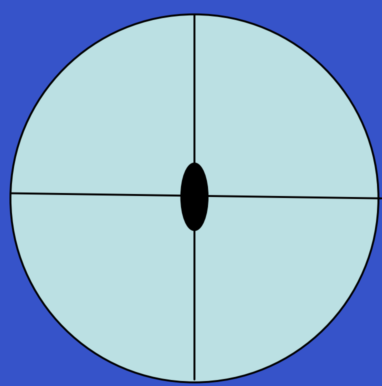
Stereographic projections of symmetry groups

Types of pure rotation symmetry

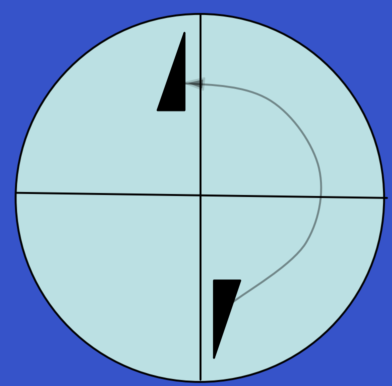
Rotation 1, 2, 3, 4, 6

Rotoinversion $\bar{1}$ (= i), $\bar{2}$ (= m), $\bar{3}$, $\bar{4}$, $\bar{6}$

Draw point group diagrams (stereographic projections)



symmetry elements



equivalent points

Stereographic projections of symmetry groups

Types of pure rotation symmetry

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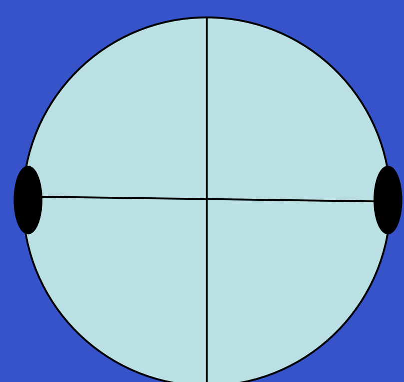
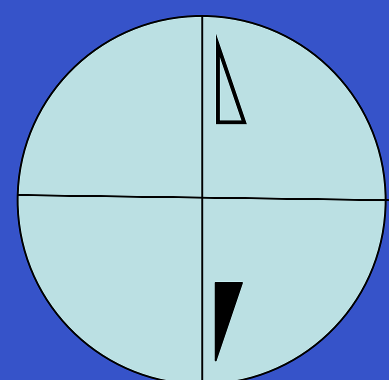


symmetry elements



equivalent points

Stereographic projections of symmetry groups

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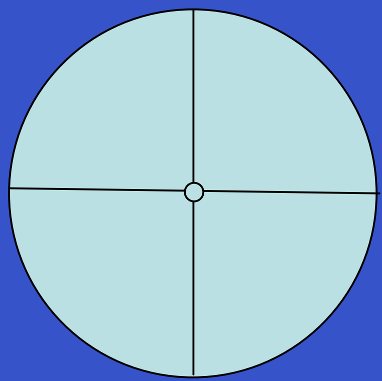
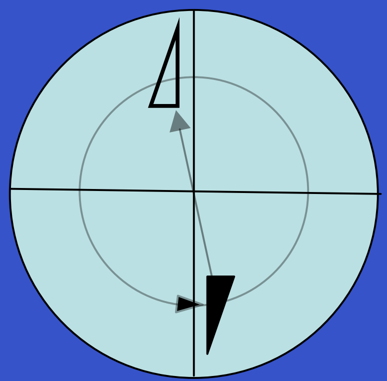


symmetry elements



equivalent points

Stereographic projections of symmetry groups

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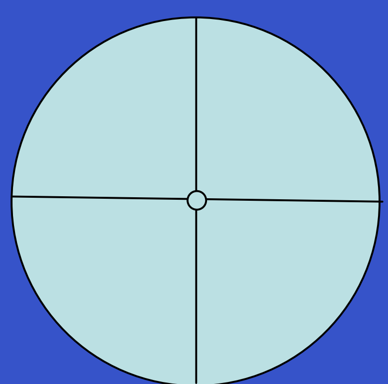
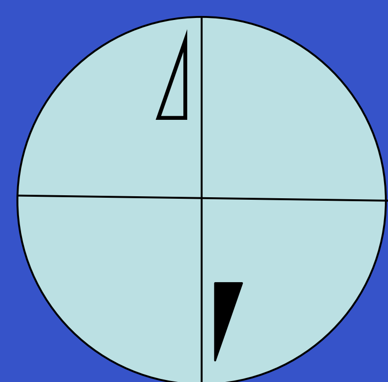


symmetry elements



equivalent points

All objects, structures with *i* symmetry are centric

Stereographic projections of symmetry groups

Types of pure rotation symmetry

Rotation 1, 2, 3, 4, 6

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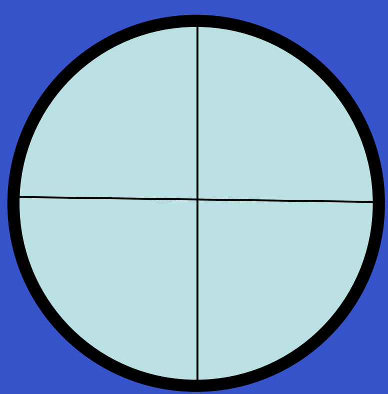
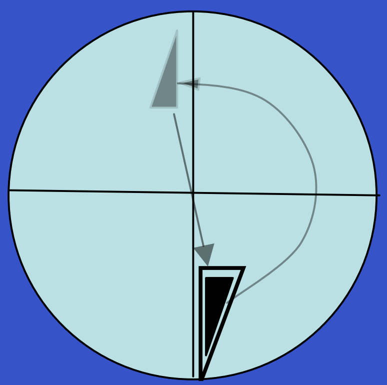


symmetry elements



equivalent points

Stereographic projections of symmetry groups

Types of pure rotation symmetry

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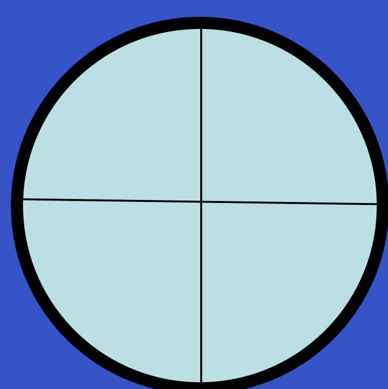
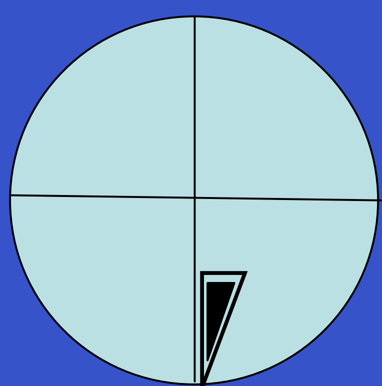


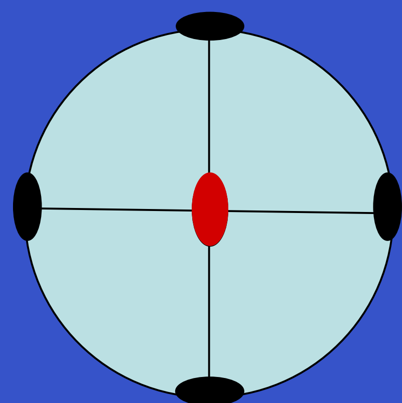
symmetry elements

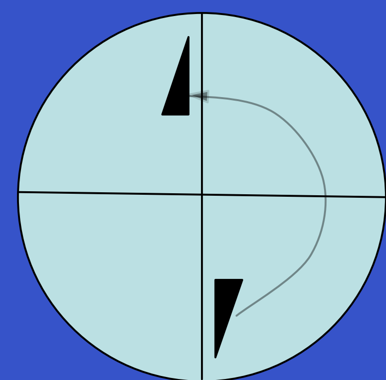


equivalent points

Stereographic projections of symmetry groups

More than one rotation axis - point group 222


symmetry elements


equivalent points

Stereographic projections of symmetry groups

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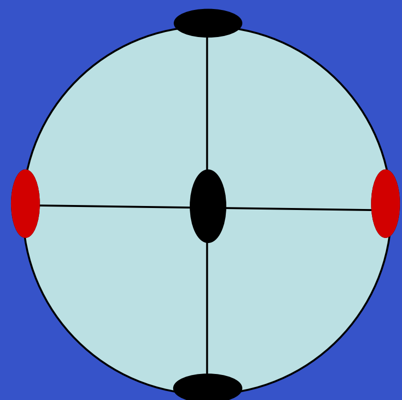
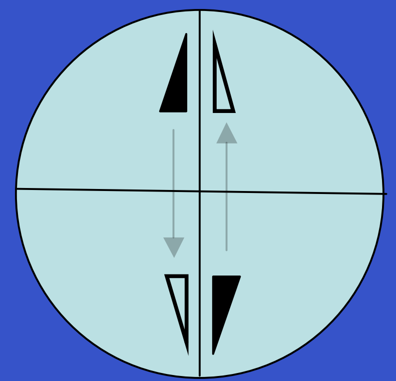


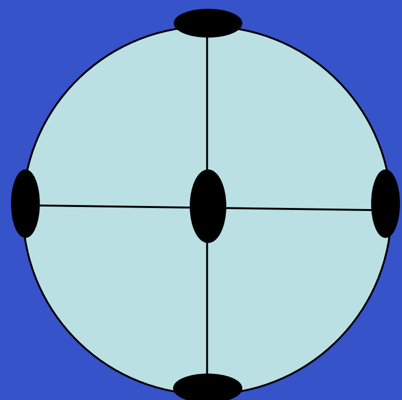
symmetry elements



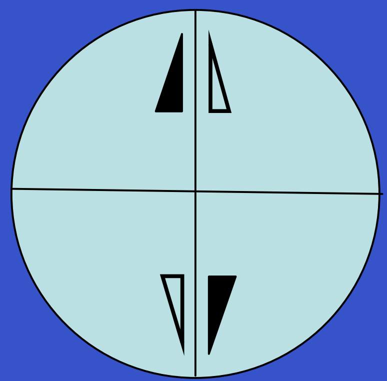
equivalent points

Stereographic projections of symmetry groups

More than one rotation axis - point group 222



symmetry elements

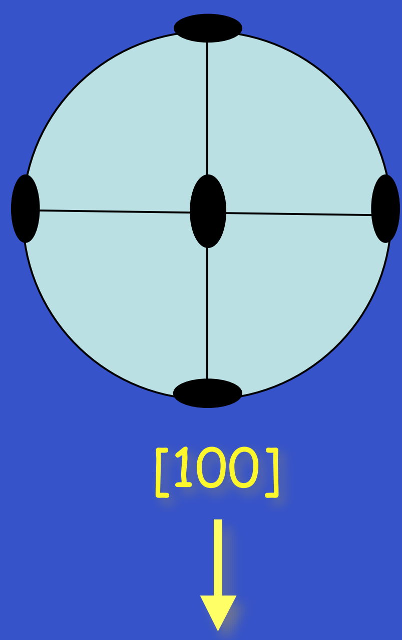


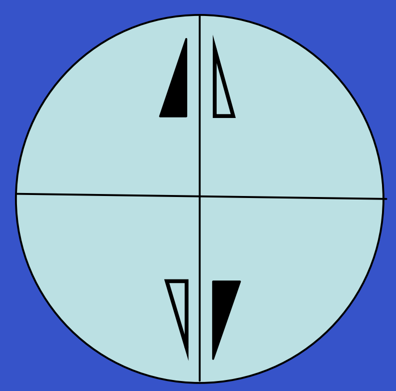
equivalent points

orthorhombic

Stereographic projections of symmetry groups

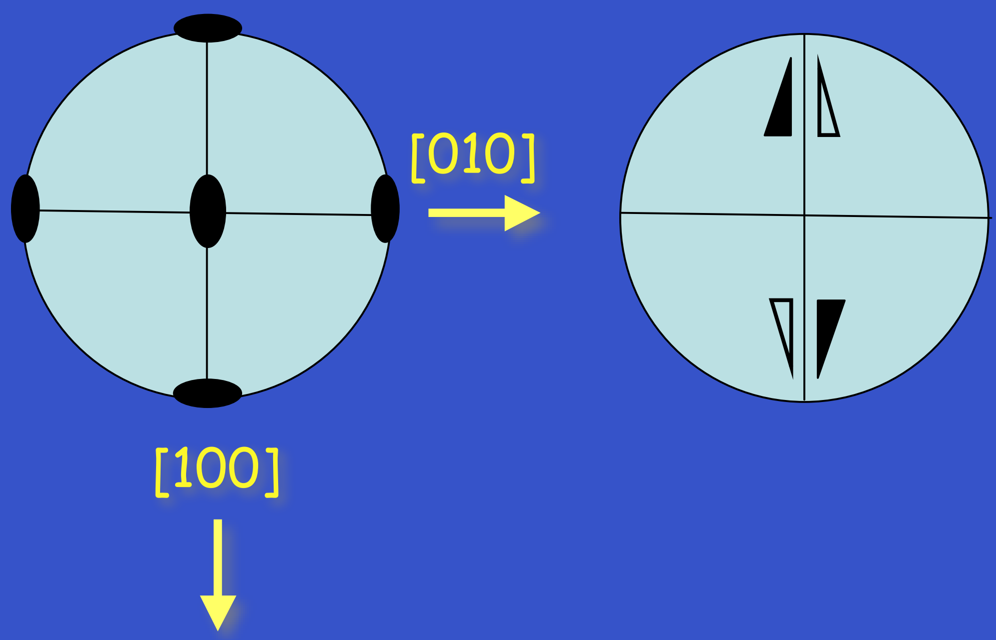
More than one rotation axis - point group $\boxed{2}22$





Stereographic projections of symmetry groups

More than one rotation axis - point group 222



Stereographic projections of symmetry groups

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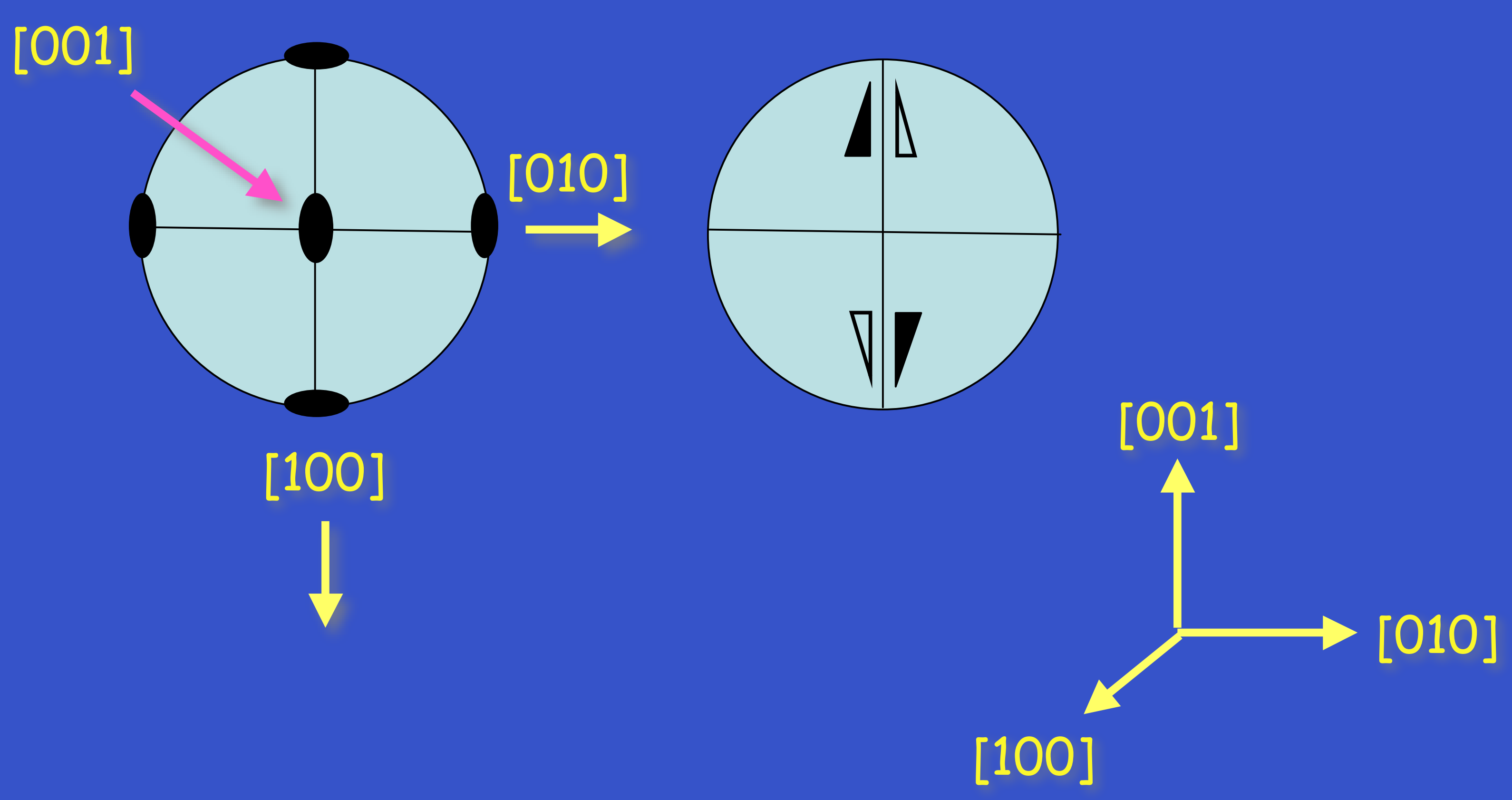
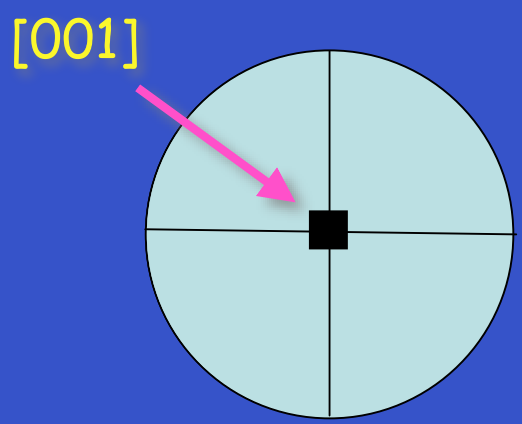
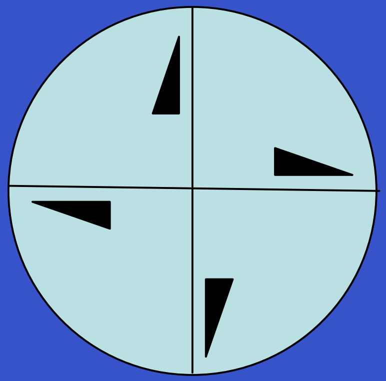


Stereographic projections of symmetry groups

Rotation + mirrors - point group 4mm





Stereographic projections of symmetry groups

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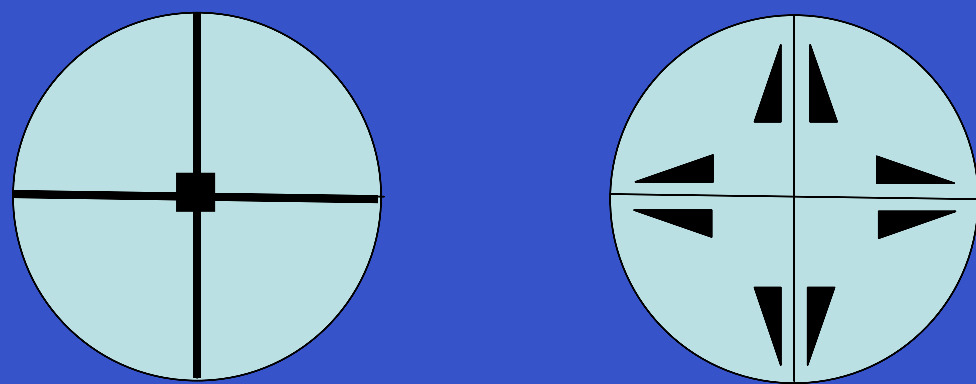
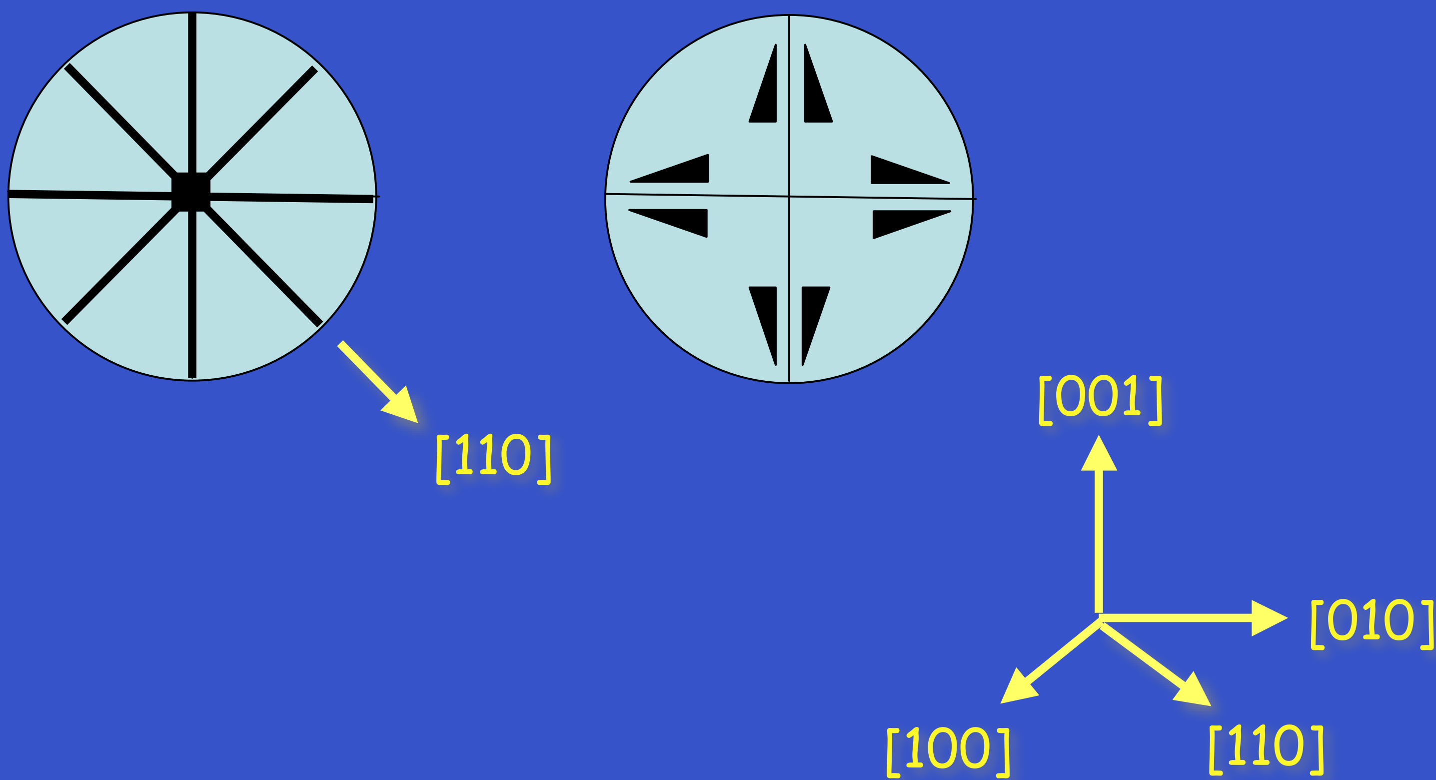


[100]

Stereographic projections of symmetry groups

Rotation + mirrors - point group 4mm



Stereographic projections of symmetry groups

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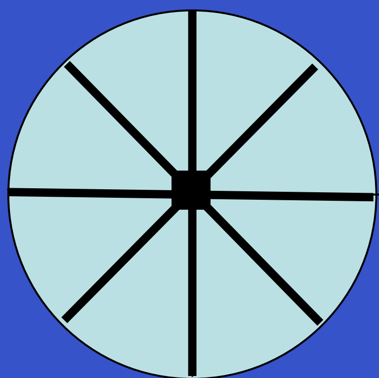
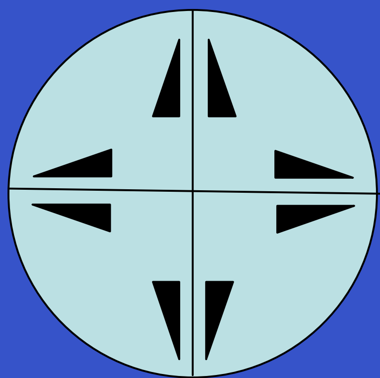


symmetry elements

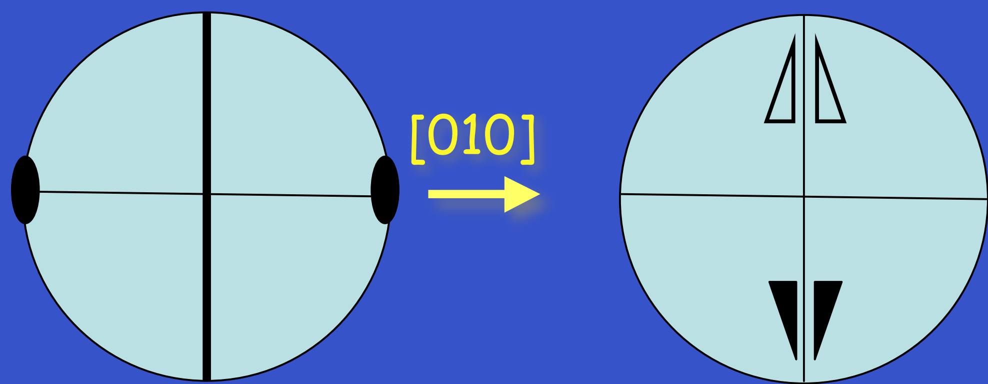


equivalent points

tetragonal

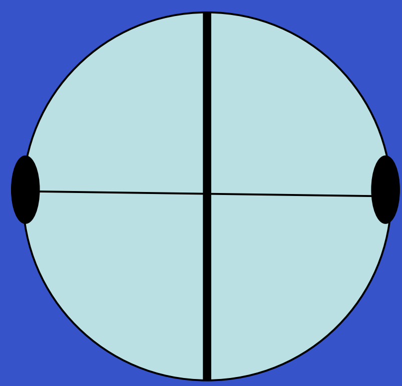
Stereographic projections of symmetry groups

Rotation + mirrors - point group 2/m

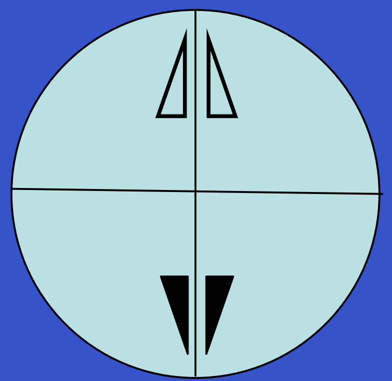


Stereographic projections of symmetry groups

Rotation + mirrors - point group 2/m



symmetry elements



equivalent points

monoclinic

Stereographic projections of symmetry groups

Use this table for symmetry directions

System	1st symbol	2nd symbol	3rd symbol
Triclinic	–	–	–
Monoclinic	[010]	–	–
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	[100]	[110]
Cubic	[100]	[111]	[110]
Hexagonal	[001]	[100]	[210]
Trigonal	[001]	[100]	[210]

Use this table to assign point groups to crystal systems

System	Minimum symmetry
Triclinic	1 or $\bar{1}$
Monoclinic	2 or $\bar{2}$
Orthorhombic	three 2s or $\bar{2}$s
Tetragonal	4 or $\bar{4}$
Cubic	four 3s or $\bar{3}$s
Hexagonal	6 or $\bar{6}$
Trigonal	3 or $\bar{3}$

And here are the 32 point groups

System	Point groups
Triclinic	$1, \bar{1}$
Monoclinic	$2, m, 2/m$
Orthorhombic	$222, mm2, 2/m\ 2/m\ 2/m$
Tetragonal	$4, \bar{4}, 4/m, 422, \bar{4}2m, 4mm, 4/m\ 2/m\ 2/m$
Cubic	$23, 2/m\ \bar{3}, 432, \bar{4}3m, 4/m\ \bar{3}\ 2/m$
Hexagonal	$6, \bar{6}, 6/m, 622, \bar{6}2m, 6mm, 6/m\ 2/m\ 2/m$
Trigonal	$3, \bar{3}, 32, 3m, \bar{3}\ 2/m$