Coordination Number

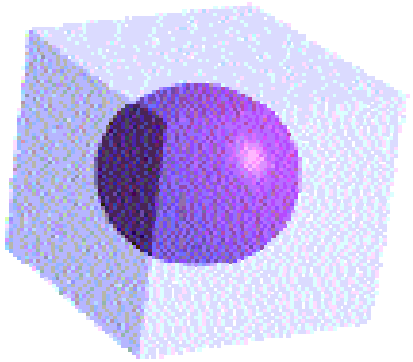
- Coordination Number (CN) : The Bravais lattice points closest to a given point are the nearest neighbours.

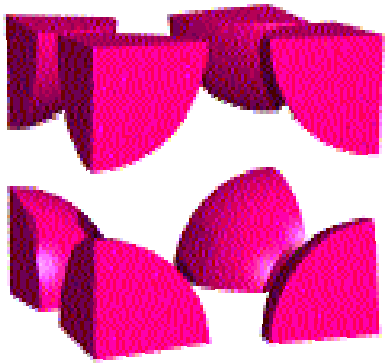
- Because the Bravais lattice is periodic, all points have the same number of nearest neighbours or coordination number. It is a property of the lattice.

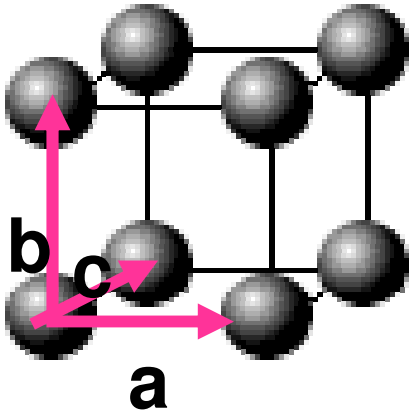
- A simple cubic has coordination number 6; a body-centered cubic lattice, 8; and a face-centered cubic lattice,12.

Examlple 1: Coordination Number for SC

- Simple Cubic has one lattice point so its primitive cell.
- In the unit cell on the left, the atoms at the corners are cut because only a portion (in this case 1/8) belongs to that cell. The rest of the atom belongs to neighboring cells.
- Coordinatination number of simple cubic is 6.

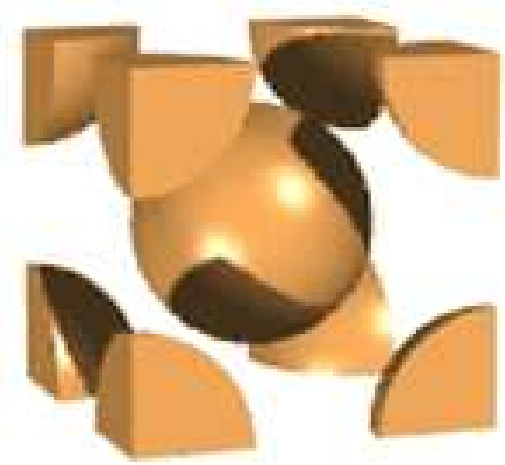


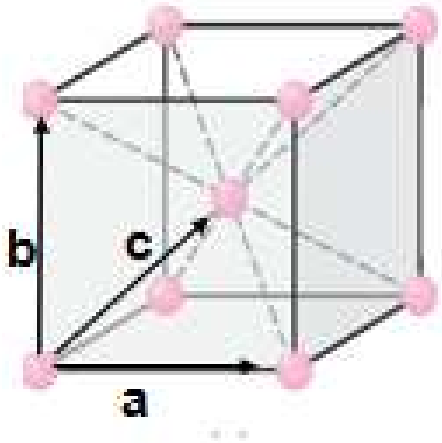




Example 2: Coordination Number for BCC

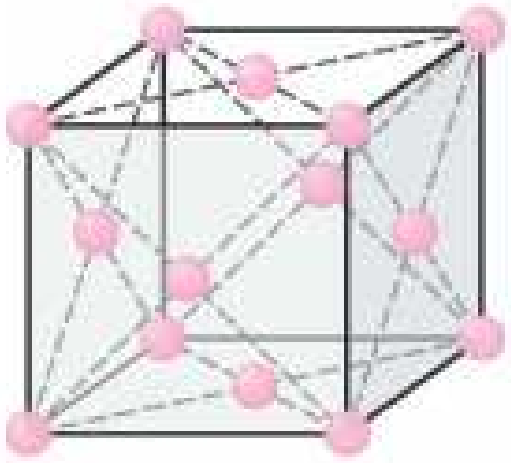
- BCC has two lattice points so BCC is a non-primitive cell.
- BCC has eight nearest neighbors. Each atom is in contact with its neighbors only along the body-diagonal directions.
- Many metals (Fe,Li,Na..etc), including the alkalis and several transition elements choose the BCC structure.

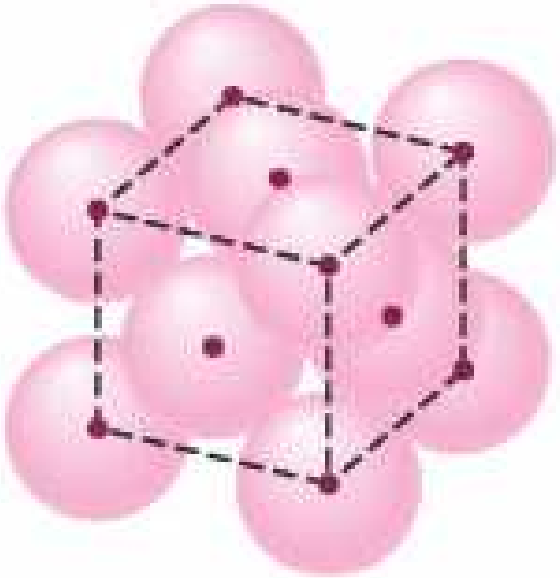


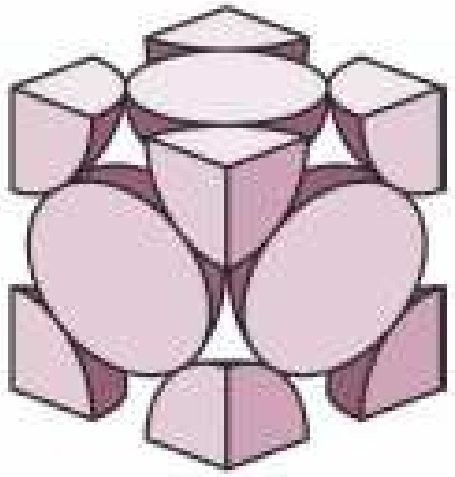


Example 3: Coordination Number for FCC

- There are atoms at the corners of the unit cell and at the center of each face.
- Face centered cubic has 4 atoms so its non primitive cell.
- Many of common metals (Cu,Ni,Pb..etc) crystallize in FCC structure.







Unit cell contents

Counting the number of atoms within the unit cell

Atoms	Shared Between:	Each atom counts:
corner	8 cells	1/8
face centre	2 cells	1/2
body centre	1 cell	1
edge centre	2 cells	1/2

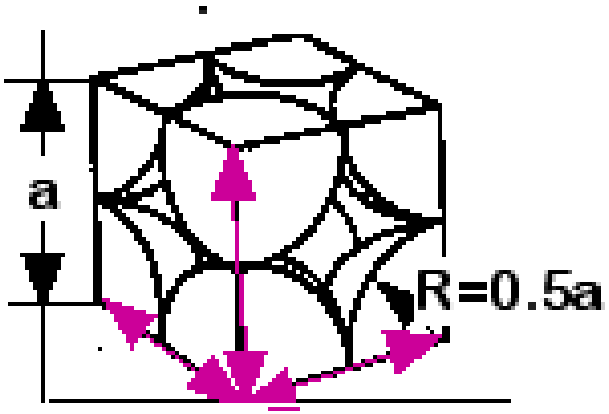
lattice type	cell contents	
P	1	[=8 x 1/8]
I	2	[=(8 x 1/8) + (1 x 1)]
F	4	[=(8 x 1/8) + (6 x 1/2)]
C	2	[=(8 x 1/8) + (2 x 1/2)]

Atomic Packing Factor

- **Atomic Packing Factor (APF) is defined as the volume of atoms within the unit cell divided by the volume of the unit cell.**

$$\text{APF} = \frac{\text{Volume of Atoms in Unit Cell}}{\text{Volume of Unit Cell}}$$

Example 1: Atomic Packing Factor for SC

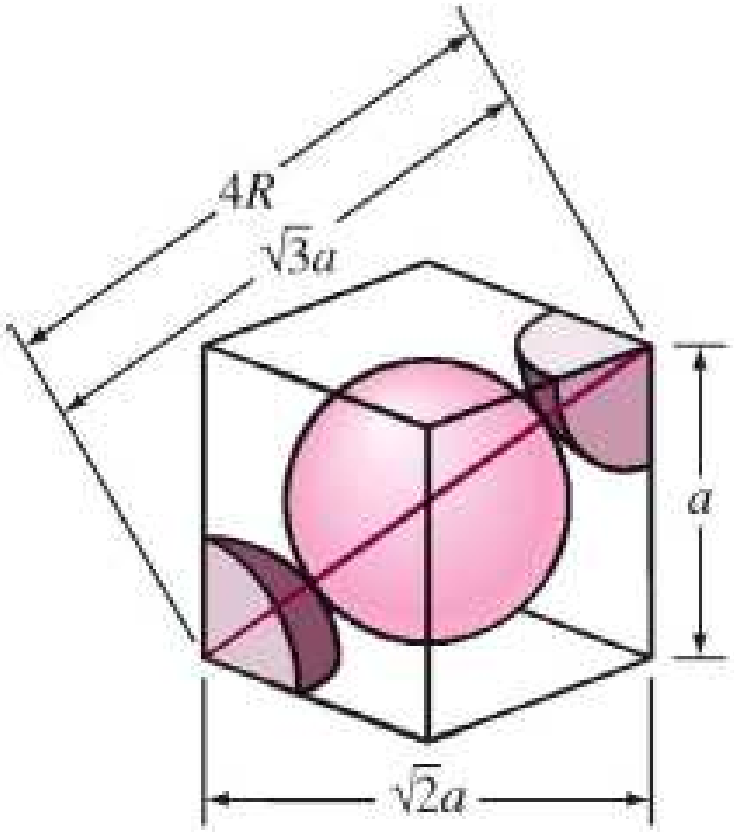


contains 8 x 1/8 =
1atom/unit cell

APF = 0.52 for simple cubic

$$APF = \frac{\frac{\text{atom}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}}}{\frac{\text{volume}}{\text{unit cell}}} = \frac{1 \cdot \frac{4}{3}\pi (0.5a)^3}{a^3}$$

Example 2: Atomic Packing Factor for BCC



$\sqrt{3}a = 4R$

atom / unit cell

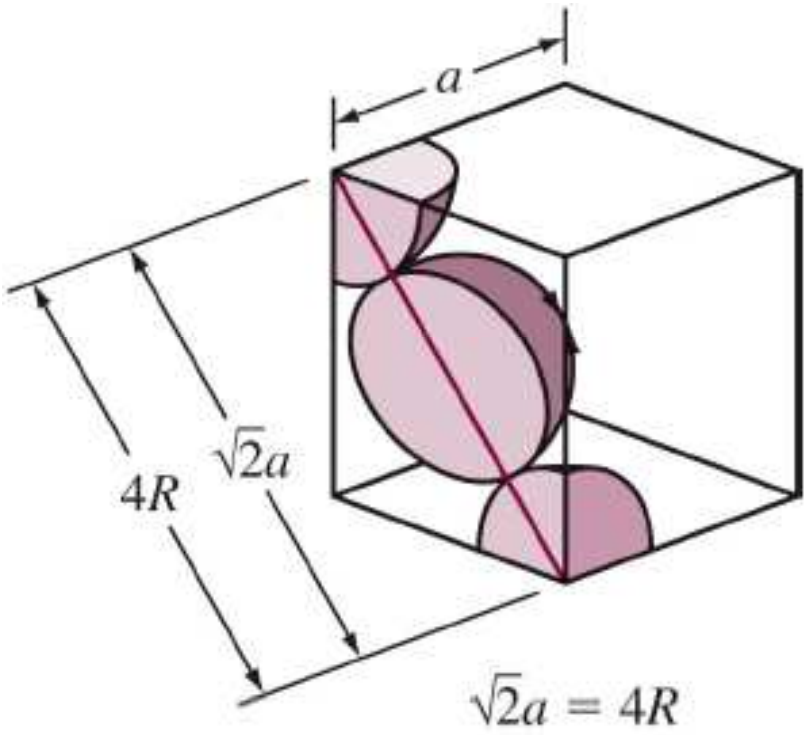
volume / atom

volume / unit cell

$$APF = \frac{2 \cdot \frac{4}{3}\pi (0{,}433a)^3}{a^3}$$

$$APF_{BCC} = \frac{V_{atoms}}{V_{unit\ cell}} = 0.68$$

Example 3: Atomic Packing Factor for FCC



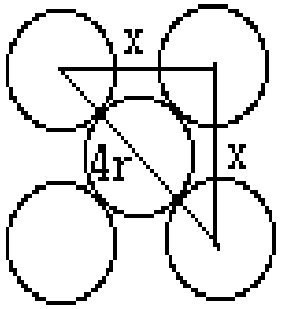
$$APF_{FCC} = \frac{V_{atoms}}{V_{unit\ cell}} = 0{,}74$$

$$APF = \frac{\dfrac{\text{atom}}{\text{unit cell}} \left[1 \; \frac{4}{3}\pi (0.5a)^3 \right] \dfrac{\text{volume}}{\text{atom}}}{a^3 \; \dfrac{\text{volume}}{\text{unit cell}}}$$

Comprehensive details for APF for FCC

It is very easy to show that the filling of space by spheres is 74%
e.g. for the fcc unit cell of cubic close packing (CCP) with an ABC layer repeat

For spheres of radius, r, touching along the **face diagonal**, the cubic unit cell parameter is calculated as $x = 2\sqrt{2}\,r$



total unit cell volume = x^3

$= 16\sqrt{2}\,r^3$

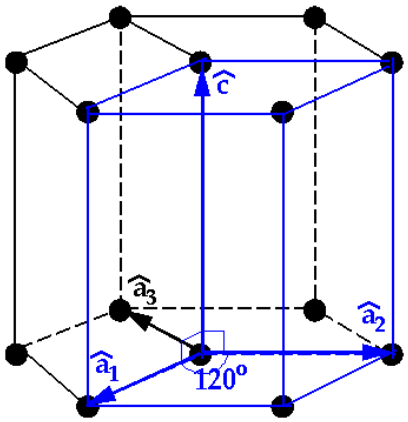
occupied volume = 4 spheres

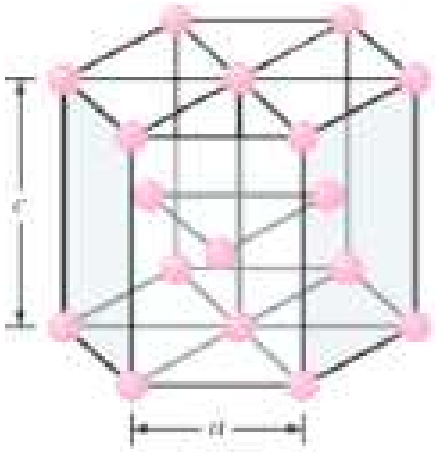
$= \frac{16\pi r^3}{3}$

space filling = $\frac{\pi}{3\sqrt{2}}$ = **74.05 %**

HEXAGONAL SYSTEM

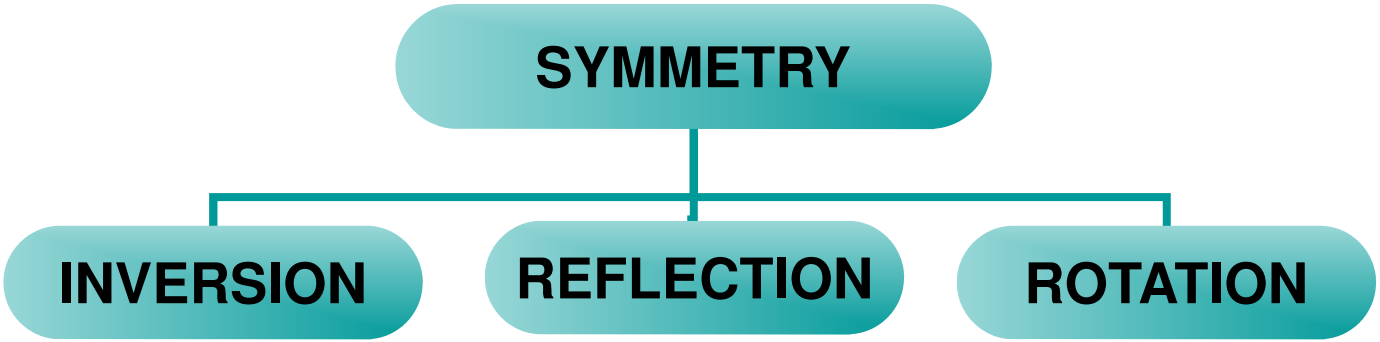
- A crystal system in which three equal coplanar axes intersect at an angle of 60 , and a perpendicular to the others, is of a different length.





ELEMENTS OF SYMMETRY

- Each of the unit cells of the 14 Bravais lattices has one or more types of symmetry properties, such as inversion, reflection or rotation,etc.



Lattice goes into itself through Symmetry without translation

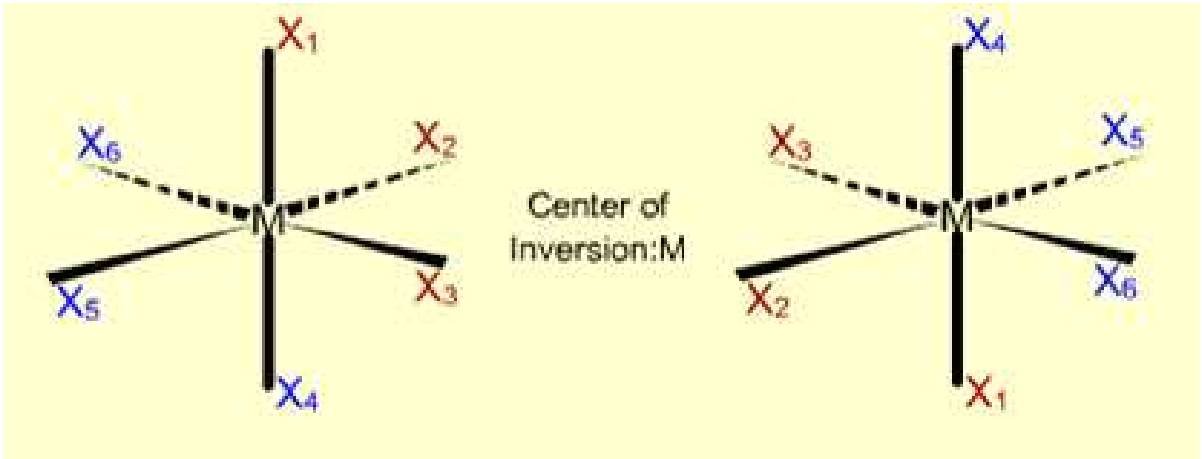
Operation	Element
Inversion	Point
Reflection	Plane
Rotation	Axis
Rotoinversion	Axes

Inversion Center

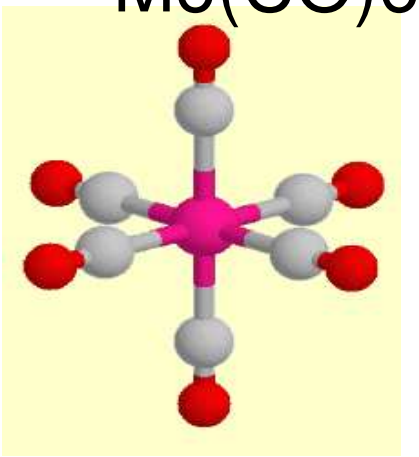
- **A center of symmetry: A point at the center of the molecule.**

  (x,y,z) --> (-x,-y,-z)

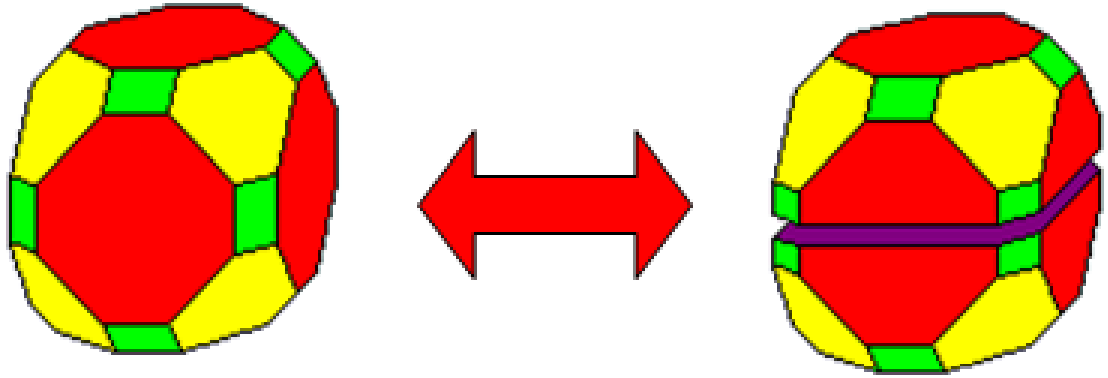
- **Center of inversion can only be in a molecule. It is not necessary to have an atom in the center (benzene, ethane). Tetrahedral, triangles, pentagons don't have a center of inversion symmetry. All Bravais lattices are inversion symmetric.**



Mo(CO)6

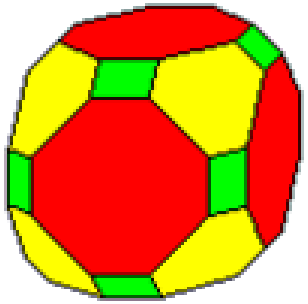


Reflection Plane

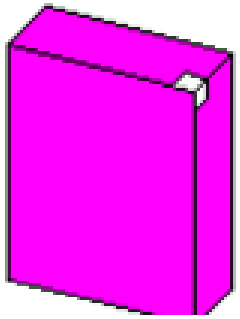


- A plane in a cell such that, when a mirror reflection in this plane is performed, the cell remains invariant.

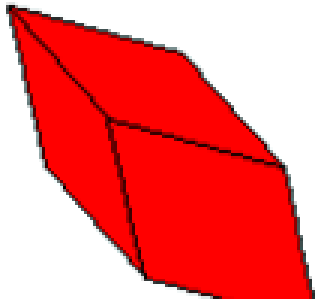
Examples



Monoclinic



Triclinic



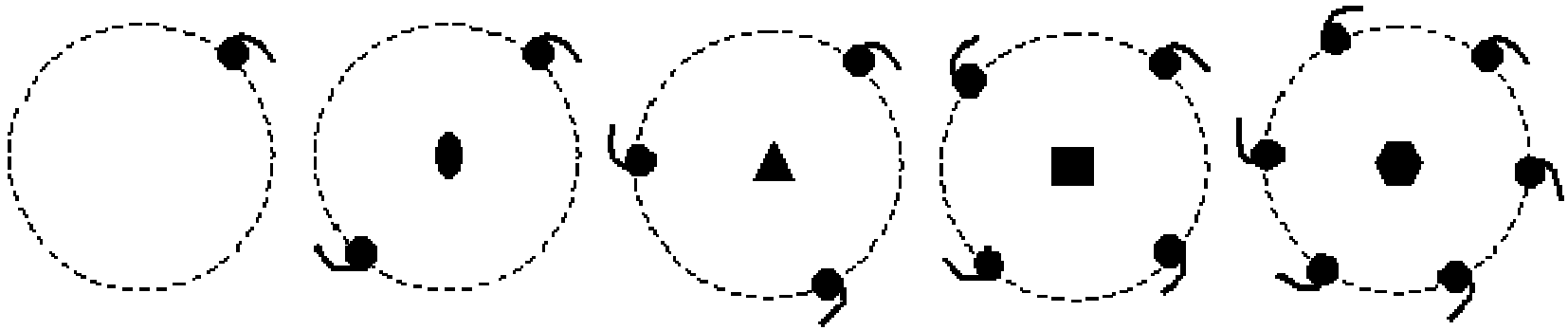
- Triclinic has no reflection plane.
- Monoclinic has one plane midway between and parallel to the bases, and so forth.

Rotation Symmetry

We can not find a lattice that goes into itself under other rotations

- A single molecule can have any degree of rotational symmetry, but an infinite periodic lattice – can not.

Axis of Rotation



Fold (n)	1	2	3	4	6
Angles	360	180	120	90	60

Axis of Rotation

1-fold	2-fold	3-fold	4-fold	6-fold
Objects with symmetry:				
a	Z	▼	✚	❄
identity