Symmetry elements in 3D

- All four symmetry elements in 2D
  - Rotation
  - Reflection
  - Translation
  - Glide reflection

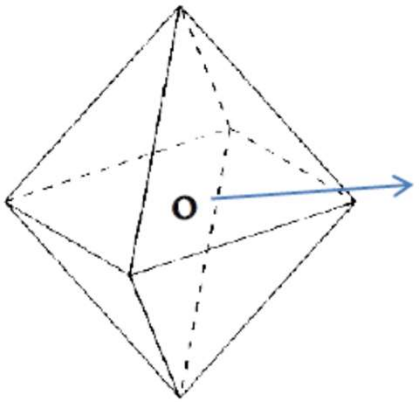
- In addition to these there are
  - Inversion centers
  - Rotation and Inversion = Rotoinversion
  - Screw
  - Glide in 3D

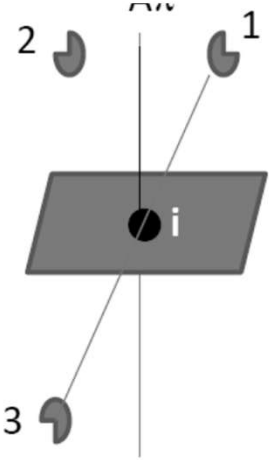
Additional Symmetry elements in 3D

- Mirror lines in 2D become mirror planes in 3D
- Inversion center or Symmetry center
- Combination of rotation and inversion
- Rotoinversion axis is improper rotation axis
- Rotoinversion axis = Inversion axis
- Screw axes
- Glide in 3D

Inversion center

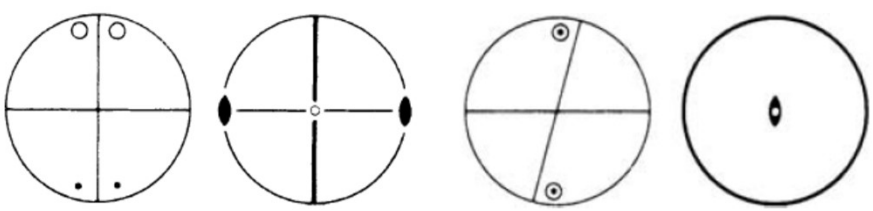
- r to $\bar{r}$ that is $\vec{r}$ goes to -$\vec{r}$
- (x, y, z) to (-x, -y, -z)
- In 2D if mirrors intersect; (x, y) to (-x, -y)
- This is by a 2 fold rotation
- In 3D one needs a 2 fold intersecting with a mirror
- In 3D, (x, y, z) to (-x, -y, z) by 2 fold
- A mirror perpendicular to z axis will take (-x, -y, z) to (-x, -y, -z)



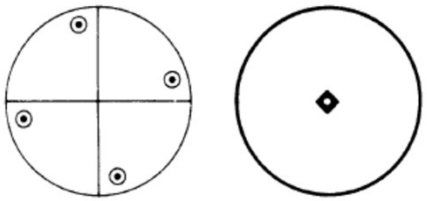


More on mirrors

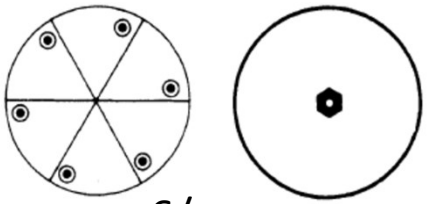
- Mirror perpendicular to rotation axis is 2/m
- 4/m and 6/m exist
- m out of plane possible, simply m
- 3/m is not there



2/m



4/m



6/m

Note the rotation symmetry symbols and inversion symbol

Inversion center

- Most inorganic crystals have center of inversion
- Centre of inversion is chosen as origin
- Balancing of forces about the center
- Point groups with center of symmetry are called Laue groups

Inversion axis or rotoinversion

- Rotation + center of inversion = Inversion axis
- $\bar{1}, \bar{2}, \bar{3}, \bar{4}, \bar{6}$
- $\bar{2}$ is equivalent to m
- $\bar{6}$ is equivalent to 3/m

$\bar{1} \rightarrow$ o

$\bar{2} \rightarrow m$

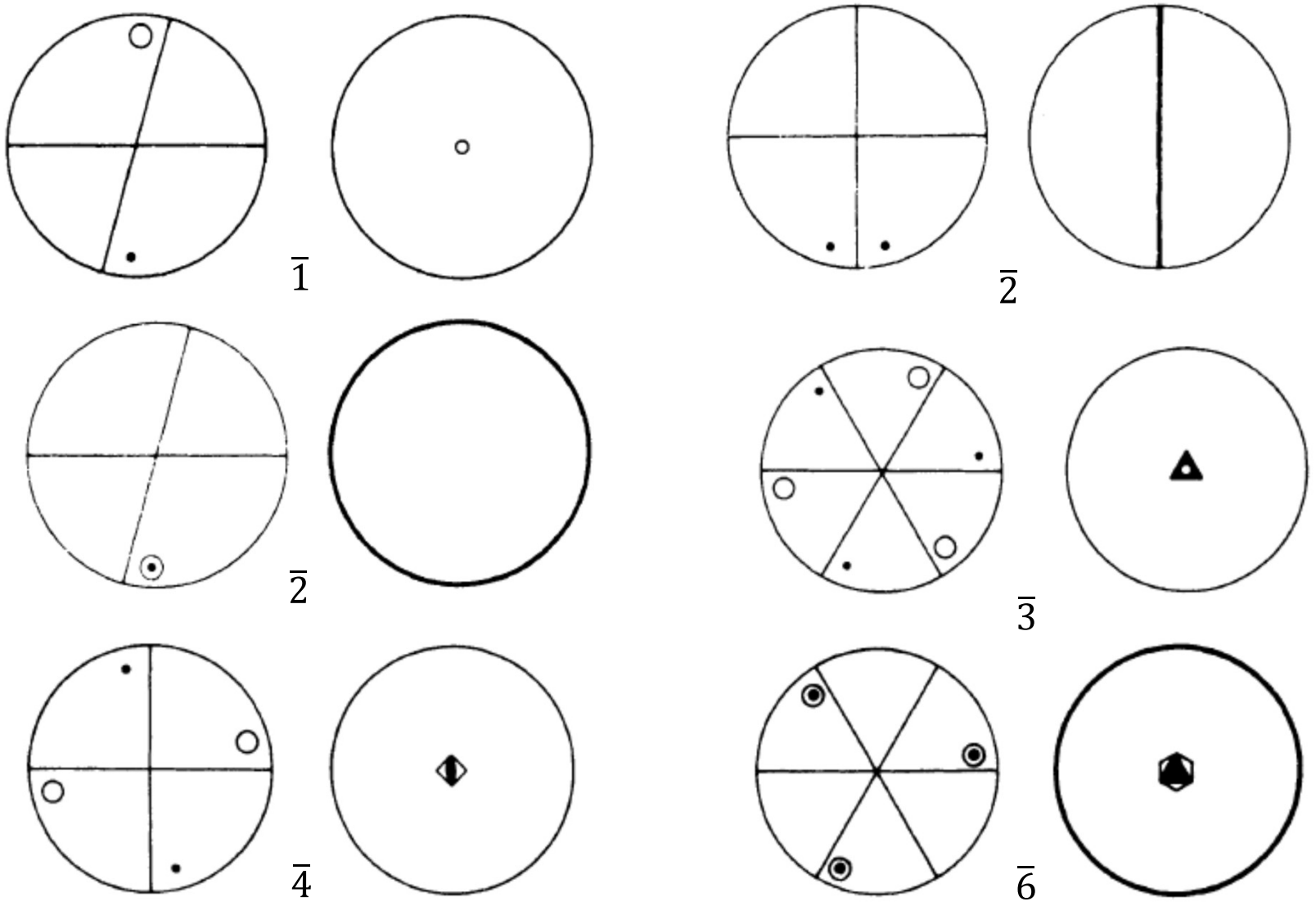
$\bar{3} \rightarrow$ 

$\bar{4} \rightarrow$

$\bar{6} \rightarrow$ 

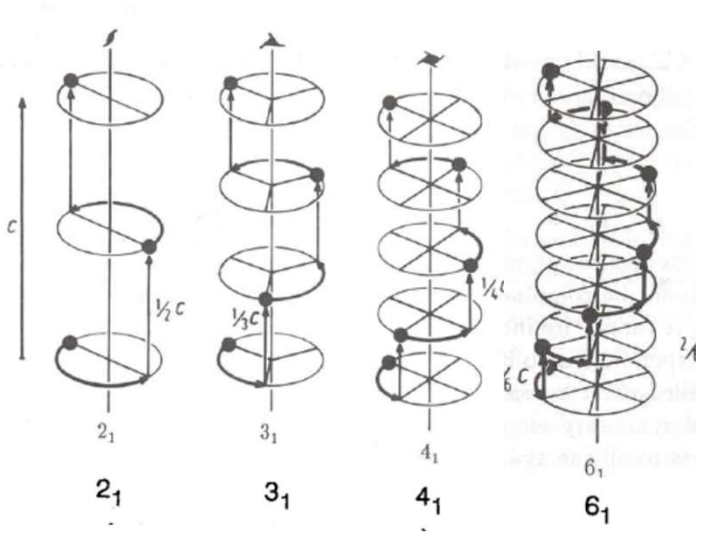
- Improper rotation axes
- Two objects related by axis of inversion are enantimorphs
- Enantiomorphs have different handedness

Rotoinversion axes stereographic projection

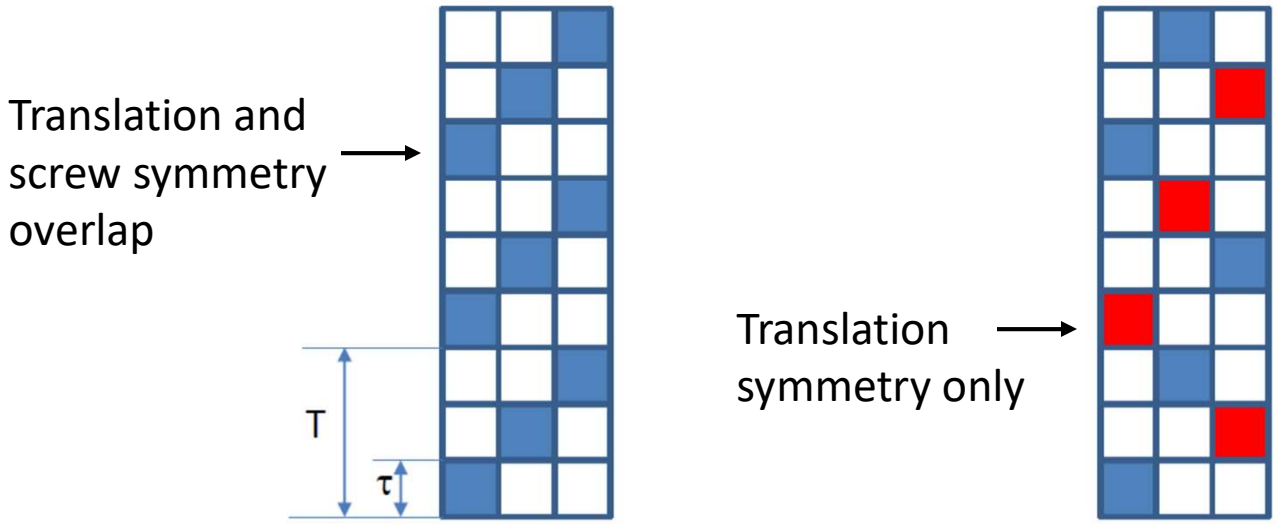


Screw axes

- Rotation + translation in axial direction
- n_m screw axis
- n fold rotation m/n translation
- m < n

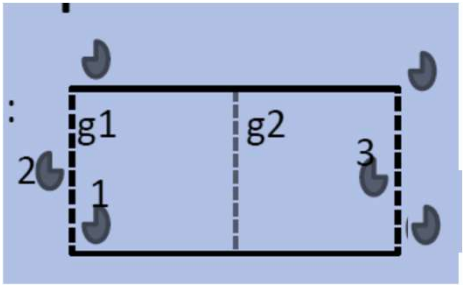


- Screw axes 3_1 and 3_2
- Rotation by 120 degree and translation by 1/3 and 2/3 along the axis
- Left one is 3_1 and right one is 3_2



Glide reflection

- Glide reflection in 3D
- Glide is on a plane so different ways of representing it
- a glide or b glide or c glide: a/2. b/2, c/2
- n glide is (a + b)/2 or (a-b)/2 Diagonal glide
- Diamond glide is (a + b)/4 or (a + b + c)/4 denoted by d in centered lattice



3D point groups

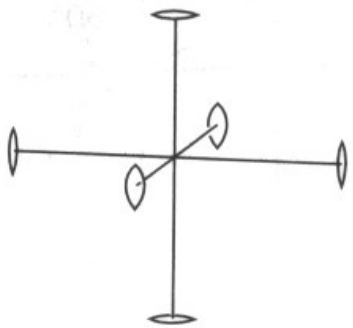
- Combination of symmetry elements in 3D
- Rotation, reflection, inversion and rotoinversion
- Easiest is combination of rotation

  1, 2, 3, 4, 6

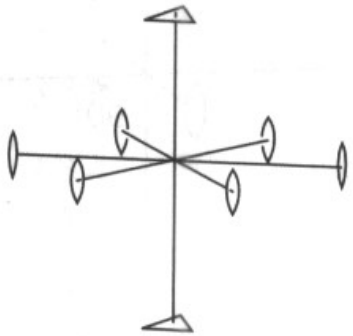
  222, 322, 422, 622

  23, 432

  32 and 321 and 312



222



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- Rotoinversion

  $\bar{1}, \bar{2}, \bar{3}, \bar{4}, \bar{6}$

- With mirror in plane of rotation axis
  - mm2, 4mm, 6mm
  - 3m, 3m1, 31m
  - m3m

- With mirror perpendicular to rotation axis
  - 2/m, 4/m, 6/m

- With combination of mirrors and rotation axis

  mmm or 2/m 2/m 2/m

  4/m 2/m 2/m or 4/mmm

  6/m 2/m 2/m or 6/mmm

- With combination of mirrors and rotoinversion axis

  $\bar{4}$2m, $\bar{4}$3m, m$\bar{3}$m, $\bar{6}$2m

  $\bar{3}$m1 or $\bar{3}$2/m1 and $\bar{3}$1m or $\bar{3}$12/m

- With rotoinversion and perpendicular mirror

  4/m $\bar{3}$ 2/m

Crystal System	32 Crystallographic Point Groups						
Triclinic	**1**	-1					
Monoclinic	**2**	***m***	2/*m*				
Orthorhombic	222	***mm2***	*mmm*				
Tetragonal	**4**	-4	4/*m*	422	***4mm***	-42*m*	4/*mmm*
Trigonal	**3**	-3	32	***3m***	-3*m*		
Hexagonal	**6**	-6	6/*m*	622	***6mm***	-62*m*	6/*mmm*
Cubic	23	*m-3*	432	-43*m*	*m*-3*m*		

Please refer to the attachment for more details in terms of classification of the Point groups.

http://pd.chem.ucl.ac.uk/pdnn/symm2/group32.htm

Crystal System	Laue Group	Point Group
Triclinic	-1	1, -1
Monoclinic	2/m	2, m, 2/m
Orthorhombic	mmm	222, mm2, mmm
Tetragonal	4/m	4, -4, 4/m
	4/mmm	422, 4mm, -42m, 4/mmm
Trigonal/ Rhombohedral	-3	3, -3
	-3/m	32, 3m, -3m
Hexagonal	6/m	6, -6, 6/m
	6/mmm	622, 6mm, -6m2, 6/mmm
Cubic	m3	23, m3
	m3m	432, -43m, m3m

- Point groups with center of inversion are called Laue groups
- Non centrosymmetric point groups are piezoelectric

- 32 Point groups in 3D while 10 point groups in 2D
- 7 Crystal systems and 14 Bravais lattice in 3D and
  2 crystals and 5 lattices in 2D
- 230 space groups while 17 plane groups in 2D
- 2D plane groups from glide
- 3D planes groups from glide, screw axes, inversion axes and inversion center

- Representing space group
  - P, I, F, A, B, C
  - I also called R
  - Highest symmetry first
  - mirror over 2 fold: Cmm2
  - Mirror perpendicular to rotation axis use”/”
  - P2/mmm
  - n, (a, b, c) for diagonal glide and (glide along, a, b, c)

- Triclinic

  no symmetry or inversion symmetry P1 or P-1

- Monoclinic

  P2, P2/m, C2/m

- Orthorhombic

  Pmm2, Pnma, Pnc2

- Tetragonal

  P4/mmm, $I4_1cd$

- Cubic

  Fm-3m, P23, F432

Crystal System	Symmetry Direction		
	Primary	**Secondary**	**Tertiary**
Triclinic	None		
Monoclinic	[010]≡ b		
Orthorhombic	[100]≡ a	[010] ≡ b	[001]≡ c
Tetragonal	[001] ≡ c	[100]/[010] ≡ a/b	[110]
Hexagonal/Trigonal	[001] ≡ c	[100]/[010]≡ a/b	[120]
Cubic	[100]/[010]/[001] ≡ a/b/c	[111]	[110]

- Common metals
  - Iron Im-3m, Nickel Fm-3m, Polonium Pm-3m
  - Magnesium and titanium $P6_3/mmc$

- Ceramic BaTiO3
  - Cubic Pm-3m
  - Tetragonal P4mm
  - Orthorhombic Amm2
  - Rhombohedral R3m

- Table salt NaCl is also Fm-3m

- Diamond Fd-3m

- High density polyethylene Pnam

We will revisit this
when we will study bonding