International School on Fundamental Crystallography

and

Workshop on Structural Phase Transitions

30th August – 4th September 2017, Rourkela

Bernd Souvignier

Radboud University Nijmegen, The Netherlands

Crystallographic point groups (II).

Overview

- group actions
- conjugation, normalizers
- Wyckoff positions
- overview of crystallographic point groups

From symmetry operations to abstract groups and back

- Symmetry operations of an (idealized) crystal structure leave the whole structure invariant, but map substructures to others, e.g. atoms, bonds, coordination polyhedra etc.
- For abstract groups, the concept of group actions reinstalls the fact, that the group elements can be applied to certain objects.

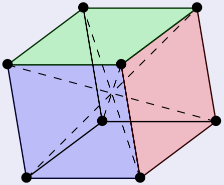
Definition

A group $\mathcal{G}$ is said to act on a set Ω if an object $\omega \in \Omega$ is moved to another object $g(\omega) \in \Omega$ by $g \in \mathcal{G}$ such that:

(i) $h(g(\omega)) = (hg)(\omega)$, i.e. applying two group elements consecutively is the same as applying their product;

(ii) $e(\omega) = \omega$, i.e. applying the identity element of $\mathcal{G}$ has no effect.

Example: Symmetry group $\mathcal{G}$ of a cube



- $\mathcal{G}$ acts on the 8 corners of the cube, but also on its 12 edges, its 6 faces and its 4 space diagonals.
- Since the cube is imbedded in 3D-space $\mathbb{R}^3$, $\mathcal{G}$ acts on the points in $\mathbb{R}^3$, but also on the 1D-lines and 2D-planes in $\mathbb{R}^3$.
- The action on lines and planes can be restricted to the subsets of lines and planes containing the center of the cube.

Two concepts and a theorem

Definition

- The set
$$\mathcal{G}(\omega) = \{g(\omega) \mid g \in \mathcal{G}\}$$
of objects to which ω is moved by the elements of $\mathcal{G}$ is called the orbit of ω under $\mathcal{G}$.
- The set
$$S_{\mathcal{G}}(\omega) = \{g \in \mathcal{G} \mid g(\omega) = \omega\}$$
of group elements that do not move ω is a subgroup of $\mathcal{G}$, called the stabilizer of ω in $\mathcal{G}$.

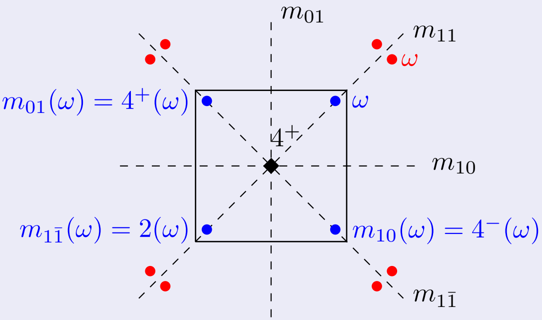
Orbit-stabilizer theorem

- The length $|\mathcal{G}(\omega)|$ of the orbit $\mathcal{G}(\omega)$ is equal to the index $[\mathcal{G} : S_{\mathcal{G}}(\omega)]$ of the stabilizer in $\mathcal{G}$, i.e. to the number of cosets of $\mathcal{G}$ relative to $S_{\mathcal{G}}(\omega)$.
- In particular, the length of the orbit divides the group order $|\mathcal{G}|$.
- More precisely, if

$$\mathcal{G} = g_1 S_{\mathcal{G}}(\omega) \cup g_2 S_{\mathcal{G}}(\omega) \cup \ldots \cup g_m S_{\mathcal{G}}(\omega)$$

  is the coset decomposition of $\mathcal{G}$ relative to $S_{\mathcal{G}}(\omega)$, then
  - $g_1(\omega), g_2(\omega), \ldots, g_m(\omega)$ is the full orbit $\mathcal{G}(\omega)$ and
  - the coset $g_i S_{\mathcal{G}}(\omega)$ collects together precisely those elements of $\mathcal{G}$ that move ω to $g_i(\omega)$.

Example: Orbits of $4mm$



- point $\omega =$ •: trivial stabilizer $\{1\} \to$ point in general position
- point $\omega =$ •: stabilizer $\{1, m_{11}\} \to$ point in special position

Not-so-quick quiz

Every point in an orbit gives rise to the same orbit $\mathcal{G}(g(\omega)) = \mathcal{G}(\omega)$, but what is the relation between the stabilizers $S_{\mathcal{G}}(\omega)$ and $S_{\mathcal{G}}(g(\omega))$?

Not-so-quick quiz

Every point in an orbit gives rise to the same orbit $\mathcal{G}(g(\omega)) = \mathcal{G}(\omega)$, but what is the relation between the stabilizers $S_{\mathcal{G}}(\omega)$ and $S_{\mathcal{G}}(g(\omega))$?

Answer

- If $h \in S_{\mathcal{G}}(\omega)$ and $\omega' = g(\omega)$, then

$$ghg^{-1}(\omega') = ghg^{-1}g(\omega) = gh(\omega) = g(\omega) = \omega'$$

  i.e. ghg^{-1} lies in the stabilizer of $g(\omega)$.
- Reversing the roles of ω and ω' shows that

$$gS_{\mathcal{G}}(\omega)g^{-1} = \{ghg^{-1} \mid h \in S_{\mathcal{G}}(\omega)\}$$

  is the full stabilizer of $\omega' = g(\omega)$.

Conjugate elements

- Two elements h and ghg^{-1} are said to be conjugate by g.
- Conjugation is a group action $g(h) = ghg^{-1}$ of $\mathcal{G}$ on its elements.
- Conjugate elements lie in the same orbit, the orbits are called conjugacy classes of elements
- The stabilizer of an element is called its centralizer

$$\mathcal{C}_{\mathcal{G}}(h) = \{g \in \mathcal{G} \mid ghg^{-1} = h\} = \{g \in \mathcal{G} \mid gh = hg\}$$

and consists of the elements of $\mathcal{G}$ commuting with h.

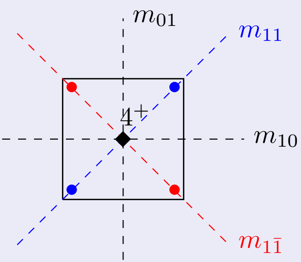
Conjugate subgroups

- Two subgroups $\mathcal{H}$ and $g\mathcal{H}g^{-1} = \{ghg^{-1} \mid h \in \mathcal{H}\}$ are said to be conjugate subgroups by g.
- Conjugation is a group action $g(\mathcal{H}) = g\mathcal{H}g^{-1}$ of $\mathcal{G}$ on its subgroups.
- Conjugate subgroups lie in the same orbit, the orbits are called conjugacy classes of subgroups
- The stabilizer of a subgroup is called its normalizer

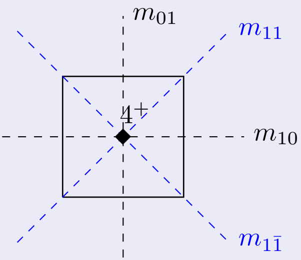
$$\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \{g \in \mathcal{G} \mid g\mathcal{H}g^{-1} = \mathcal{H}\} = \{g \in \mathcal{G} \mid g\mathcal{H} = \mathcal{H}g\}$$

  and consists of the elements of $\mathcal{G}$ that conjugate all the elements of $\mathcal{H}$ into $\mathcal{H}$.

Example: Normalizers in $\mathcal{G} = 4mm$



- 2-fold rotation 2 interchanges the $\bullet$ points, and thus conjugates their stabilizers
- both points have the same stabilizer $\mathcal{H} = \{1, m_{11}\}$, hence 2 lies in the normalizer of $\mathcal{H}$
- 4^+ moves the $\bullet$ points to the $\bullet$ points with stabilizer $\mathcal{H}' = \{1, m_{1\bar{1}}\} \neq \mathcal{H}$
- $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \langle m_{11}, 2\rangle = \{1, 2, m_{11}, m_{1\bar{1}}\}$



- $\mathcal{H} = \{1, 2, m_{11}, m_{1\bar{1}}\}$,
- 4^+ interchanges the reflection lines but fixes the pair of reflection lines
- $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{G}$
- The normalizer describes the symmetry of the symmetries.

Normal subgroups

Definition

A subgroup $\mathcal{H}$ of $\mathcal{G}$ is called a normal subgroup if $g\mathcal{H}g^{-1} = \mathcal{H}$ for all $g \in \mathcal{G}$, i.e. if $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{G}$. Notation: $\mathcal{H} \trianglelefteq \mathcal{G}$.

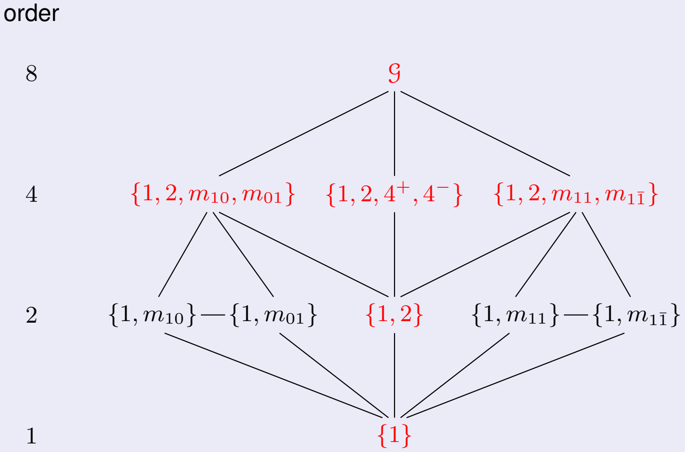
Properties of normal subgroups

- Each left coset $g\mathcal{H}$ coincides with the right coset $\mathcal{H}g$ with the same representative.
- A subgroup of index 2 is always a normal subgroup.
- In an abelian group, every subgroup is a normal subgroup.
- The cosets relative to $\mathcal{H}$ form a group with the product

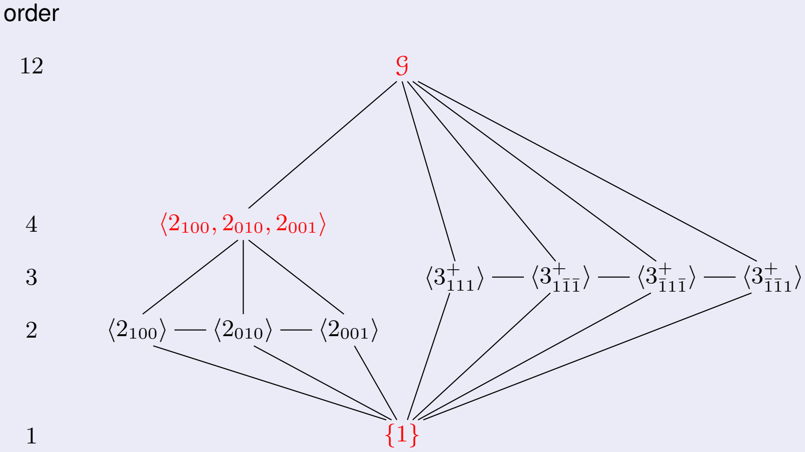
$$(g\mathcal{H}) \circ (g'\mathcal{H}) = (gg')\mathcal{H}$$

  (representative of the product is the product of the representatives), called the factor group of $\mathcal{G}$ by $\mathcal{H}$ and denoted by $\mathcal{G}/\mathcal{H}$.

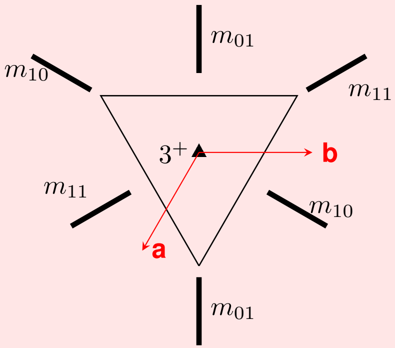
Normal subgroups in $\mathcal{G} = 4mm$



Normal subgroups of the tetrahedral group $\mathcal{G} = 23$



Exercise

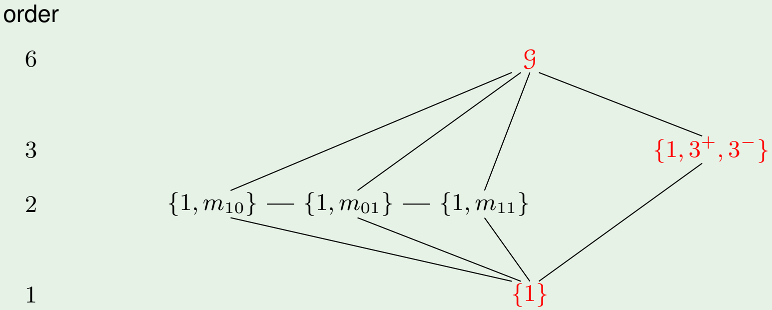


Determine

- the subgroup diagram,
- conjugation relations between subgroups,
- the normal subgroups

of the symmetry group $\mathcal{G} = 3m$ of an equilateral triangle.

Answer



Construction of 2D point groups

Crystallographic restriction

- crystallographic symmetry operation: acting on the translation lattice of a periodic crystal pattern
- n-fold rotation by angle $\theta = \frac{360^\circ}{n}$ has matrix $\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$ with respect to orthonormal basis
- matrix with respect to lattice basis is integral
  $\Rightarrow$ trace $2\cos\theta$ is an integer (trace is invariant under basis transformation)
- the only possibilities for $\cos\theta$ are $0, \pm\frac{1}{2}, \pm 1$

$\cos\theta$	θ	$n = 360^\circ/\theta$
1	$360^\circ = 0^\circ$	1
$\frac{1}{2}$	60°	6
0	90°	4
$-\frac{1}{2}$	120°	3
-1	180°	2

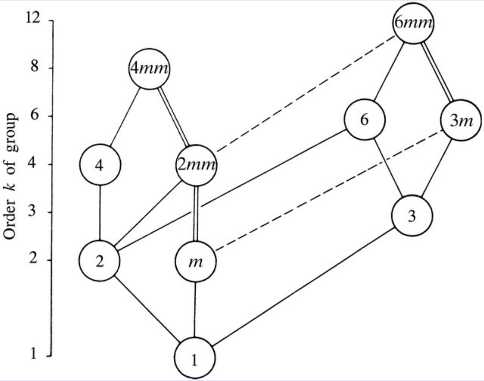
Overview of 2D point groups

- rotation groups of order $1, 2, 3, 4, 6$
- adding a reflection to an n-fold rotation gives dihedral group of order $2n$

object	rotation group	symmetry group
trapezium	1	m
rectangle	2	$2mm$
triangle	3	$3m$
square	4	$4mm$
hexagon	6	$6mm$

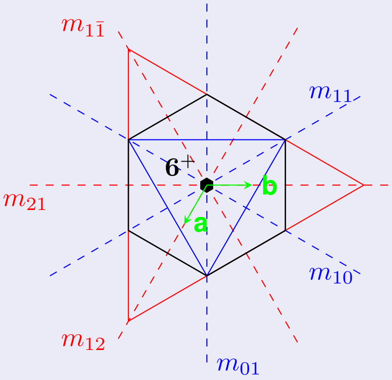
Overview of 2D point groups

Combined and contracted subgroup diagram



- solid line: normal subgroup;
- double/triple solid line: two/three (non-conjugate) normal subgroups of this type;
- dashed line: non-normal subgroups (number $=$ index).

Maximal subgroups of $\mathcal{G} = 6mm$



- type 6: $\{1, 2, 3^+, 3^-, 6^+, 6^-\}$
- type $3m$: $\{1, 3^+, 3^-, m_{10}, m_{01}, m_{11}\}$
- type $3m$: $\{1, 3^+, 3^-, m_{21}, m_{12}, m_{1\bar{1}}\}$

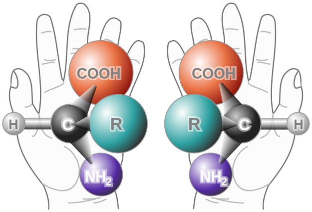
Symmetry operations in 3D

Rotations: $\det = +1$

- n-fold rotation: $n^+_{001} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$

  $\Rightarrow$ same crystallographic restriction as in 2D: $n = 2, 3, 4, 6$

Improper rotations: $\det = -1$ (reversing chirality)

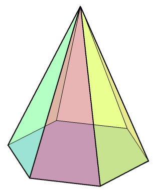
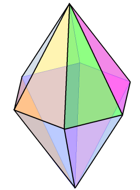
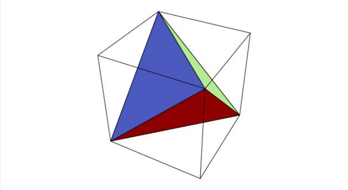


- reflection: $m_{001} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
- inversion: $\bar{1} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
- n-fold rotoinversion (n-fold rotation composed with inversion):

  $\bar{n}^+_{001} = \begin{pmatrix} -\cos\theta & \sin\theta & 0 \\ -\sin\theta & -\cos\theta & 0 \\ 0 & 0 & -1 \end{pmatrix}$ (note that $\bar{2} = m$)

Construction of 3D point groups

Proper rotation groups

- cyclic groups $1, 2, 3, 4, 6$: rotation groups of pyramids
- dihedral groups $222, 32, 422, 622$: rotation groups of double pyramids
- cubic groups $23, 432$: rotation groups of tetrahedron and cube

Group $\mathcal{G}$ containing improper rotations

- proper rotations form rotational subgroup $\mathcal{H}$ of index 2 in $\mathcal{G}$
- two cases: $\mathcal{G}$ contains inversion $\bar{1}$ or not:
  - $\bar{1} \in \mathcal{G}$: coset decomposition $\mathcal{G} = \mathcal{H} \cup \bar{1}\mathcal{H} \Rightarrow \mathcal{G} = \mathcal{H} \times \langle \bar{1} \rangle$
  - $\bar{1} \notin \mathcal{G}$: coset decomposition $\mathcal{G} = \mathcal{H} \cup g\mathcal{H}$ for an improper rotation g $-g = \bar{1} \cdot g$ is a proper rotation and $\tilde{\mathcal{G}} = \mathcal{H} \cup (-g)\mathcal{H}$ is a rotational group containing $\mathcal{H}$ as a subgroup of index 2
- two construction methods from a rotational group $\mathcal{H}$:
  - rotational group $\mathcal{H}$ yields $\mathcal{G} = \mathcal{H} \times \langle \bar{1} \rangle$
  - rotational group $\mathcal{H}$ with subgroup $\mathcal{H}'$ of index 2 and coset decomposition $\mathcal{H} = \mathcal{H}' \cup g\mathcal{H}'$ yields $\mathcal{G} = \mathcal{H}(\mathcal{H}') = \mathcal{H}' \cup (-g)\mathcal{H}'$
  - note that $\mathcal{H}(\mathcal{H}')$ is a subgroup of index 2 in $\mathcal{H} \times \langle \bar{1} \rangle$

Example: $\mathcal{H} = 4 = \{1, 2_{001}, 4^+_{001}, 4^-_{001}\}$

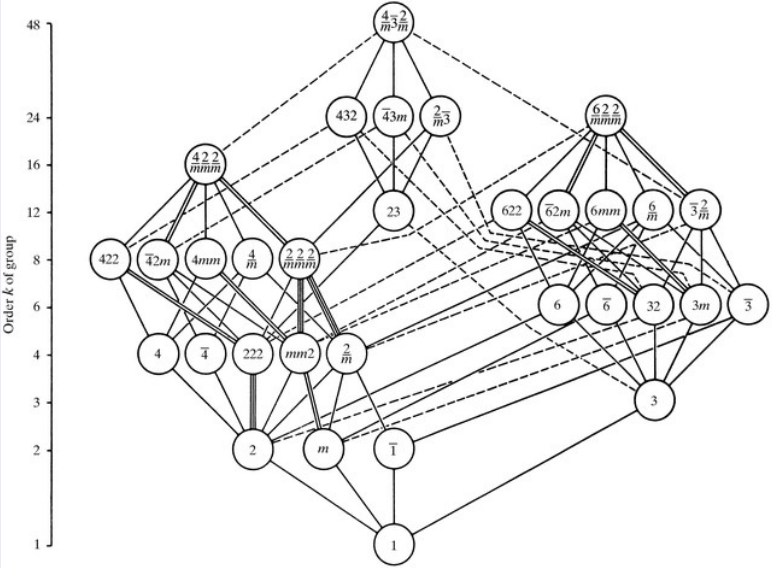
- $\mathcal{H} \times \langle \bar{1} \rangle = 4/m = \{1, 2_{001}, 4^+_{001}, 4^-_{001}, \bar{1}, m_{001}, \bar{4}^+_{001}, \bar{4}^-_{001}\}$
- $\mathcal{H}' = 2$: $4(2) = \bar{4} = \{1, 2_{001}, \bar{4}^+_{001}, \bar{4}^+_{001}\}$

Overview of 3D crystallographic point groups

	$\mathcal{H}$	$\mathcal{H} \times \langle \bar{1} \rangle$	$\mathcal{H}'$	$\mathcal{H}(\mathcal{H}')$
cyclic	1	$\bar{1}$		
	2	$2/m$	1	m
	3	$\bar{3}$		
	4	$4/m$	2	$\bar{4}$
	6	$6/m$	3	$\bar{6}$
dihedral	222	mmm	2	$mm2$
	32	$\bar{3}m$	3	$3m$
	422	$4/mmm$	4	$4mm$
			222	$\bar{4}2m$
	622	$6/mmm$	6	$6mm$
			32	$\bar{6}2m$
cubic	23	$m\bar{3}$		
	432	$m\bar{3}m$	23	$\bar{4}3m$

Subgroup relations of 3D point groups

Combined and contracted subgroup diagram



Wyckoff positions

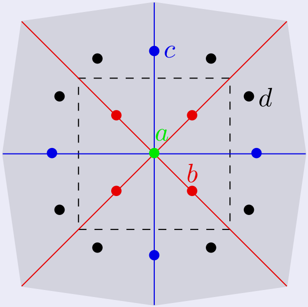
Specific terminology for (2D or 3D) point groups

- For a point group $\mathcal{G}$ acting on $\mathbb{R}^2$ or $\mathbb{R}^3$, the stabilizer of a point $X = (x, y)$ or $X = (x, y, z)$ is called the site-symmetry group of X, denoted by $\mathcal{S}_X$.
- The length of the orbit of X under $\mathcal{G}$ is called the multiplicity of X.
- By the orbit-stabilizer theorem, the multiplicity of X is $|\mathcal{G}|/|\mathcal{S}_X|$.
- A point X with $|\mathcal{S}_X| = \{1\}$ is called a point in general position, a point with $|\mathcal{S}_X| > \{1\}$ is called a point in special position.

Definition

- Two points X and Y belong to the same Wyckoff position of $\mathcal{G}$ if their site-symmetry groups $\mathcal{S}_X$ and $\mathcal{S}_Y$ are conjugate subgroups of $\mathcal{G}$.
- In particular, points in the same orbit under $\mathcal{G}$ belong to the same Wyckoff position.

Example: $\mathcal{G} = 4mm$ (in 2D)

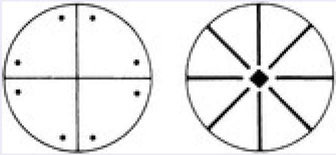


multiplicity,
letter,
site-symmetry

8	d	1	(x, y)	$(-x, -y)$	$(-y, x)$	$(y, -x)$
			$(x, -y)$	$(-x, y)$	$(-y, -x)$	(y, x)
4	c	$.m.$	$(x, 0)$	$(-x, 0)$	$(0, x)$	$(0, -x)$
4	b	$..m$	(x, x)	$(-x, -x)$	$(-x, x)$	$(x, -x)$
1	a	$4mm$	$(0, 0)$			

Example: $\mathcal{G} = 4mm$ (in 3D)

- stereographic projection

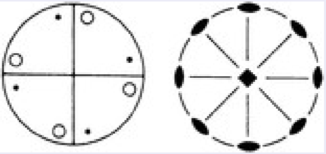


- $\mathcal{G} = \langle 4^{+}_{001}, m_{100} \rangle$
- all $g \in \mathcal{G}$ leave z-coordinate fixed
  $\Rightarrow$ same Wyckoff positions as for 2D-group $4mm$ (with general z-coordinate added)

8	d	1	(x, y, z)	$(-x, -y, z)$	$(-y, x, z)$	$(y, -x, z)$
			$(x, -y, z)$	$(-x, y, z)$	$(-y, -x, z)$	(y, x, z)
4	c	$.m.$	$(x, 0, z)$	$(-x, 0, z)$	$(0, x, z)$	$(0, -x, z)$
4	b	$..m$	(x, x, z)	$(-x, -x, z)$	$(-x, x, z)$	$(x, -x, z)$
1	a	$4mm$	$(0, 0, z)$			

Example: $\mathcal{G} = 422$ (in 3D)

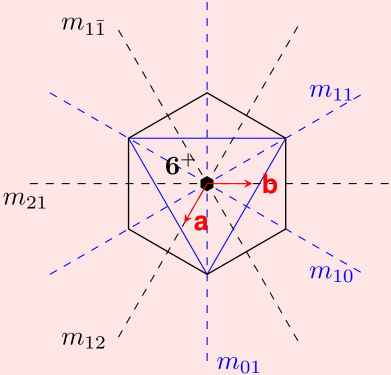
- stereographic projection



- $\mathcal{G} = \langle 4^+_{001}, 2_{100} \rangle$
- 2-fold rotations (corresponding to reflections in 2D $4mm$) map z-coordinate to $-z$

8	e	1	(x, y, z)	$(-x, -y, z)$	$(-y, x, z)$	$(y, -x, z)$
			$(-x, y, -z)$	$(x, -y, -z)$	$(y, x, -z)$	$(-y, -x, -z)$
4	d	.2.	$(x, 0, 0)$	$(-x, 0, 0)$	$(0, x, 0)$	$(0, -x, 0)$
4	c	..2	$(x, x, 0)$	$(-x, -x, 0)$	$(-x, x, 0)$	$(x, -x, 0)$
2	b	4..	$(0, 0, z)$	$(0, 0, -z)$		
1	a	422	$(0, 0, 0)$			

Exercise



Determine the Wyckoff positions of the groups:

- $3m = \left\langle 3^+ = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix},\ m_{10} = \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix} \right\rangle$ (triangle);
- $6mm = \left\langle 6^+ = \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix},\ m_{10} = \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix} \right\rangle$ (hexagon).

Answer $3m$

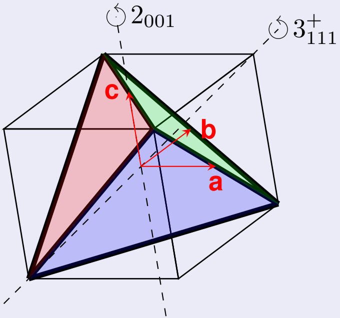
multiplicity,
letter,
site-symmetry

6	c	1	(x,y)	$(-y,x-y)$	$(-x+y,-x)$
			$(-x+y,y)$	$(-y,-x)$	$(x,x-y)$
3	b	$.m.$	$(x,2x)$	$(-2x,-x)$	$(x,-x)$
1	a	$3m$	$(0,0)$		

Answer $6mm$

12	d	1	(x,y)	$(-y,x-y)$	$(-x+y,-x)$
			$(-x,-y)$	$(y,-x+y)$	$(x-y,x)$
			$(-x+y,y)$	$(-y,-x)$	$(x,x-y)$
			$(x-y,-y)$	(y,x)	$(-x,-x+y)$
6	c	$.m.$	$(x,2x)$	$(-2x,-x)$	$(x,-x)$
			$(-x,-2x)$	$(2x,x)$	$(-x,x)$
6	b	$..m$	$(x,0)$	$(0,x)$	$(-x,-x)$
			$(-x,0)$	$(0,-x)$	(x,x)
1	a	$6mm$	$(0,0)$		

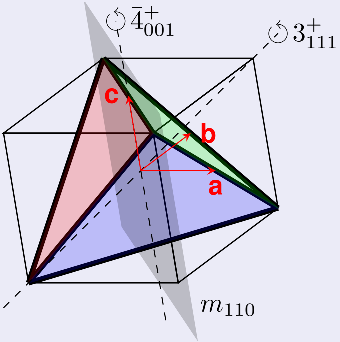
Example: Rotation group 23 of a tetrahedron



- points in special position are points on the rotation axes

12	d	1	(x,y,z)	$(-x,-y,z)$	$(-x,y,-z)$	$(x,-y,-z)$
			(z,x,y)	$(z,-x,-y)$	$(-z,-x,y)$	$(-z,x,-y)$
			(y,z,x)	$(-y,z,-x)$	$(y,-z,-x)$	$(-y,-z,x)$
6	c	2..	$(x,0,0)$	$(-x,0,0)$	$(0,x,0)$	$(0,-x,0)$
			$(0,0,x)$	$(0,0,-x)$		
4	b	.3.	(x,x,x)	$(-x,-x,x)$	$(-x,x,-x)$	$(x,-x,-x)$
1	a	23.	$(0,0,0)$			

Example: Full symmetry group $\bar{4}3m$ of a tetrahedron



- group of order 24
- 2-fold rotation axes become 4-fold rotoinversion axes $\Rightarrow$ 6 additional elements: $\bar{4}^{\pm}_{100}$, $\bar{4}^{\pm}_{010}$, $\bar{4}^{\pm}_{001}$
- 6 additional reflections in planes containing face diagonals: m_{110}, $m_{1\bar{1}0}$, m_{101}, $m_{10\bar{1}}$, m_{011}, $m_{01\bar{1}}$

24	e	1	$(x, y, z)\ldots$	general position
12	d	$..m$	$(x, x, z)\ldots$	on one mirror plane
6	c	$2.mm$	$(x, 0, 0)\ldots$	on 2-fold axis and two mirror planes
4	b	$.3m$	$(x, x, x)\ldots$	on 3-fold axis and three mirror planes
1	a	$\bar{4}3m$	$(0, 0, 0)$	origin

Splitting of Wyckoff positions for group-subgroup pairs

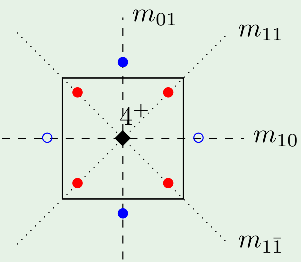
Group-subgroup pair $\mathcal{G} > \mathcal{H}$ with index $[i]$

- Let X be a point with site-symmetry group $\mathcal{S}_X$ and multiplicity m_X under the action of $\mathcal{G}$.
- Orbit-stabilizer theorem: $|\mathcal{G}| = m_X \cdot |\mathcal{S}_X|$.
- Transition to subgroup $\mathcal{H}$: site-symmetry group $\mathcal{S}'_X$ and multiplicity m'_X under the action of $\mathcal{H}$, $|\mathcal{H}| = m'_X \cdot |\mathcal{S}'_X|$.
- Divide equations: $[i] = \frac{|\mathcal{G}|}{|\mathcal{H}|} = \frac{m_X}{m'_X} \cdot \frac{|\mathcal{S}_X|}{|\mathcal{S}'_X|}$ implies that multiplicity or site-symmetry or both must be reduced.
- If the multiplicity is reduced, the orbit $\mathcal{G}(X)$ of X under $\mathcal{G}$ splits into two or more orbits under $\mathcal{H}$ which can belong to the same or to different Wyckoff positions of $\mathcal{H}$.
- An orbit for the general position of $\mathcal{G}$ always splits into $[i]$ orbits for the general position of $\mathcal{H}$.

Special case of index $[i] = 2$

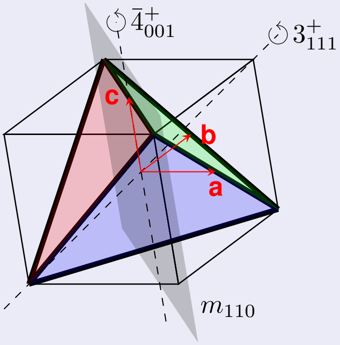
- $\dfrac{m_X}{m'_X} \cdot \dfrac{|\mathcal{S}_X|}{|\mathcal{S}'_X|} = 2$
- 2 cases:
  - multiplicity remains the same and site-symmetry is reduced by a factor of 2
  - site-symmetry remains the same and multiplicity is halved, in this case the orbit under $\mathcal{G}$ splits into two orbits of half the size under $\mathcal{H}$

Example: $\mathcal{G} = 4mm$, $\mathcal{H} = \{1, 2, m_{10}, m_{01}\} = 2mm$



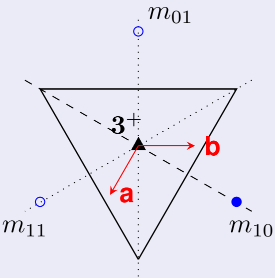
- point (x, x): multiplicity remains 4, site-symmetry is reduced from $\{1, m_{1\bar{1}}\}$ to 1 (general position for $\mathcal{H}$)
- point $(x, 0)$: site-symmetry remains $\{1, m_{01}\}$, orbit splits into two orbits $\{(x, 0), (-x, 0)\}$ and $\{(0, x), (0, -x)\}$ belonging to different Wyckoff positions of $\mathcal{H}$

Example: Splitting from $\bar{4}3m$ to 23



Wyckoff positions of $\bar{4}3m$				$\longrightarrow$	Wyckoff positions of 23			
24	e	1	$(x,y,z)\ldots$	$\longrightarrow$	12	d	1	$(x,y,z)\ldots$
				$\longrightarrow$	12	d	1	$(y,x,z)\ldots$
12	d	$..m$	$(x,x,z)\ldots$	$\longrightarrow$	12	d	1	$(x,x,z)\ldots$
6	c	$2.mm$	$(x,0,0)\ldots$	$\longrightarrow$	6	c	$2..$	$(x,0,0)\ldots$
4	b	$.3m$	$(x,x,x)\ldots$	$\longrightarrow$	4	b	$.3.$	$(x,x,x)\ldots$
1	a	$\bar{4}3m$	$(0,0,0)$	$\longrightarrow$	1	a	$23.$	$(0,0,0)$

Example with $[i] > 2$



- $\mathcal{G} = \{1, 3^+, 3^-, m_{10}, m_{01}, m_{11}\}$
- $\mathcal{H} = \{1, m_{10}\}$ has index 3 in $\mathcal{G}$
- point $(x, 2x)$ has orbit $(x, 2x)$, $(-2x, -x)$, $(x, -x)$ under $\mathcal{G}$

- site-symmetry remains the same $\Rightarrow$ multiplicity is reduced from 3 to 1
- orbit splits into two orbits under $\mathcal{H}$:
  - $(x, 2x)$: multiplicity 1, site-symmetry of order 2;
  - $(-2x, -x)$, $(x, -x)$: multiplicity 2, site-symmetry 1 (general position)
- Wyckoff position $3b$ of $\mathcal{G}$ splits into $1a + 2b$ of $\mathcal{H}$.