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Twin point groups

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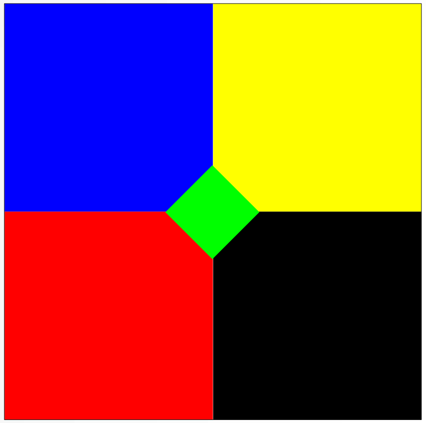
What is a twin point group?

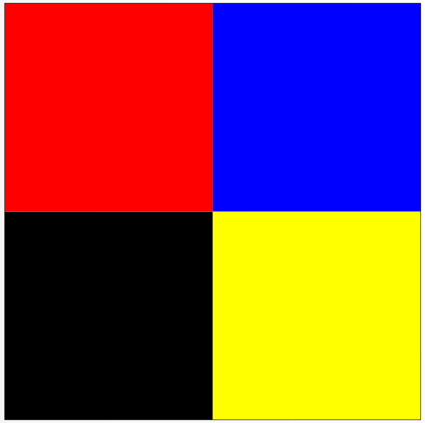
- A twin point group is a **chromatic crystallographic** point group.
- We assign to each individual of a twin a **color**.
- Symmetry operations of the **individual** are **achromatic**; operations mapping the orientation of an individual onto that of another individual are **chromatic**.
- Twin point groups are thus obtained as **extensions** of the **achromatic H* intersection group** by the **chromatic twin operation(s)**.

Symmetry operations in a chromatic group

- **Achromatic** operation: it does not exchange the colors.
- **Grey** operation: it exchange the colors without moving the object (no application in twinning)
- **Totally chromatic** operation: it exchanges a number of colors equal to the order of the operation without leaving fixed any color.
- **Partially chromatic** operation: it leaves fixed one or more colors

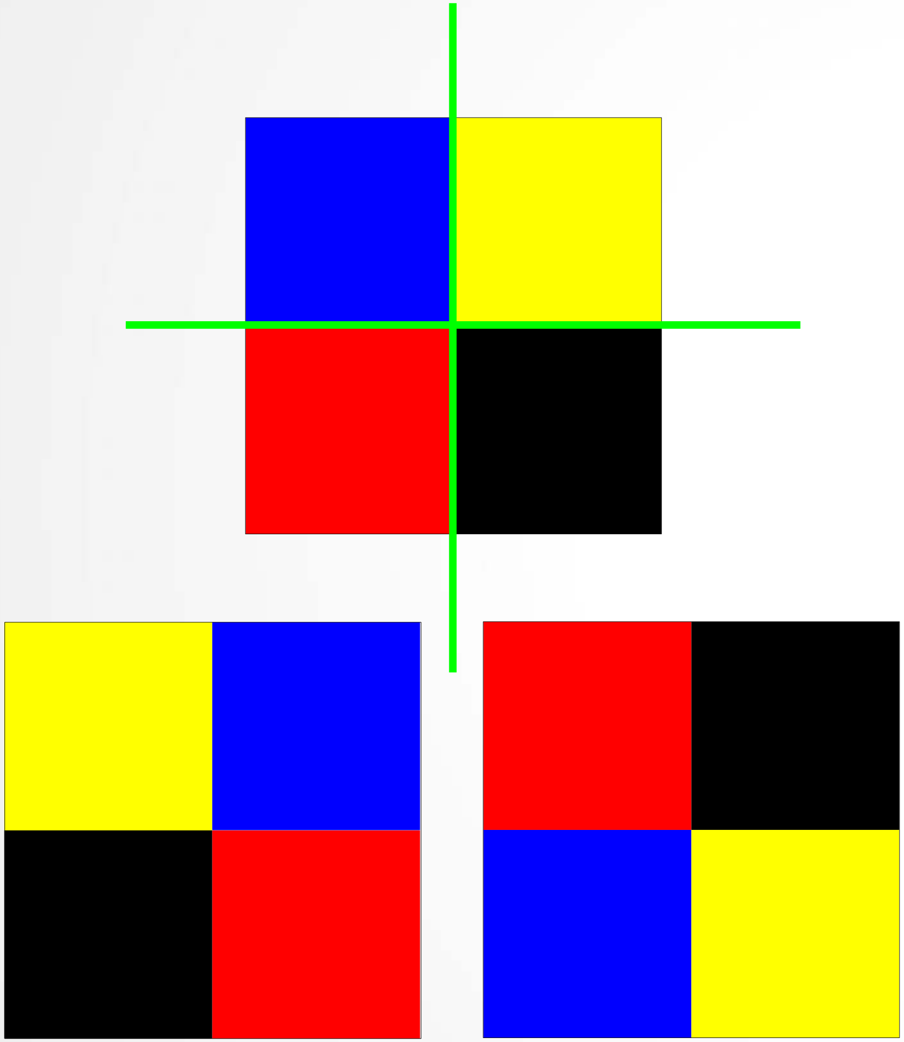
Example





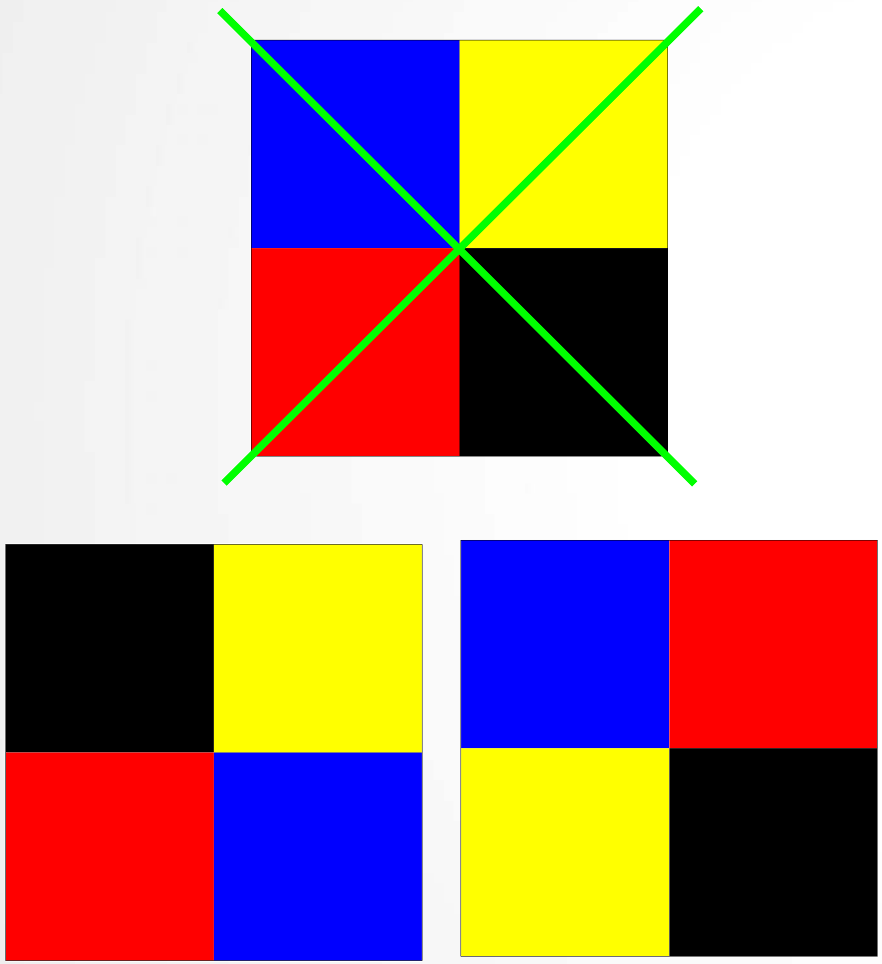
Fourfold axis totally chromatic: it exchanges ***four colors***.

Example



Two mirror planes totally chromatic: each of them exchanges ***two pairs*** of colors.

Example



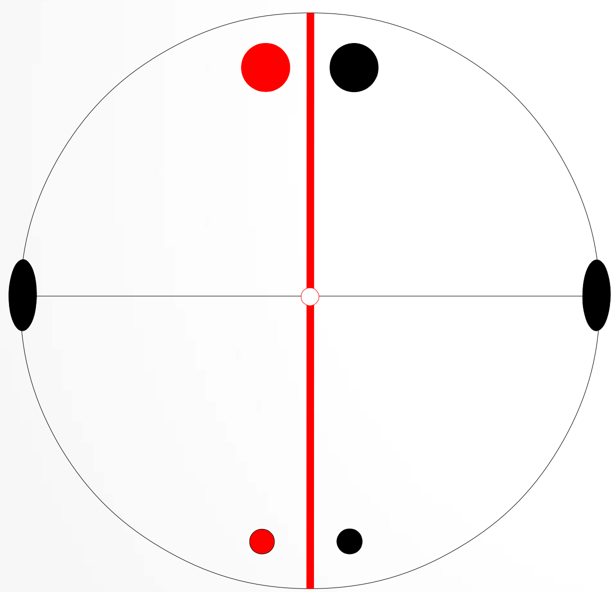
Two mirror planes partially chromatic: each of them exchanges ***one pair*** of colors and leaves fixed the other pair.

Categories of chromatic point groups

- **Dichromatic** crystallographic point groups: **Shubnikov groups** $K^{(2)}$
- **Polychromatic invariant** extension of crystallographic point groups (no partially chromatic operation): **Koptsik groups** $K^{(p>2)}$
- **Polychromatic non-invariant** extension of crystallographic point groups (with partially chromatic operations): **Van der Waerden-Burckhardt** groups $K_{WB}^{(p>2)}$

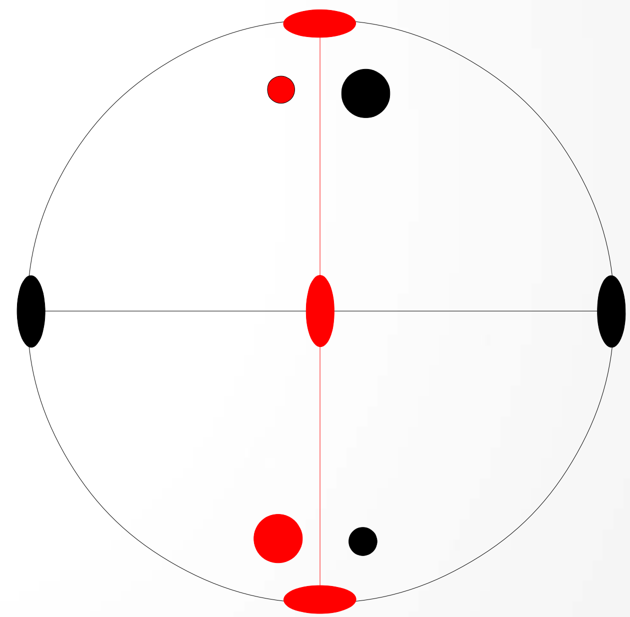
Example of dichromatic (Shubnikov) $K^{(2)}$ groups

$H^* = 2$



$K^{(2)} = 2/m'$

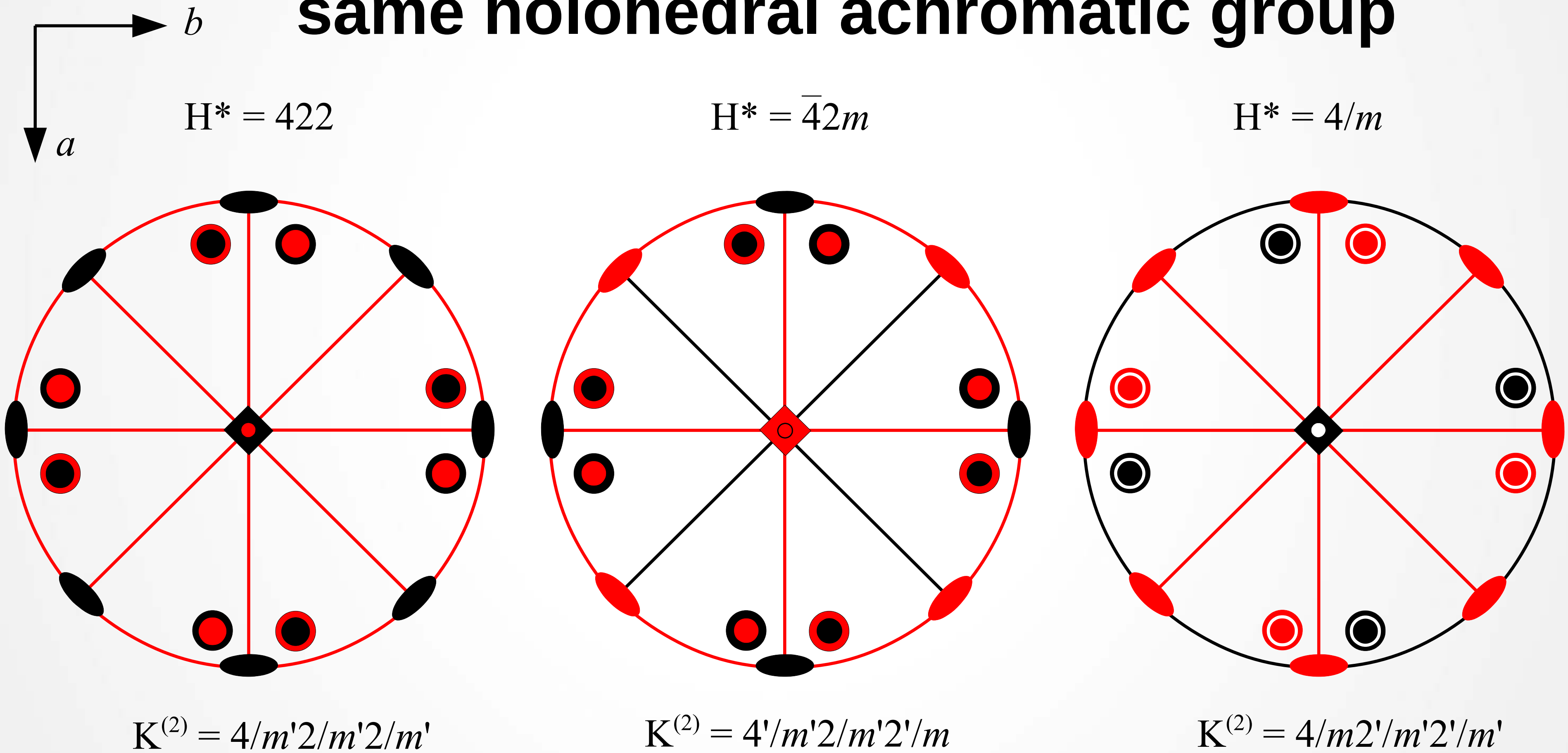
$H^* = 2$



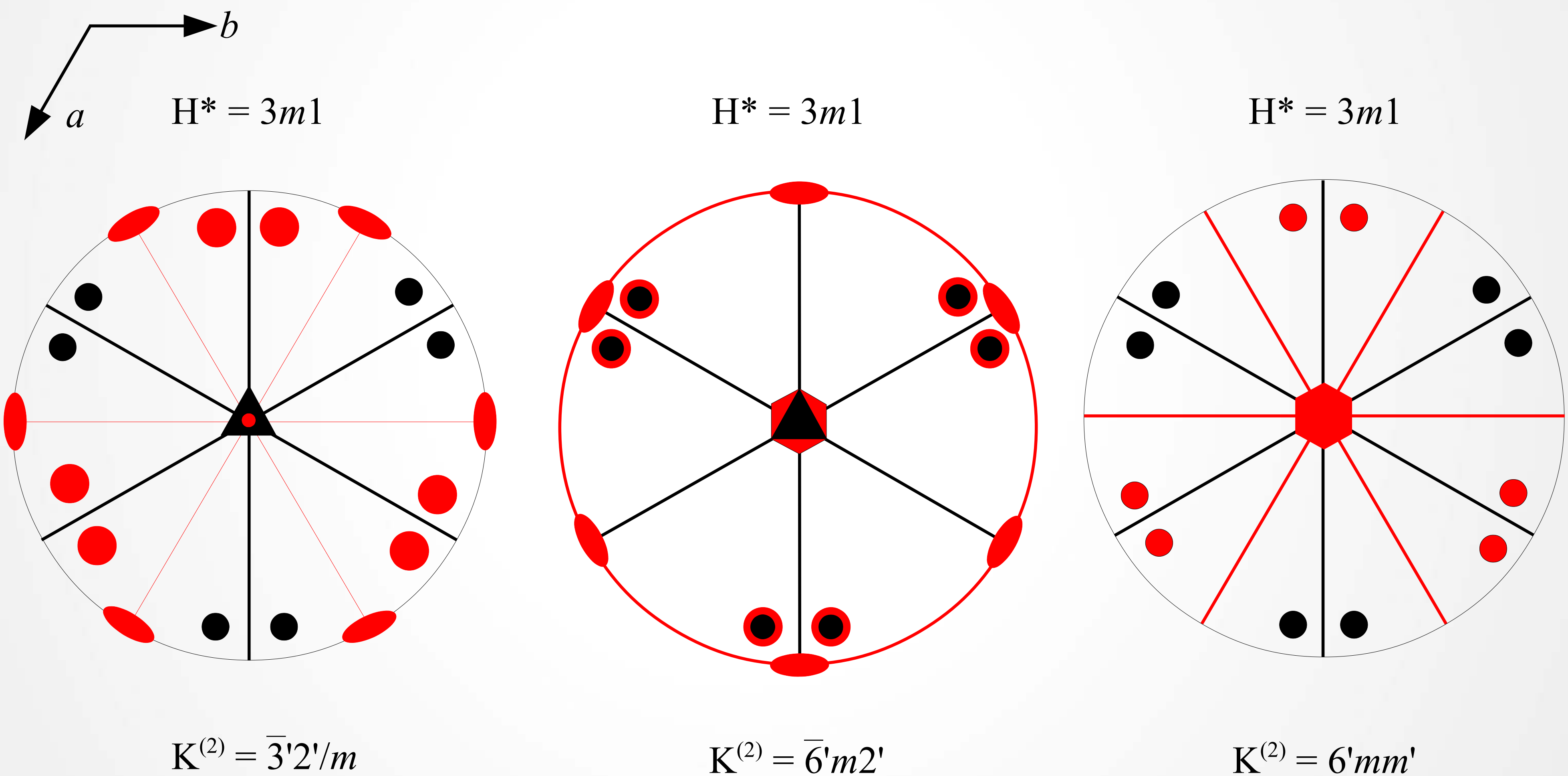
$K^{(2)} = 2'22'$

A simple exercise on dichromatic (Shubnikov) groups

Three $K^{(2)}$ groups corresponding to the same holohedral achromatic group



A simple exercise on dichromatic (Shubnikov) groups: obtain the possible $K^{(2)}$ from the given H*



Exercise

Find the twin point group of two individuals with H = 222 related by a twin mirror plane (010). What type of twin is it?

Exercise

Find the twin point group of two individuals with H = 222 related by a fourfold twin axis parallel to [001]. What type of twin is it?

Exercise

Find the twin point group of two individuals with H = *mmm* related by a fourfold twin axis parallel to [001]. What type of twin is it?

Exercise

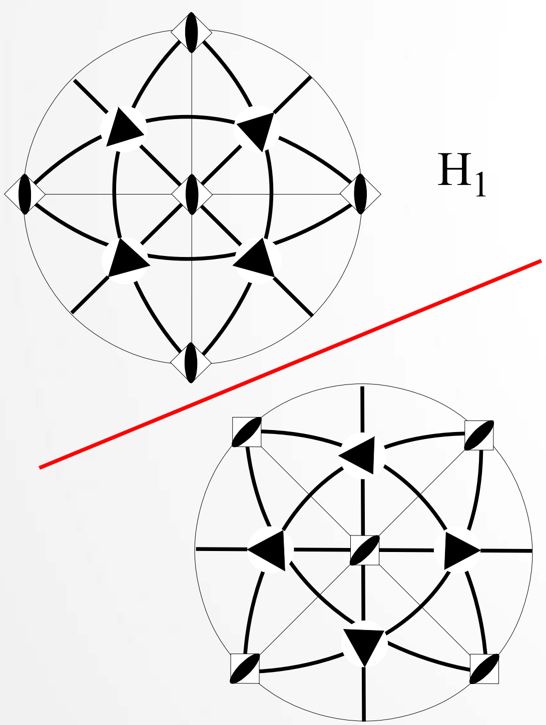
Find the twin point group of two individuals with H = 2 and β = 90° related by a twofold twin axis parallel to [100]. What type of twin is it?

Exercise

Find the twin point group of two individuals with H = *m* and β = 90° related by a twofold twin axis parallel to [100]. What type of twin is it?

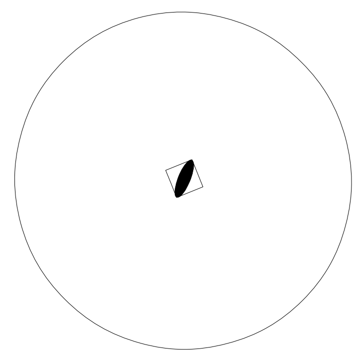
Exercise

(210) twinning in hauyne, $H = \bar{4}3m$

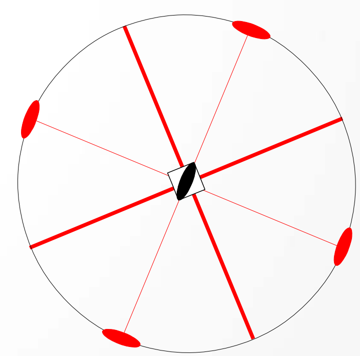


H_1

H_2



$H^* = \bar{4}$



$K = \bar{4}2'm'$

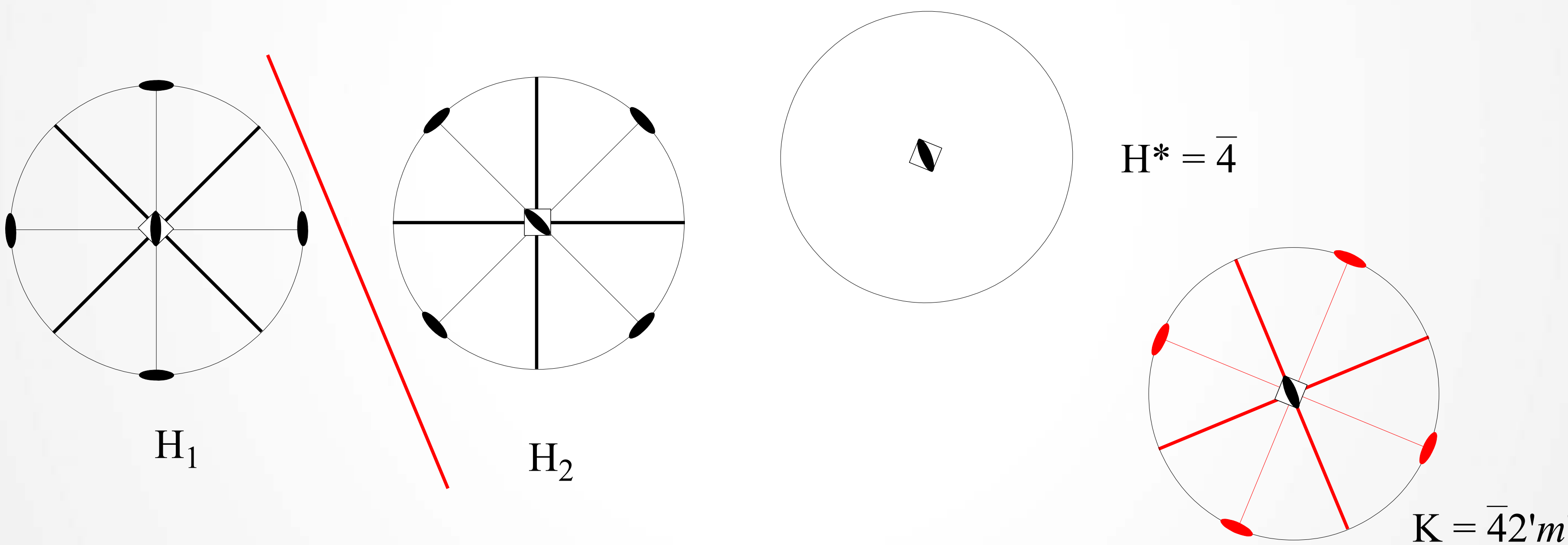
Twinning by reticular merohedry

What is the twin index?

$K \subset H$

Exercise

$(\bar{1}20)$ twinning in melilite, H = $\bar{4}2m$

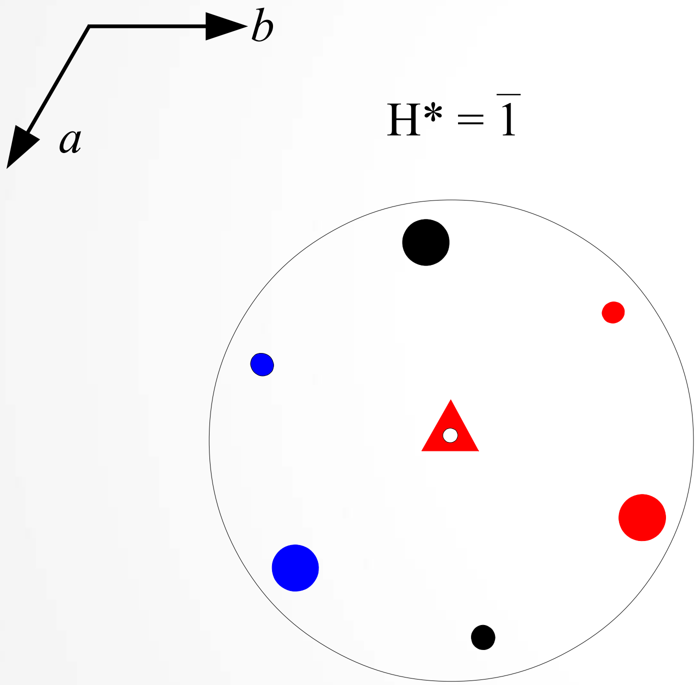


Twinning by reticular polyholohedry

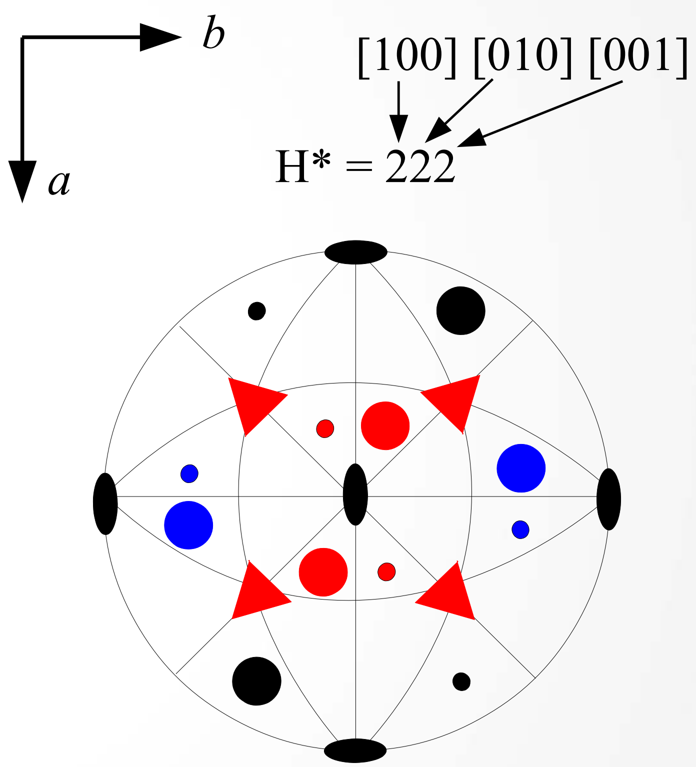
What is the twin index?

K = H

Examples of Koptsik $K^{(p)}$ groups for first-order twins



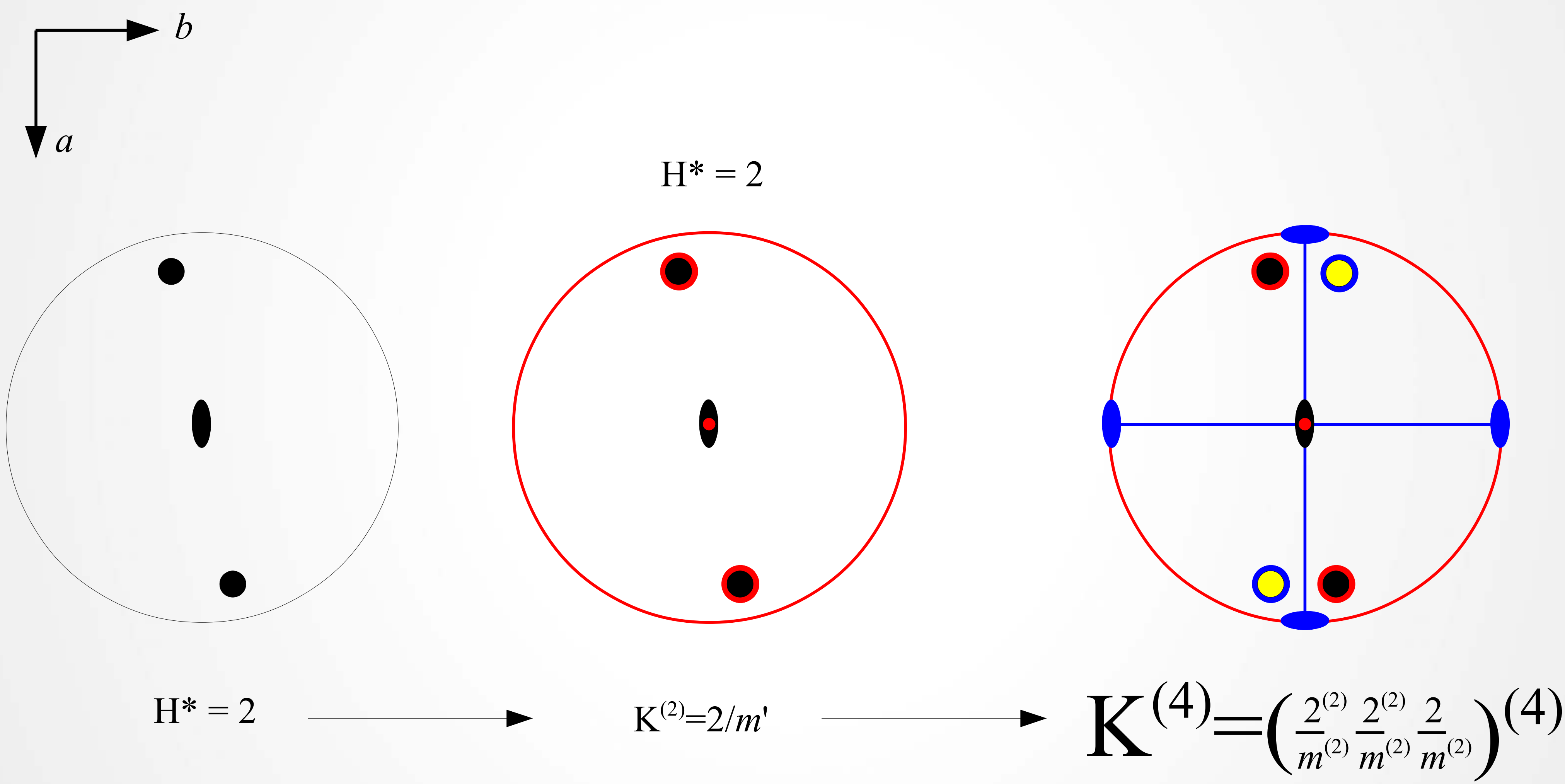
$K^{(3)} = \bar{3}^{(3)}$



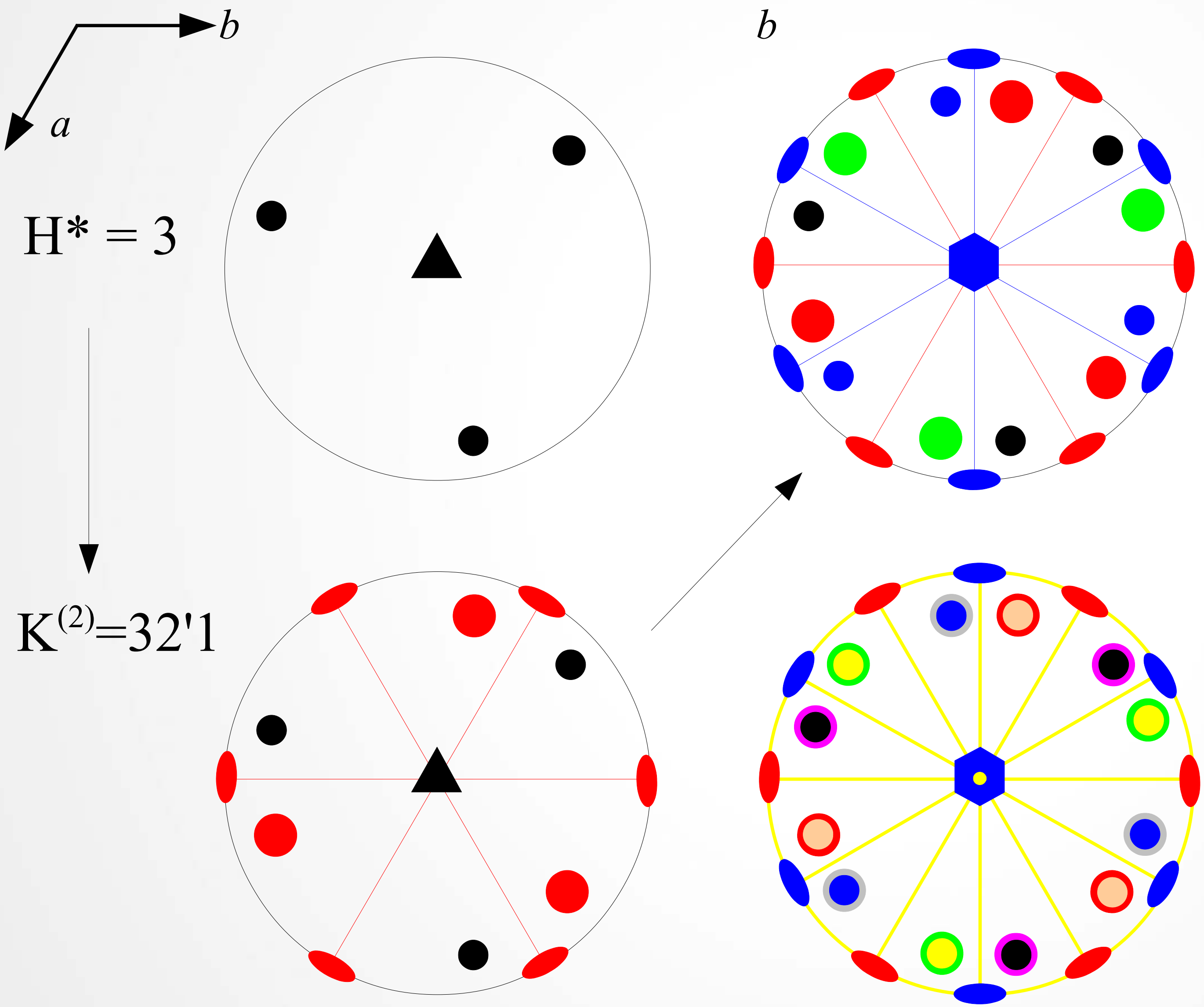
$K^{(3)} = (23^{(3)})^{(3)}$

⟨100⟩ ⟨111⟩

Examples of Koptsik $K^{(p)}$ groups for higher-order twins



Examples of Koptsik $K^{(p)}$ groups for higher-order twins



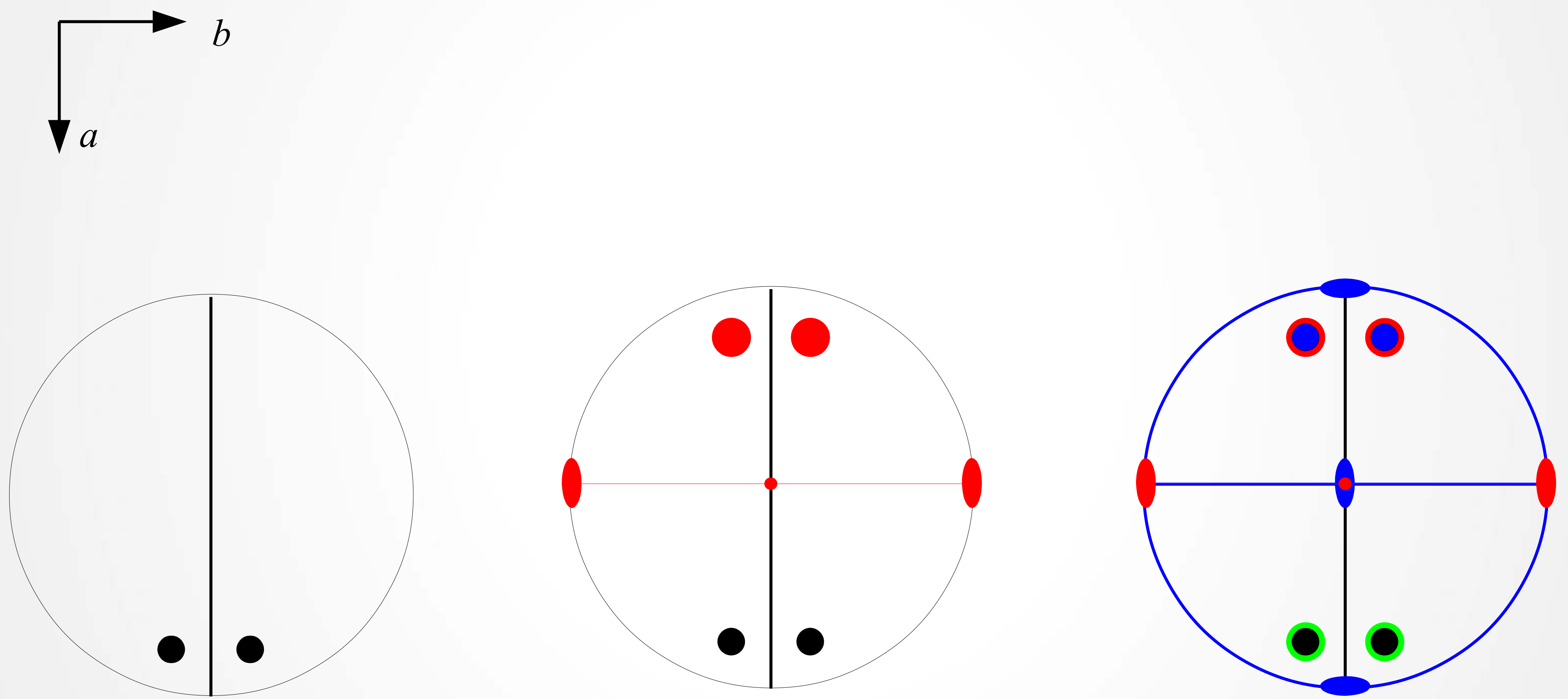
$H^* = 3$

$K^{(2)} = 32'1$

$K^{(4)} = (6^{(2)}2^{(2)}2^{(2)})^{(4)}$

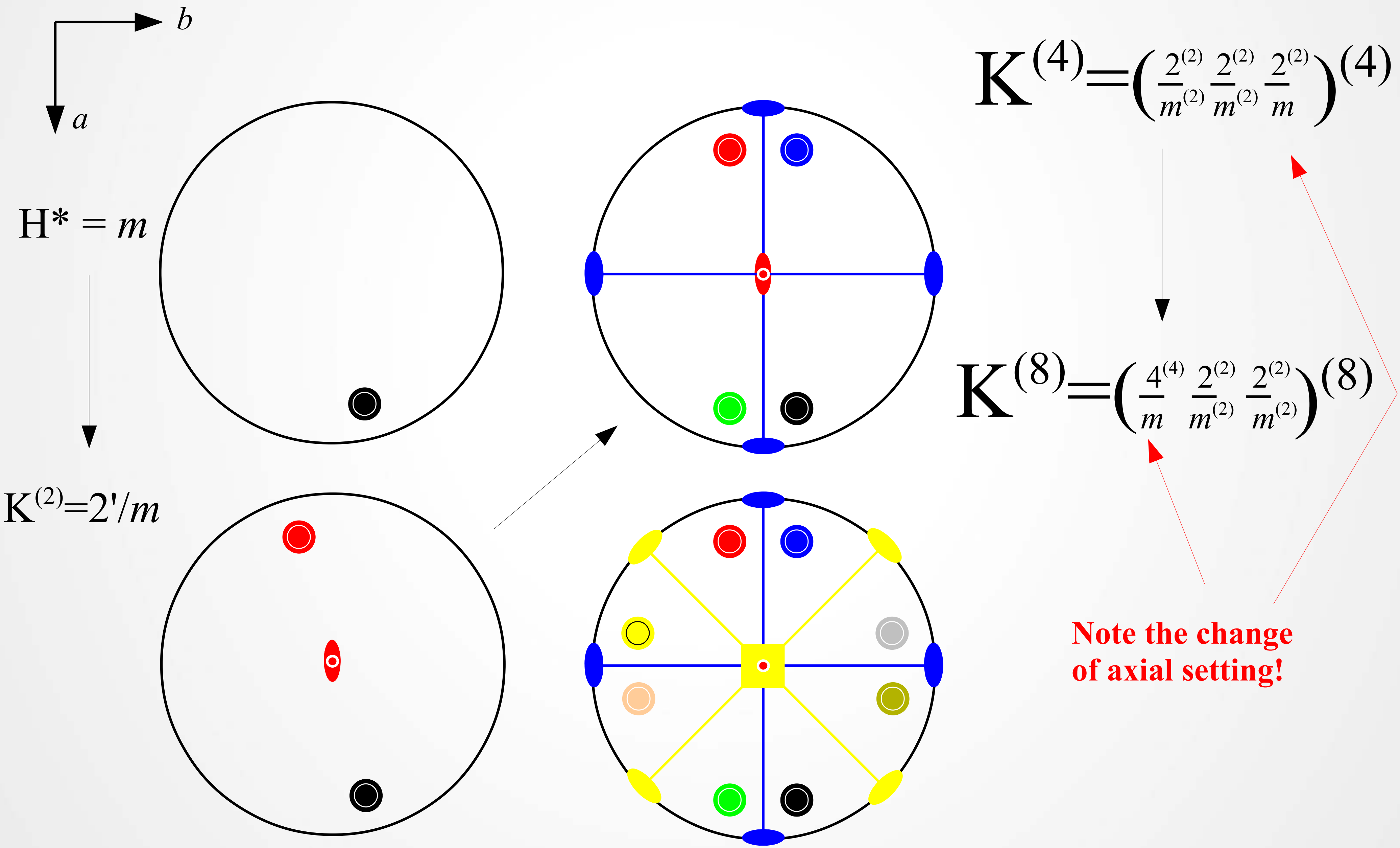
$$K^{(8)} = \left(\frac{6^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(8)}$$

A simple exercise on Koptsik groups: obtain the orthorhombic holohedral $K^{(p>2)}$ from H* = m

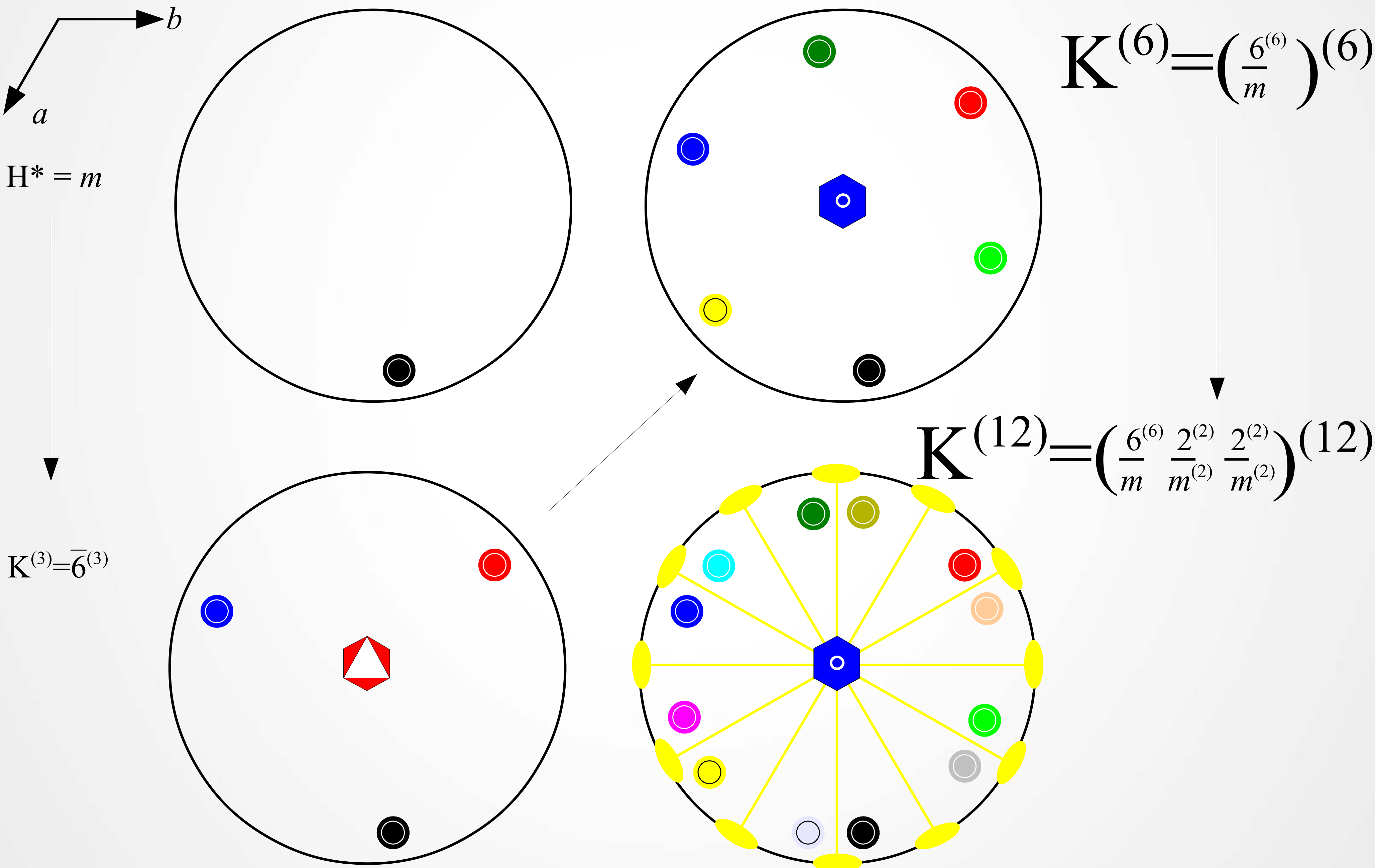


$H^* = m \longrightarrow K^{(2)} = 2'/m \longrightarrow K^{(4)} = \left(\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$

A simple exercise on Koptsik groups: obtain the tetragonal holohedral $K^{(p>2)}$ from $H^* = m$



A simple exercise on Koptsik groups: obtain the hexagoanl holohedral $K^{(p>2)}$ from H* = *m*



Exercise

Find the twin point group of four individuals with H = 2 related by 1) a mirror plane (010) and 2) a twofold twin axis parallel to [100]. What type of twin is it?

Exercise

Find the twin point group of three individuals with H = 2 related by a threefold twin axis parallel to [010]. What type of twin is it? What happens if one of the individuals does not develop or is chopped off?

Exercise

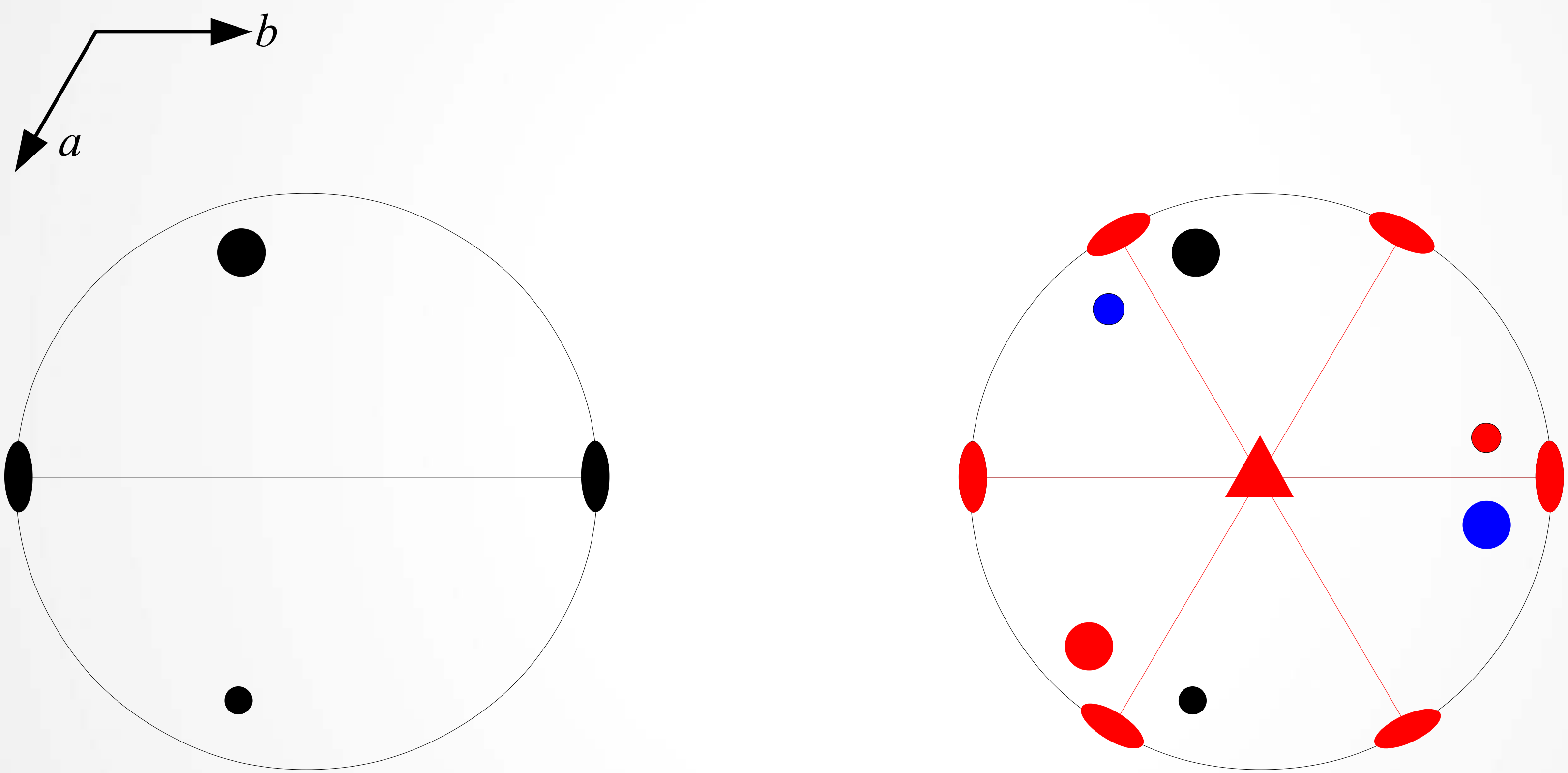
Repeat the previous exercise by adding:

→a twin mirror plane (001)

→a twofold twin axis parallel to [100]

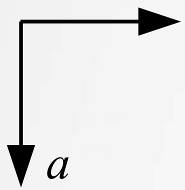
What type of twin is it? What happens if two of the individuals do not develop or are chopped off?

Examples of Van der Waerden-Burckhardt $K_{WB}^{(p)}$ groups



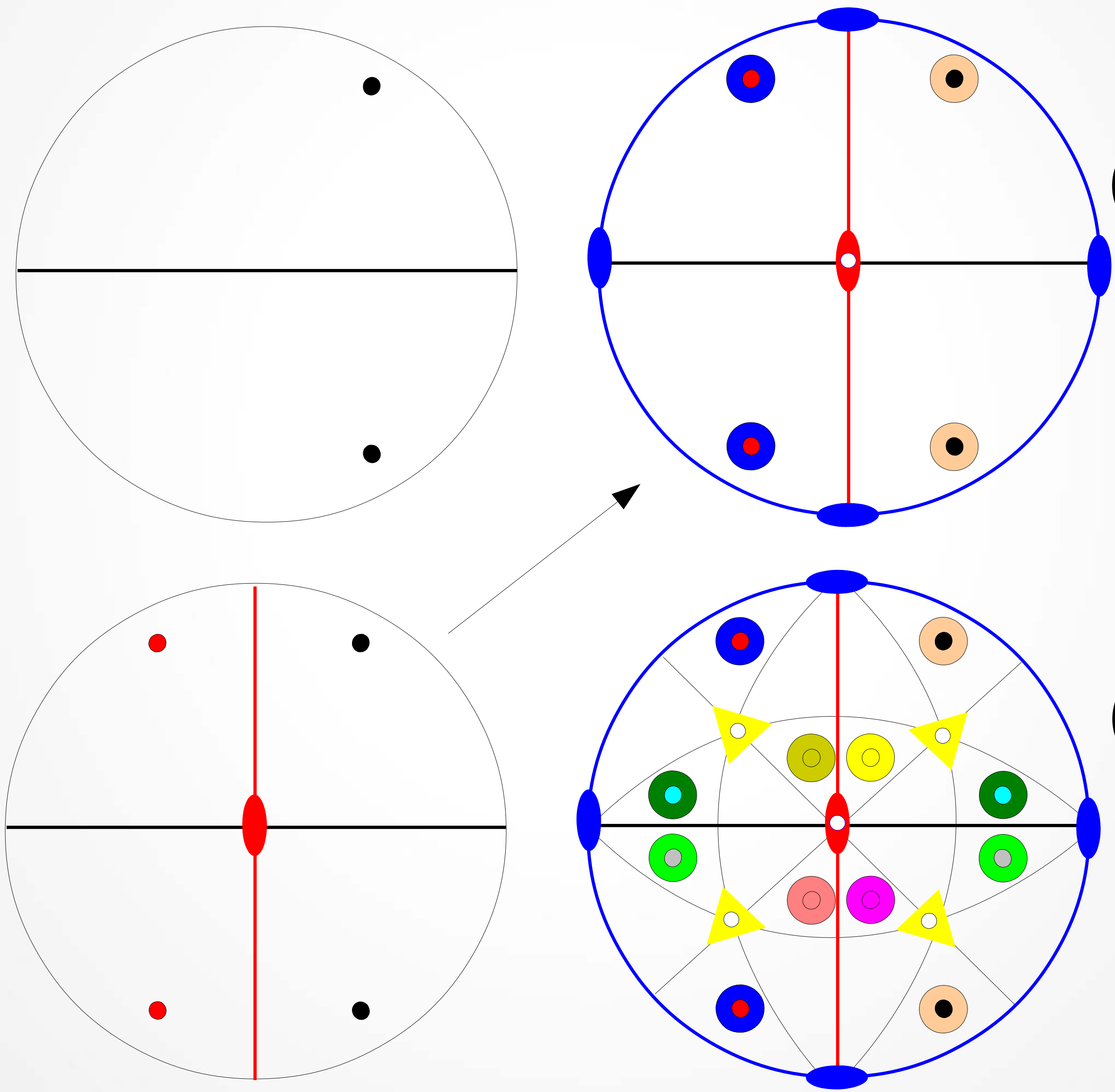
$H^* = 2 \longrightarrow K_{WB}^{(3)} = (3^{(3)}2^{(2,1)})^{(3)}$

Examples of Van der Waerden-Burckhardt $K_{WB}^{(p)}$ groups



$H^* = m$

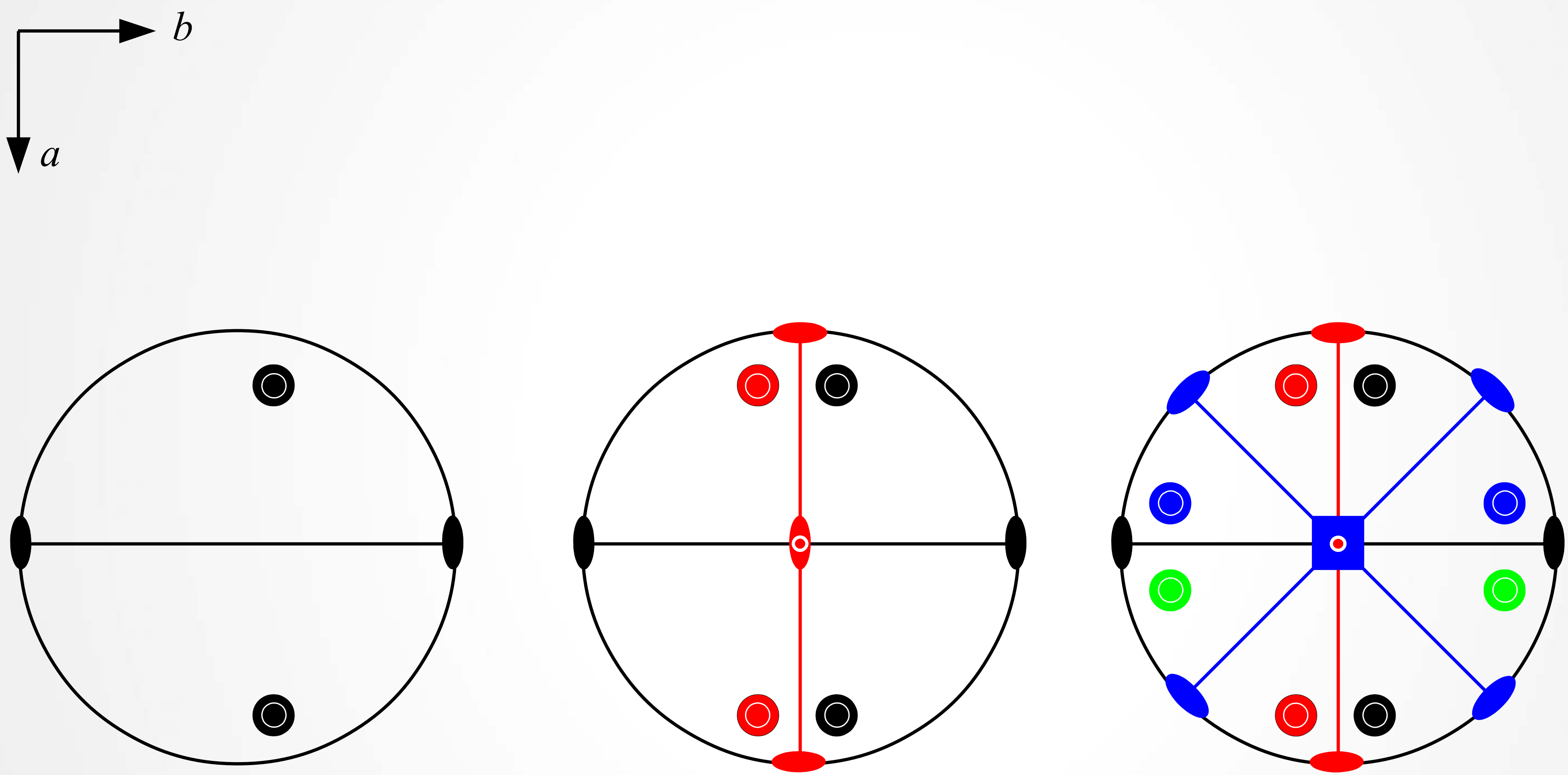
$K^{(2)} = m'm2'$



$$K^{(4)} = \left(\frac{2^{(2)}}{m}\,\frac{2^{(2)}}{m^{(2)}}\,\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$$

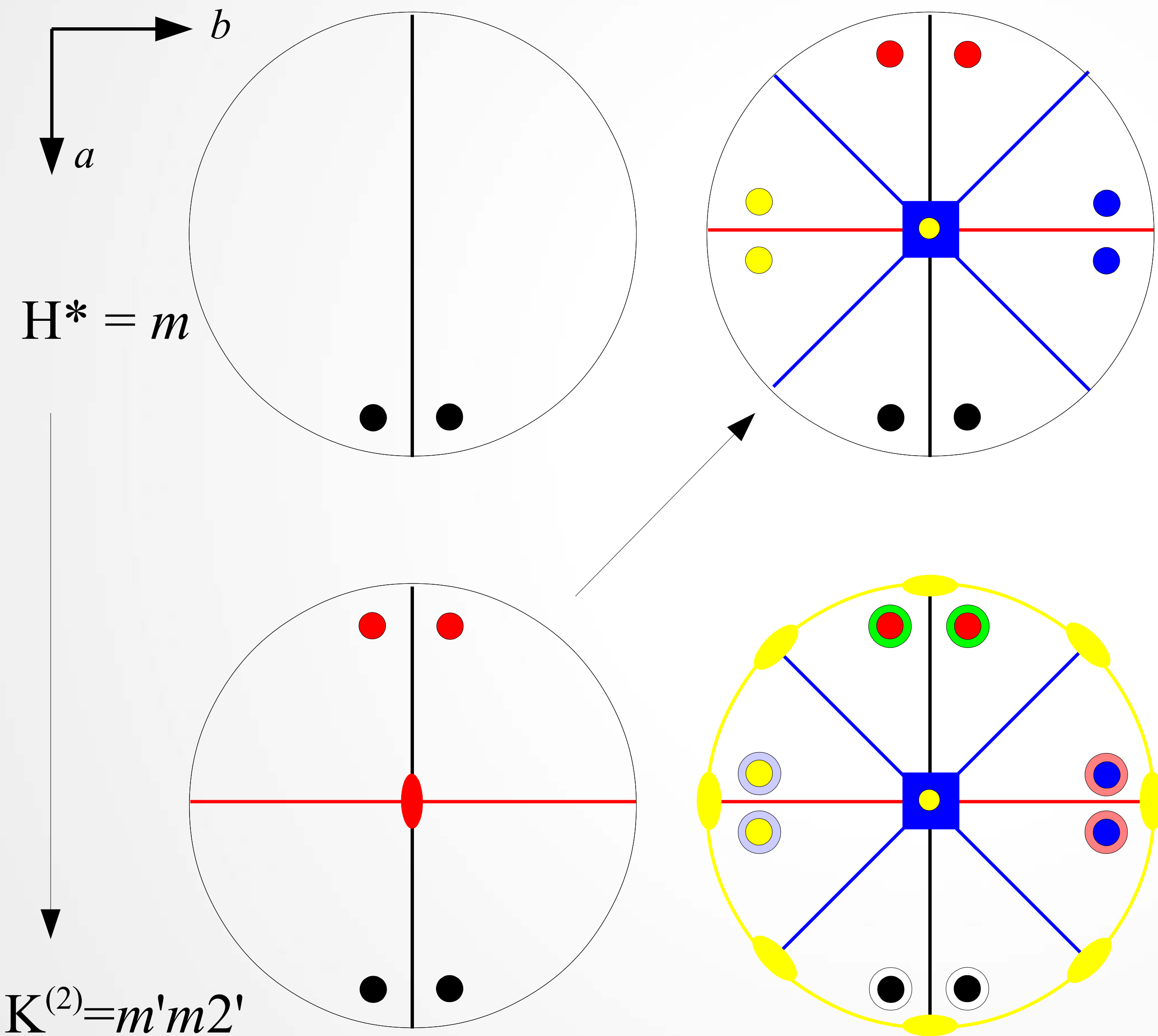
$$K_{WB}^{(12)} = \left(\frac{2^{(2)}}{m^{(2,4)}}\;\bar{3}^{(6)}\right)^{(12)}$$

Example of Van der Waerden-Burckhardt $K_{WB}^{(p)}$ groups for higher-order twins



$$H^* = m2m \longrightarrow K' = \left(\frac{2'}{m}\ \frac{2}{m'}\ \frac{2'}{m}\right) \longrightarrow K_{WB}^{(4)} = \left(\frac{4^{(4)}}{m}\ \frac{2^{(2,2)}}{m^{(2,2)}}\ \frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$$

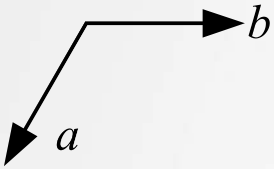
Obtain the tetragonal holohedral $K_{WB}^{(p>2)}$ from $H^* = m$



$$K_{WB}^{(4)} = (4^{(4)}\ m^{(2,2)} m^{(2)})^{(4)}$$

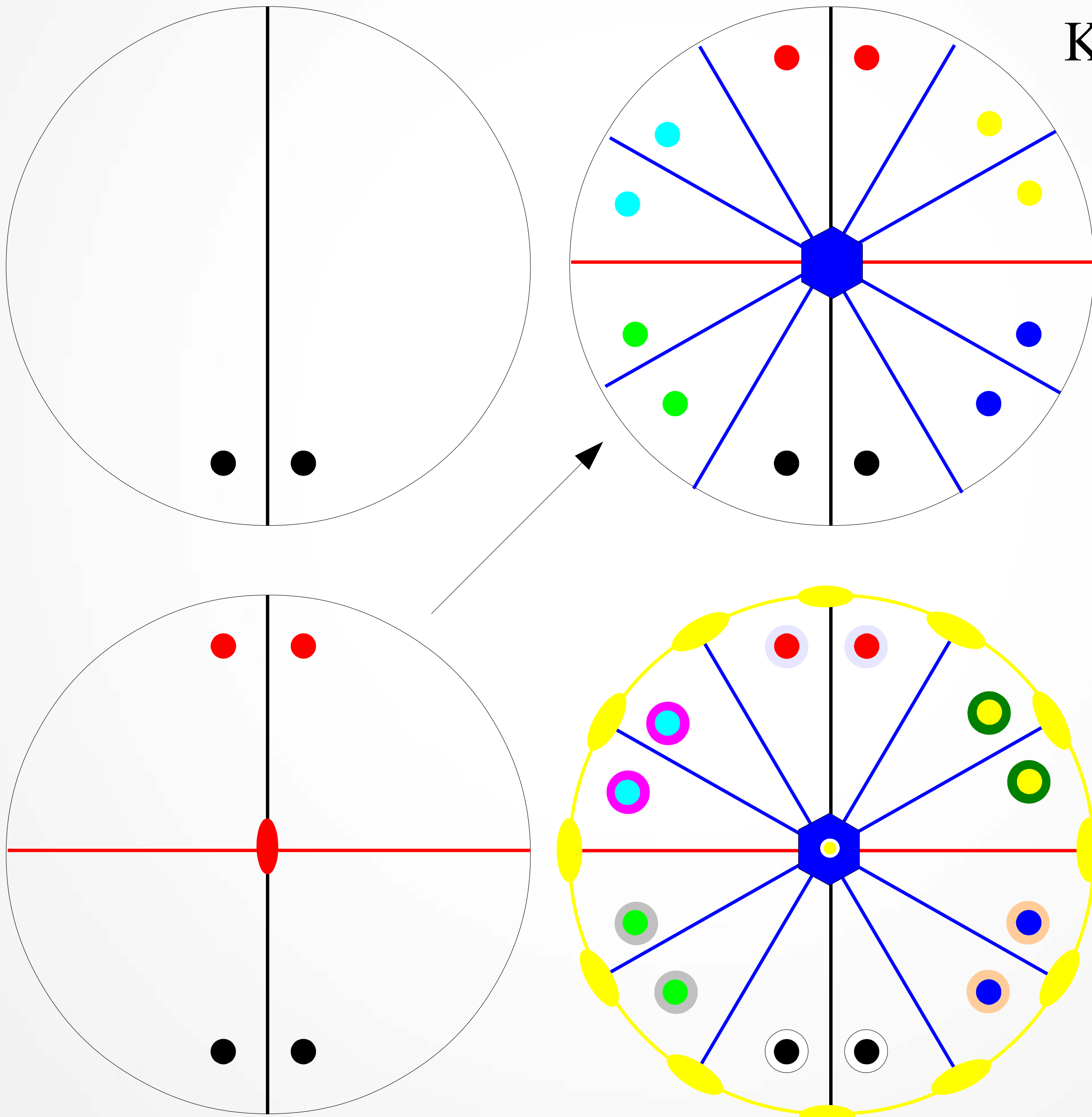
$$K_{WB}^{(8)} = \left(\frac{4^{(4)}}{m^{(2)}} \frac{2^{(2)}}{m^{(2,4)}}\ \frac{2^{(2)}}{m^{(2)}} \right)^{(4)}$$

Obtain the hexagonal holohedral $K_{WB}^{(p>2)}$ from $H^* = m$



$H^* = m$

$K^{(2)} = m'm2'$



$K_{WB}^{(6)} = (6^{(6)} m^{(2,2)} m^{(2)})^{(6)}$

$$K_{WB}^{(12)} = \left(\frac{6^{(6)}}{m^{(2)}} \frac{2^{(2)}}{m^{(2,4)}} \frac{2^{(2)}}{m^{(2)}}\right)^{(12)}$$