

# Chemical Crystallography and Structural Chemistry

(VO 270287)

Lecture 4

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## Previous Lecture

1. Laue Equations
2. Ewald Sphere Constructions
3. Bragg's Law and Resolution
4. Symmetry, Combination of Symmetry Operations

## Today's Lecture

1. Space groups and crystallographic point groups
2. Choice of unit cell
3. 7 Crystal systems and 14 Bravais lattices
4. Symmetry in reciprocal space
5. Space group determination

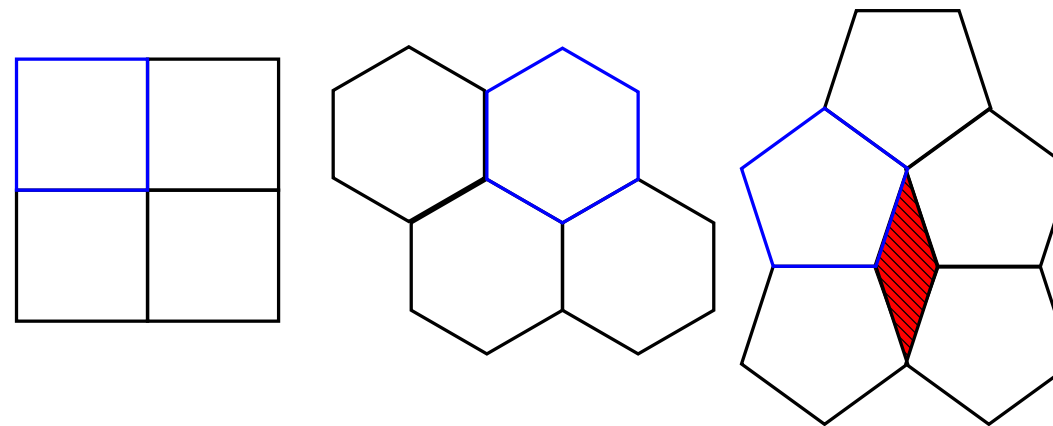
# Point groups and Space groups

# Point Groups and Space Groups

1. Classification and nomenclature
2. Symbols for symmetry elements

# Point Groups

- Point groups consider symmetry without translation
- Symmetry operations:
  1. mirror plane
  2. inversion centre
  3. n-fold rotation
- In crystallography: only 2-fold, 3-fold, 4-fold, 6-fold rotations



# Point Groups

The combination of all symmetry operations that are compatible with unit cells leads to 32 different groups, the

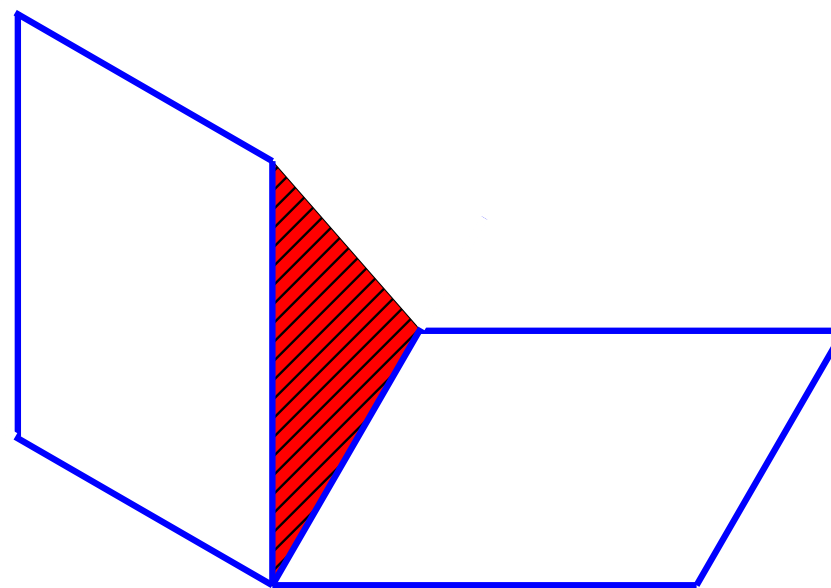
## 32 crystallographic point groups

**N.B.** There are many more point groups for molecules, only 32 are compatible with the requirements from the unit cell.

*cf.* Crystallographic point group on Wikipedia.

# Space Groups

- Point groups combined with translation of the infinite lattice
- Symmetry operations:
  1. mirror plane
  2. inversion centre
  3. n-fold rotation
  4. glide plane
  5. screw axis
- Not every unit cell type is compatible with every symmetry operation





# Space Groups

The combination of 32 point groups with translation of the infinite crystal lattice creates

## 230 space groups

- Every crystal belongs to one out of 230 different space groups.
- Chiral compounds belong to a subset, 65 different Sohncke groups <sup>1</sup>. The Sohncke groups do not violate the chirality of the compound.
- All point groups and space groups are listed in the in “*International Tables of Crystallography*”, Volume A (International Union of Crystallography, IUCr)

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<sup>1</sup>Leonhard Sohncke, 1842–1897, German mathematician and physicist

# Nomenclature

There are mainly two different types of nomenclatures for point groups and for space groups:

- Hermann-Mauguin System (primarily used in crystallography)
- Schönflies System (primarily used for symmetry of molecules, spectroscopy)

## Nomenclature: Hermann-Mauguin System

- Space groups have names like  $P2_1/c$  or  $I\bar{4}3m$ .
- subscripts can be replaced with brackets:  $P2(1)/c$
- bars can be replaced with a minus sign:  $I-43m$
- first, capital letter: lattice type (later)
- next: three positions for  $a, b, c$  axes
- by conventions, axes with '1' are dropped:  $P2_1/c = P\ 1\ 2_1/c\ 1$

(Literature: Massa "Crystal Structure Determination", Chapter. 6)

## Nomenclature: Hermann-Mauguin System

- n-fold rotation axis:  $n$
- centre of inversion:  $\bar{1}$  or  $\bar{N}$
- mirror plane:  $m$
- glide mirror plane:
  - a** translation along  $\vec{a}$ , i.e.  $1a1$  or  $11a$
  - b** translation along  $\vec{b}$ , i.e.  $b11$  or  $11b$
  - c** translation along  $\vec{c}$ , i.e.  $c11$  or  $1c1$
  - n, d** translation along diagonal
  - g** translation along arbitrary direction, needs to be followed by direction and position of mirror plane (not a standard setting).
- $1a1$ : mirror plane perpendicular to  $\vec{b}$  axis
- $11a$ : mirror plane perpendicular to  $\vec{c}$  axis

(Literature: Massa “Crystal Structure Determination”, Chapter. 6)

## List of 32 crystallographic point groups

Schönflies	Hermann-Mauguin	Schönflies	Hermann-Mauguin	Schönflies	Hermann-Mauguin	Schönflies	Hermann-Mauguin
$C_1$	1	$C_4$	4	$C_{3i} = S_6$	$\bar{3}$	$C_{6h}$	$6/m$
$C_i$	$\bar{1}$	$S_4$	$\bar{4}$	$D_3$	32	$C_{6v}$	$6mm$
$C_2$	2	$D_4$	422	$C_{3v}$	$3m$	$D_{6h}$	$6/mmm$
$C_s = C_{1v}$	m	$C_{4v}$	$4mm$	$D_{3d}$	$\bar{3}m$	$T$	23
$C_{2h}$	$2/m$	$C_{4h}$	$4/m$	$C_6$	6	$T_h$	$m\bar{3}$
$C_{2v}$	$mm2$	$D_{2d}$	$\bar{4}2m$	$C_{3h}$	$\bar{6}$	$T_d$	$\bar{4}3m$
$D_2$	222	$D_{4h}$	$4/mmm$	$D_6$	622	$O$	432
$D_{2h}$	$mmm$	$C_3$	3	$D_{3h}$	$\bar{6}m2$	$O_h$	$m\bar{3}m$

## Representation of Symmetry operators — Matrices

Each symmetry operator of the **point groups** can be expressed by a matrix:

**4-fold rotation axis about  $\vec{a}$**

$$R_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

**4-fold rotation axis about  $\vec{b}$**

$$R_2 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

**centre of inversion (at origin)**

$$R_3 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Matrices can be directly applied to atom positions with *fractional coordinates* (as e.g. the instruction file for SHELXL).

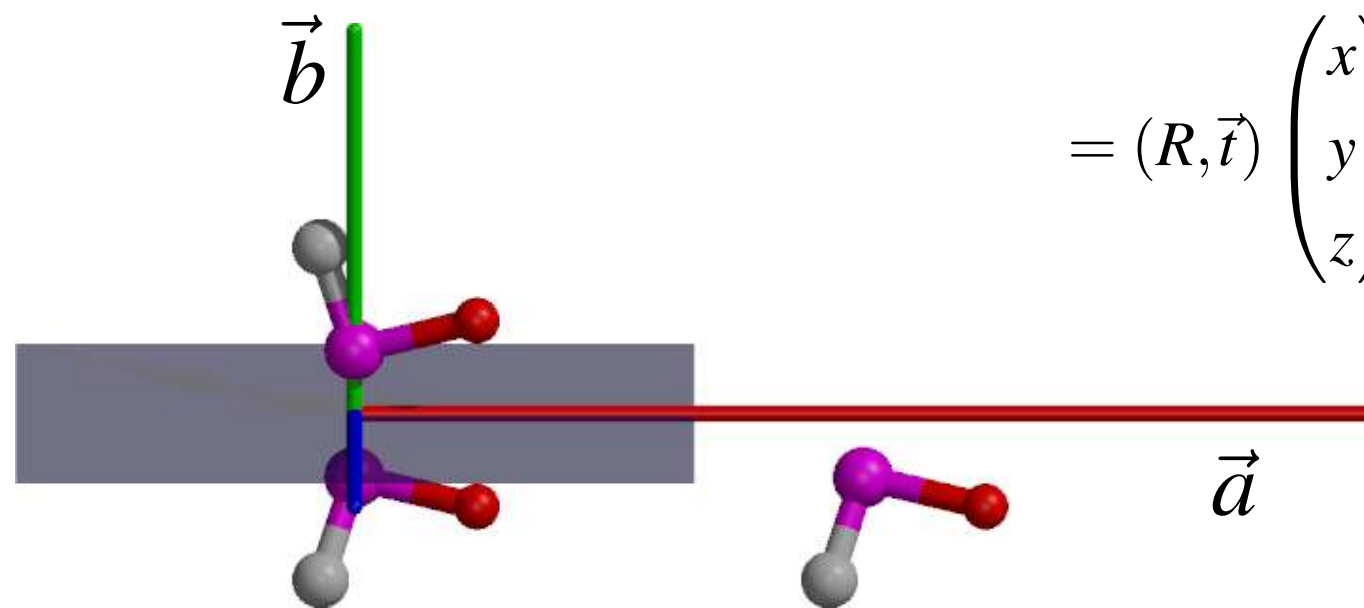
## Symmetry with Translation

**Crystal Symmetry** (Space group): the translational part has to be expressed with a vector  $\vec{t}$

Example: glide mirror plane perpendicular to  $\vec{b}$  along  $\vec{a}$ :

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 1/2 \\ 0 \\ 0 \end{pmatrix}$$

$$= (R, \vec{t}) \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$



A crystal with this type of glide mirror plane with a nitrogen atom at position  $(x, y, z)$  has an equivalent nitrogen atom at position  $(x', y', z')$

## “symmetric” — What does this mean?

**Symmetric molecule** (point groups): for every atom at position  $(x,y,z)$  of a molecule with a symmetry operator  $R$  there is an equivalent atom at position

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = R \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

.

**Symmetry in crystals** (space groups): for every atom at position  $(x,y,z)$  of a molecule with a symmetry operator  $(R, \vec{t})$  there is an equivalent atom at position

$$\begin{aligned} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} &= (R, \vec{t}) \begin{pmatrix} x \\ y \\ z \end{pmatrix} \\ &= R \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \vec{t} \end{aligned}$$

$(x, y, z)$  and  $(x', y', z')$  are **equivalent positions** of the crystal.



## Presentation of Symmetry in the *International Tables*

The *International Tables for Crystallography* contain a description for each of the 230 space groups.

Each description contains the sections

- **Symmetry Operations**
  - **Positions**

# Example Space group $R\bar{3}c$ (No. 167) *International Tables*

CONTINUED

No. 167

$R\bar{3}c$

**Symmetry operations**

For  $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})+$  set

- |  |  |  |
|--|--|--|
| (1) $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$                                     | (2) $3^+(0, 0, \frac{1}{3}) \quad \frac{1}{3}, \frac{1}{3}, z$                                   | (3) $3^-(0, 0, \frac{1}{3}) \quad \frac{1}{3}, 0, z$   |
| (4) $2(\frac{1}{2}, \frac{1}{2}, 0) \quad x, x - \frac{1}{6}, \frac{5}{12}$        | (5) $2(\frac{1}{2}, 0, 0) \quad x, \frac{1}{6}, \frac{5}{12}$                                    | (6) $2 \quad \frac{1}{3}, y, \frac{5}{12}$   |
| (7) $\bar{1} \quad \frac{1}{3}, \frac{1}{6}, \frac{1}{6}$                          | (8) $\bar{3}^+ \quad \frac{1}{3}, -\frac{1}{3}, z; \quad \frac{1}{3}, -\frac{1}{3}, \frac{1}{6}$ | (9) $\bar{3}^- \quad \frac{1}{3}, \frac{2}{3}, z; \quad \frac{1}{3}, \frac{2}{3}, \frac{1}{6}$ |
| (10) $g(\frac{1}{6}, -\frac{1}{6}, \frac{5}{6}) \quad x + \frac{1}{2}, \bar{x}, z$ | (11) $g(\frac{1}{6}, \frac{1}{3}, \frac{5}{6}) \quad x + \frac{1}{4}, 2x, z$                     | (12) $g(\frac{2}{3}, \frac{1}{3}, \frac{5}{6}) \quad 2x, x, z$                                 |

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ ; (2); (4); (7)

**Positions**

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

Reflection conditions

$(0, 0, 0)+ \quad (\frac{2}{3}, \frac{1}{3}, \frac{1}{3})+ \quad (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})+$

General:

36	<i>f</i>	1	(1) $x, y, z$	(2) $\bar{y}, x - y, z$	(3) $\bar{x} + y, \bar{x}, z$			
			(4) $y, x, \bar{z} + \frac{1}{2}$	(5) $x - y, \bar{y}, \bar{z} + \frac{1}{2}$	(6) $\bar{x}, \bar{x} + y, \bar{z} + \frac{1}{2}$			
			(7) $\bar{x}, \bar{y}, \bar{z}$	(8) $y, \bar{x} + y, \bar{z}$	(9) $x - y, x, \bar{z}$			
			(10) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(11) $\bar{x} + y, y, z + \frac{1}{2}$	(12) $x, x - y, z + \frac{1}{2}$			
			18	<i>e</i>	.2	$x, 0, \frac{1}{4}$	$0, x, \frac{1}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$

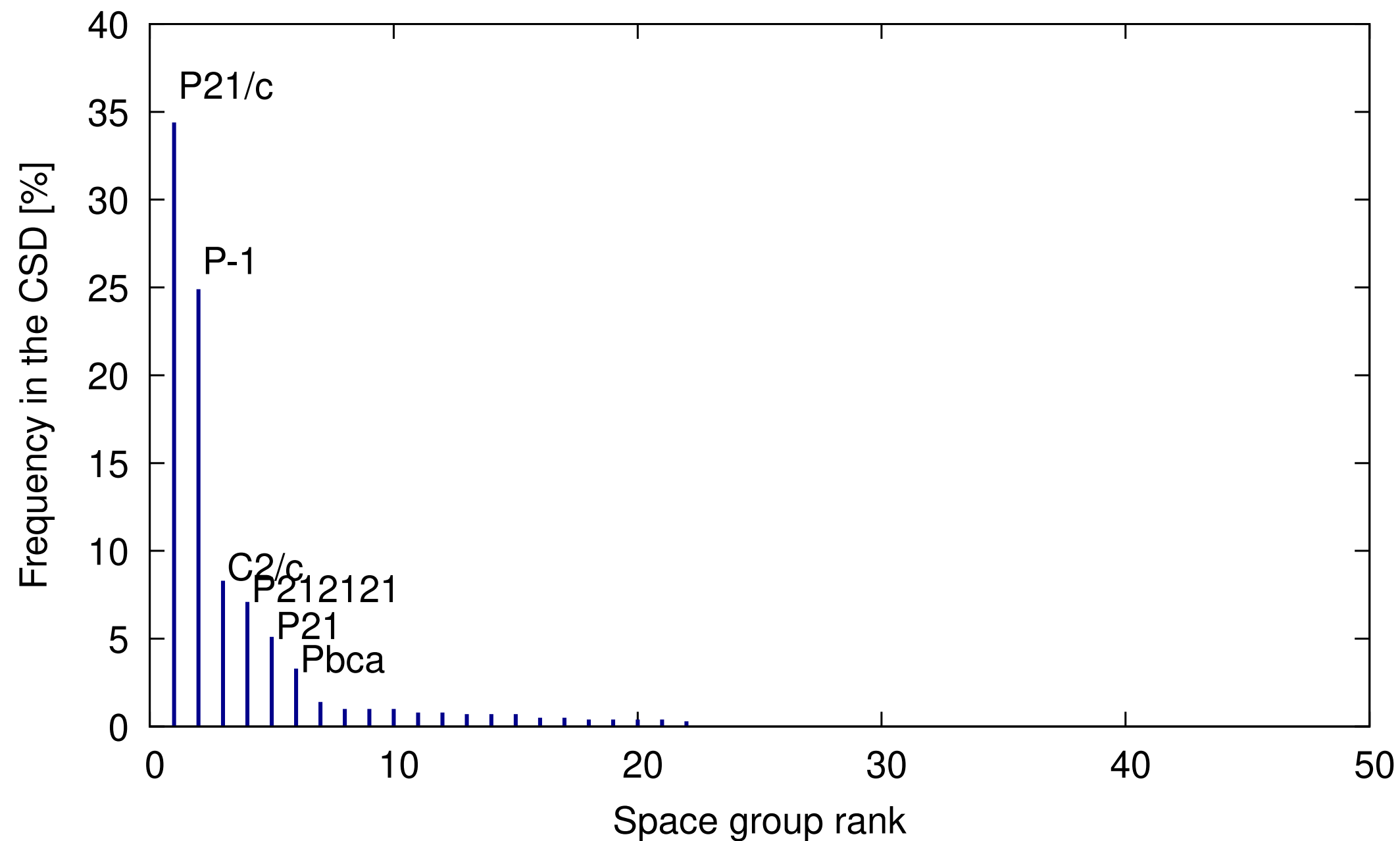
- $hkil \quad : \quad -h + k + l = 3n$
- $hki0 \quad : \quad -h + k = 3n$
- $hh\bar{2}hl \quad : \quad l = 3n$
- $h\bar{h}0l \quad : \quad h + l = 3n, \quad l = 2n$
- $000l \quad : \quad l = 6n$
- $h\bar{h}00 \quad : \quad h = 3n$

Special: as above, plus

no extra conditions

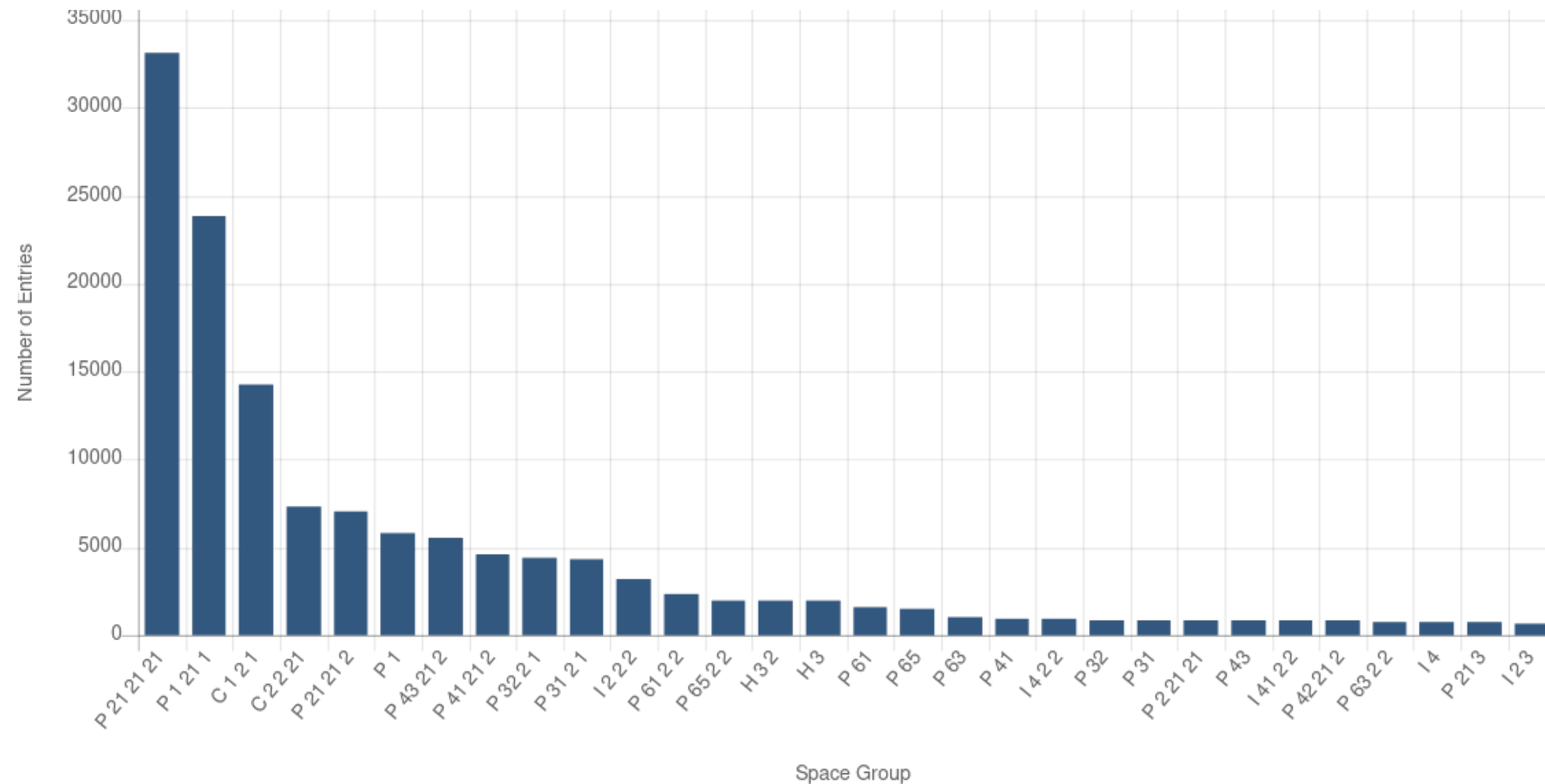
©International Tables for Crystallography (2006). Vol. A, Space group  $R\bar{3}c$  (N. 167), pp. 548-551.

# Frequency of space groups for chemical compounds (CSD, April 2020)



<http://www.ccdc.cam.ac.uk/>

# Frequency of space groups for Macromolecules (PDB, April 2020)



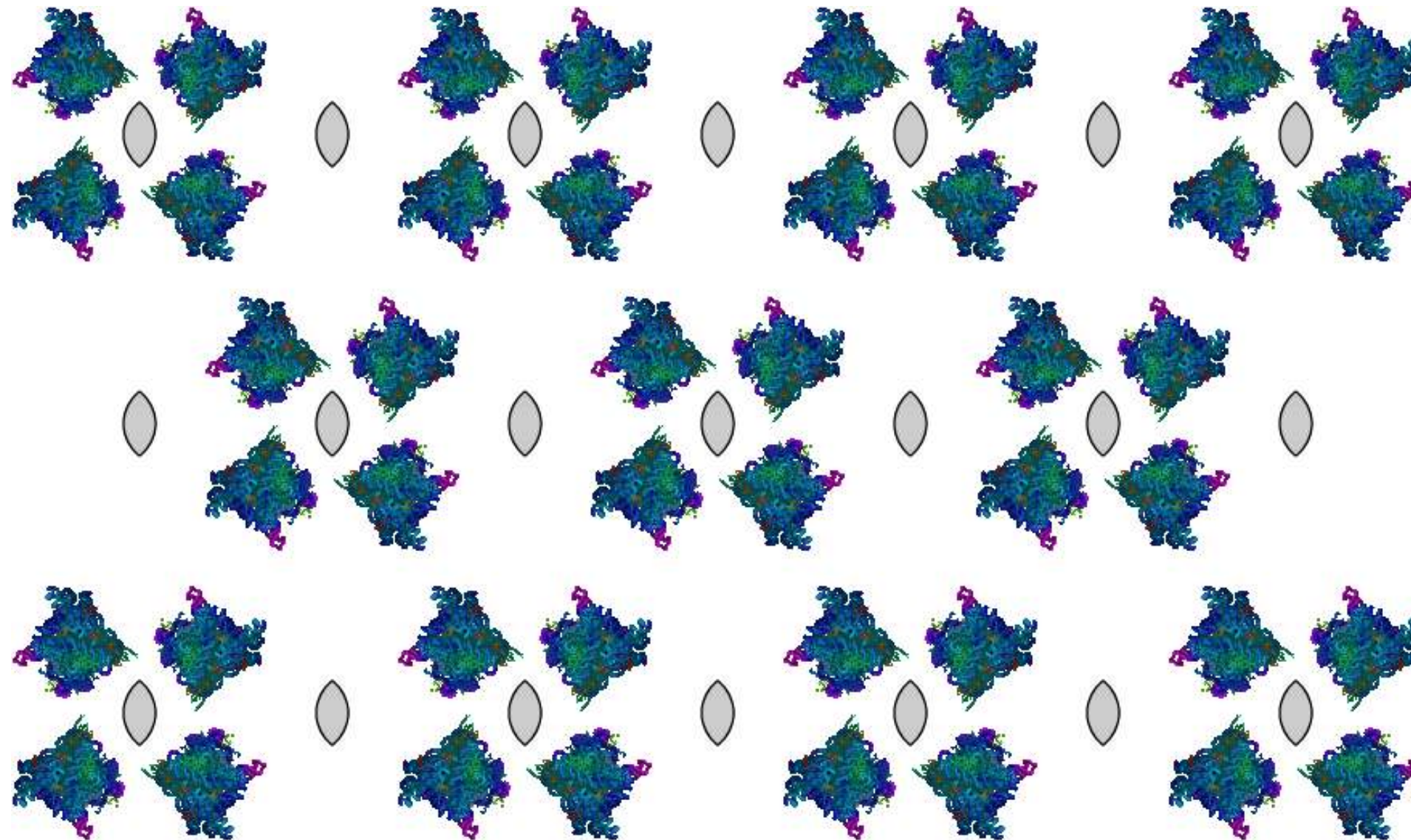
<http://www.rcsb.org>

# Choice of Unit Cell

Overview:

- primitive cell
- asymmetric unit
- 7 crystal classes
- 14 Bravais lattices

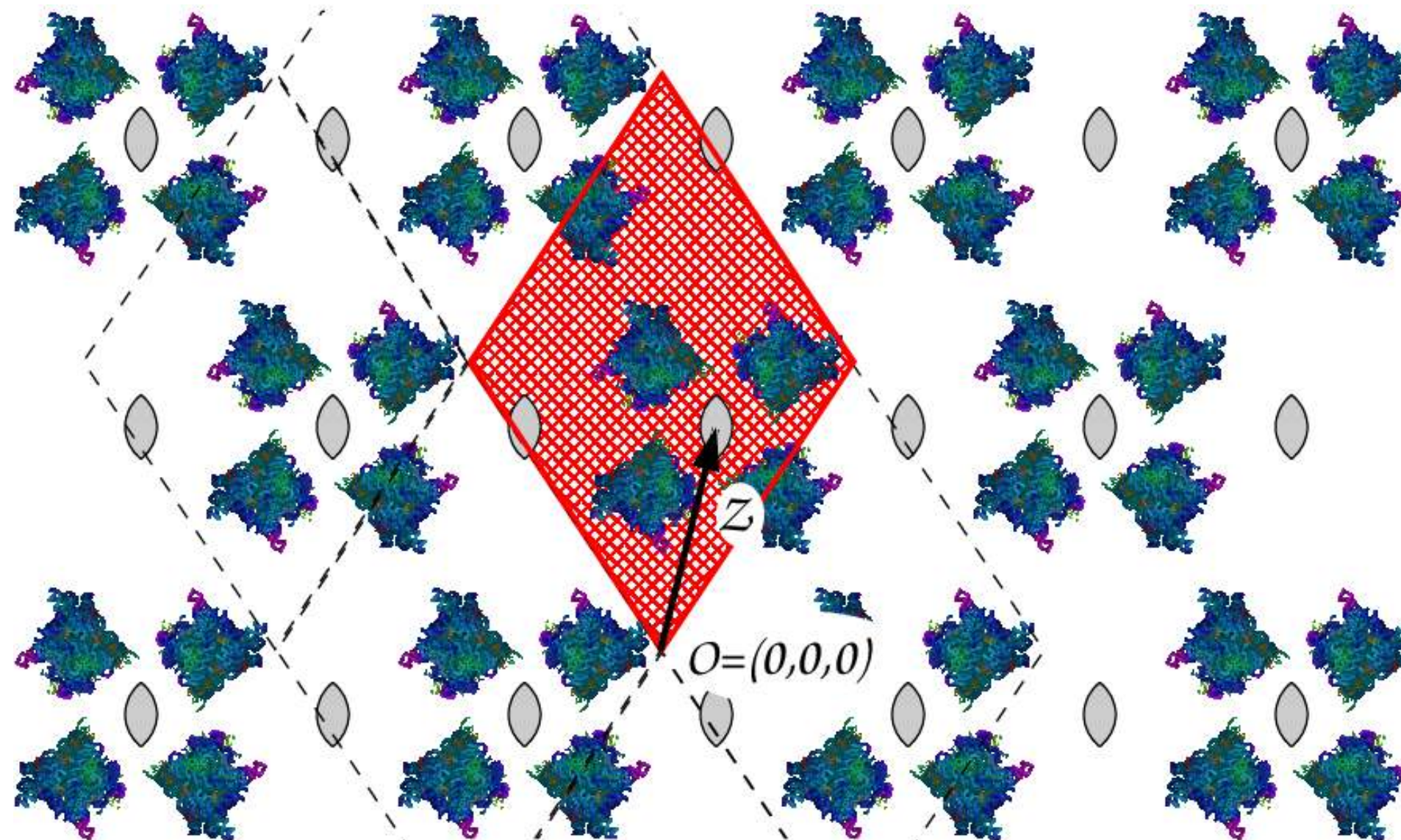
## Choice of Unit Cell



Nature determines symmetry, not *vice versa*

- The position of the molecules determines the position of the symmetry operators
- Here: **2-fold** rotation axes (not 4-fold!)

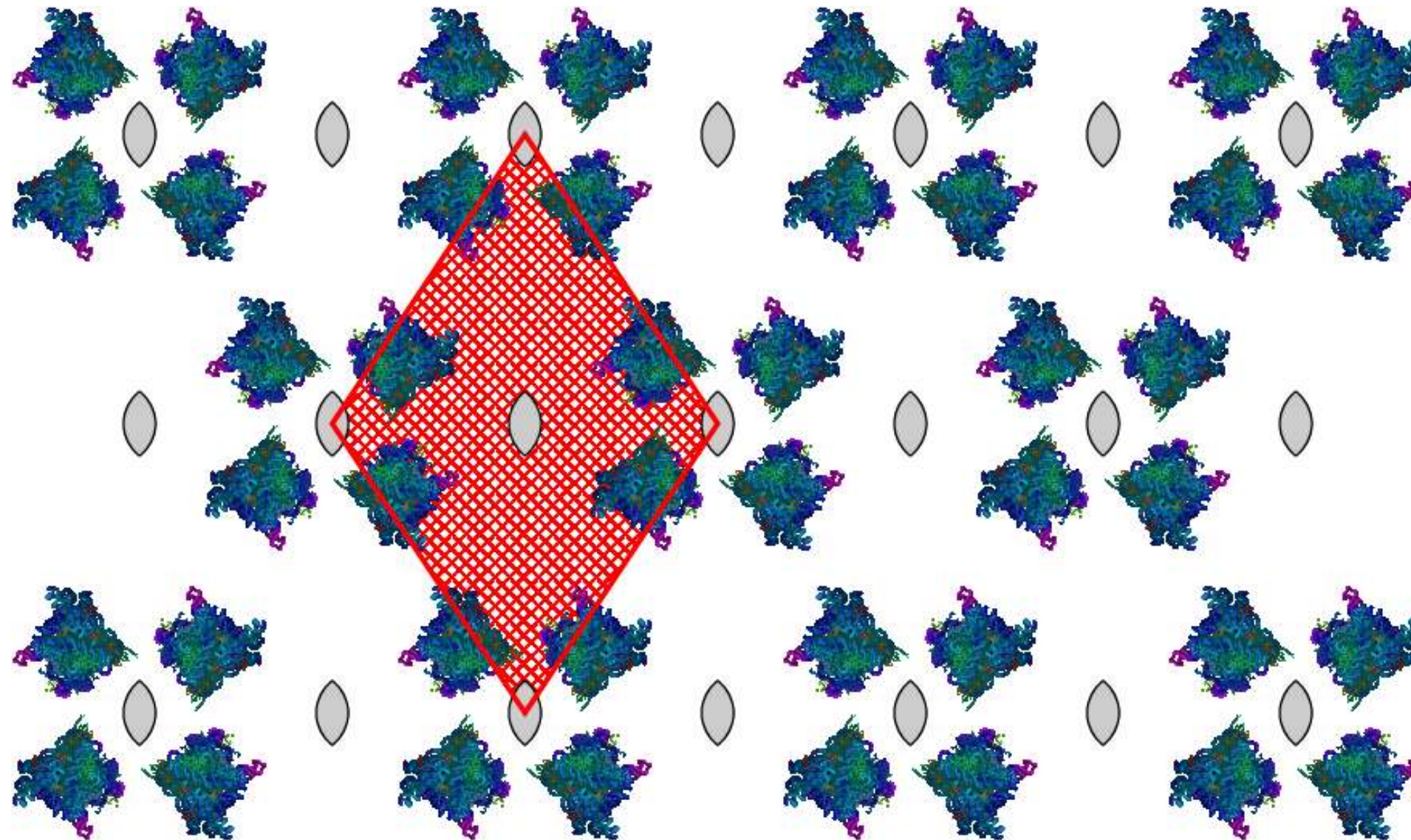
## Choice of Unit Cell



- Uni cell: Helper construction, molecules are “ignorant” of the unit cell
- Condition for unit cell: integer translations cover the entire crystal
- If placed arbitrarily: matrix description becomes awkward:

$$(x'y'z') = R((xyz) - Z) + Z$$

## Choice of Unit Cell

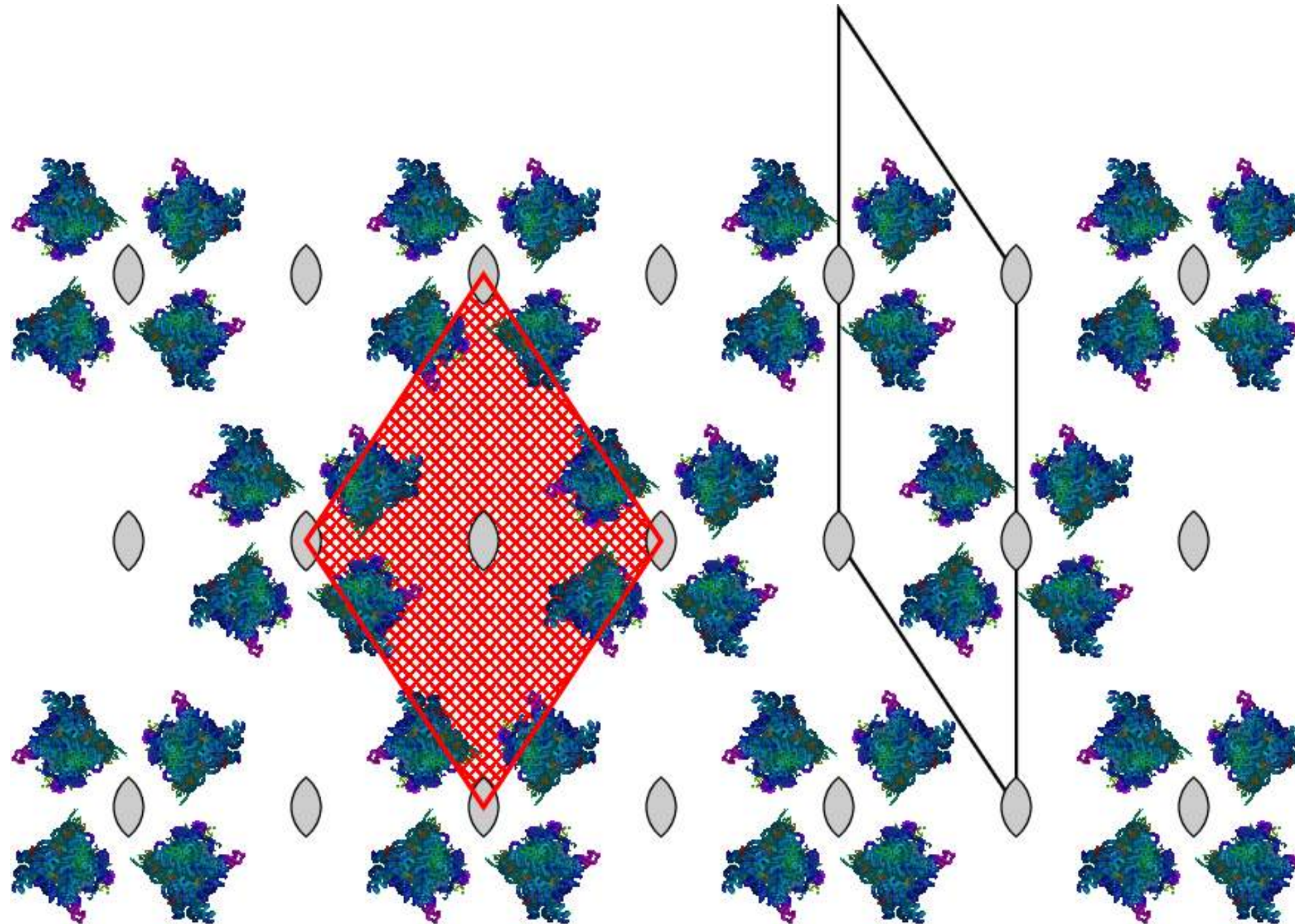


- Place origin of unit cell with position of one of the symmetry elements: simplifies matrix description:

$$(x'y'z') = R(xyz)$$

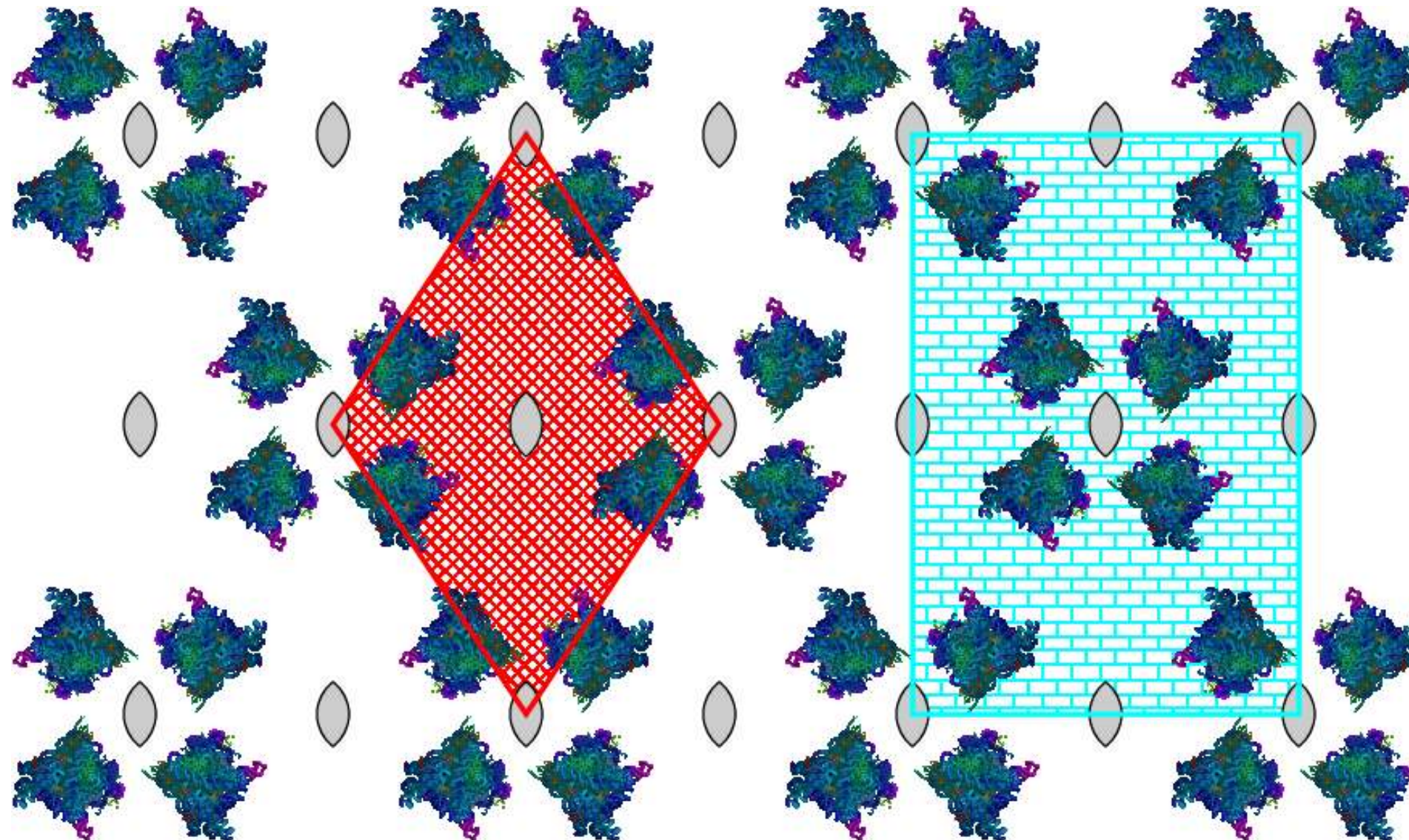


## Choice of Unit Cell



Every crystal possesses a unit cell with no symmetry element *inside* the cell.  
This unit cell is named the **primitive cell**.

## Choice of Unit Cell



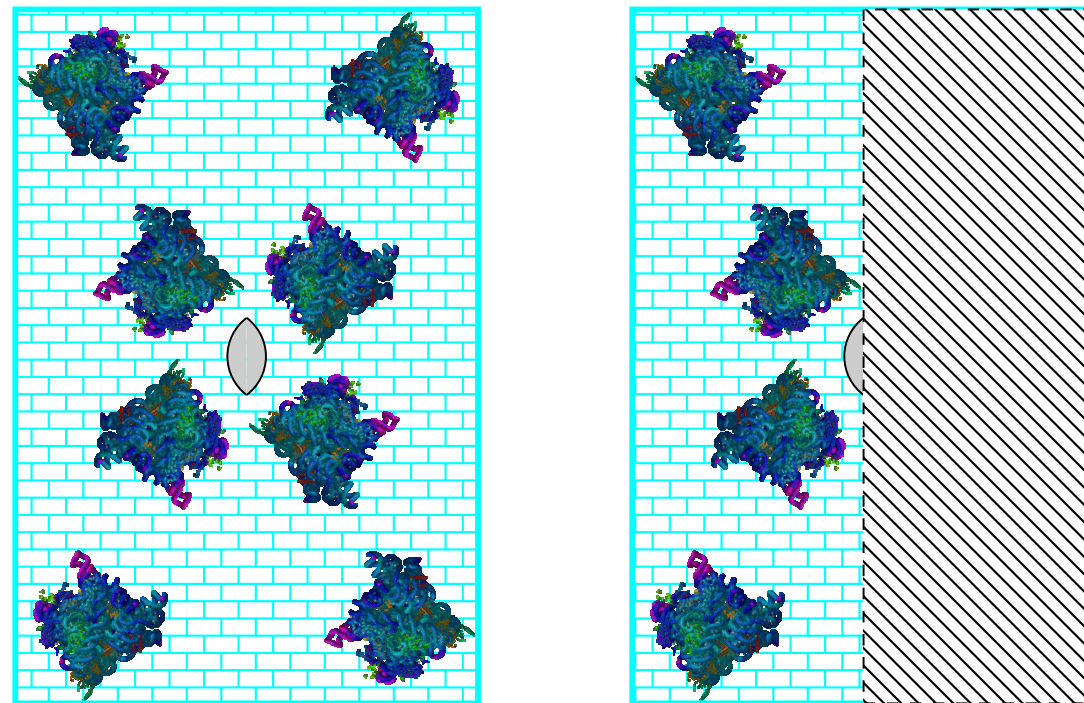
- The **primitive cell** does not necessarily reflect the crystal symmetry
- here: 2-fold axes, but angles  $\neq 90^\circ$
- By convention: choose as unit cell the smallest cell which reflects the symmetry

Example: trigonal (3-fold rotation axis) or hexagonal (6-fold rotation axis) system has conventionally: stets

$$\gamma = 120^\circ$$

## Asymmetric unit

The unit cell is the smallest box that creates the entire crystal solely by integer translations.



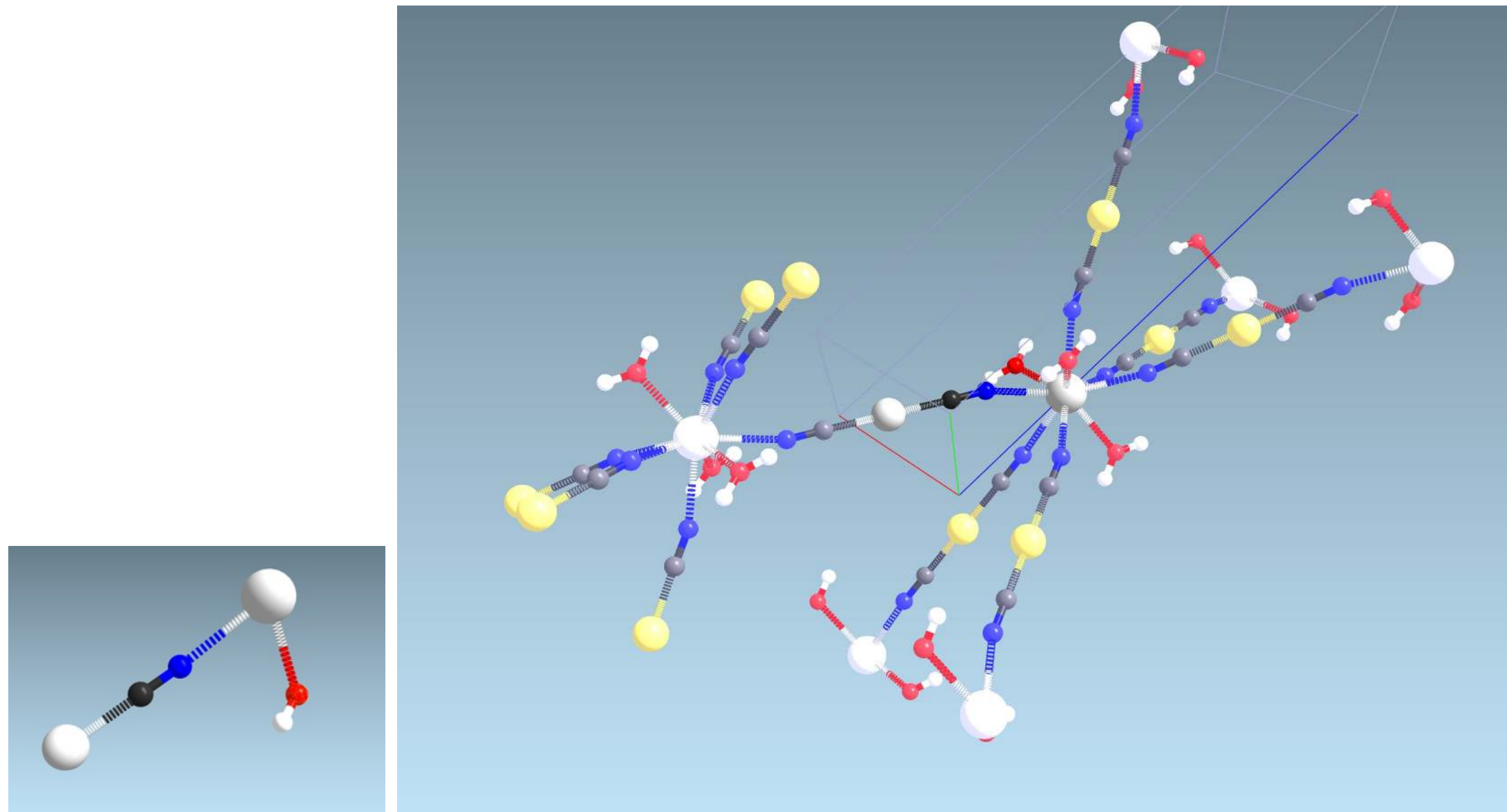
The **asymmetric unit** is the smallest box that creates the entire crystal from integer translations and all symmetry operations of the space group.

All atoms and molecules inside the asymmetric unit are independent from each other and never symmetry related

Crystallography determines the atom positions only inside the unit cell. Everything else is derived.

**Example:**  $La[Au(CN)_2]_3 \cdot 3H_2O$ , **Space group:**  $P6_3/mcm$ 

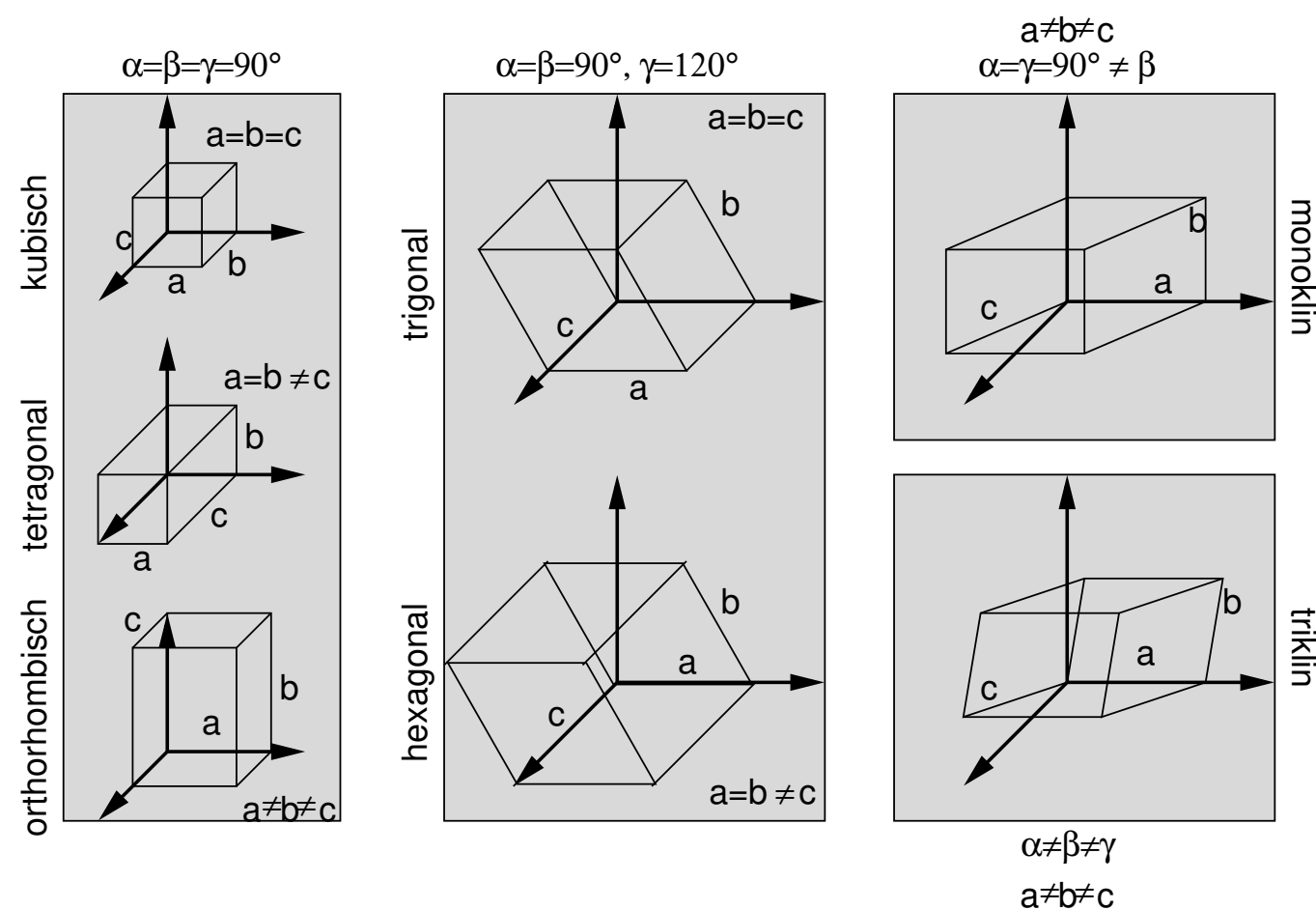
The asymmetric unit does not always make chemical sense:



(J. C. F. Colis *et al.*, *Structural studies of lanthanide ion complexes of pure gold, pure silver and mixed metal (gold-silver) dicyanides* Dalton Trans. (2005), S. 675–679)

# 7 crystal systems

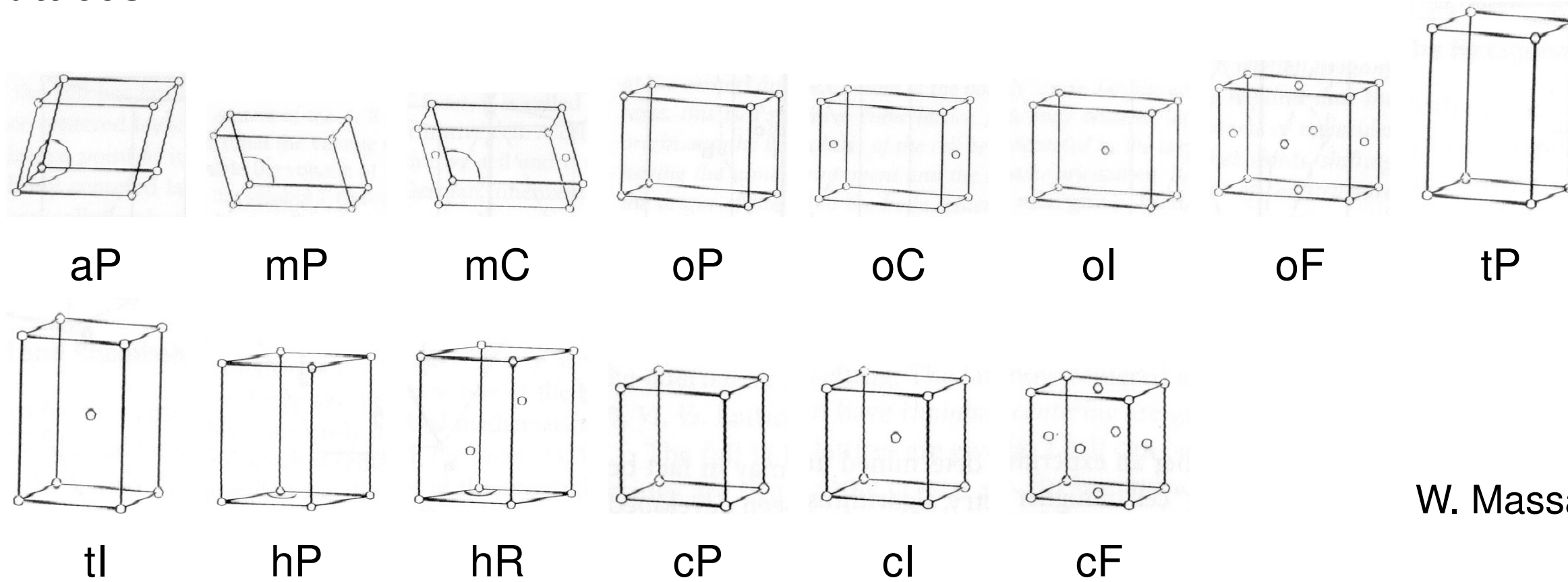
Independently from the content of the unit cell, the unit cell parameters  $a, b, c, \alpha, \beta, \gamma$ , can be classified according to regularity. These classifications result in the **seven crystal systems**



System		Conditions lengths	Conditions angles
triclinic	a	none	none
monoclinic	m	none	$\alpha = \gamma = 90^\circ$
trigonal	h	$a = b = c$	$\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$
hexagonal	h	$a = b$	$\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$
orthorhombic	o	none	$\alpha = \beta = \gamma = 90^\circ$
tetragonal	t	$a = b$	$\alpha = \beta = \gamma = 90^\circ$
cubic	c	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$

# 14 Bravais lattices

7 crystal systems plus the requirement that the unit cell reflects the symmetry results in **14 Bravais lattices**:



W. Massa

Dots: Positions of symmetry elements

## 14 Bravais lattice — naming conventions

- lower case letters (a, m, h, o, t, c): crystal system (shape of cell).
- upper case letters (P, C, F, I, R): Symmetry. They present positions of symmetry elements within the unit cell in addition to the unit cell corners.

**P** primitiv, symmetry elements only at corners

**C** C-centred: Symmetry element at centre of C-faces (spanned by  $\vec{a}$  and  $\vec{b}$ ); (correspondingly: A- and B)

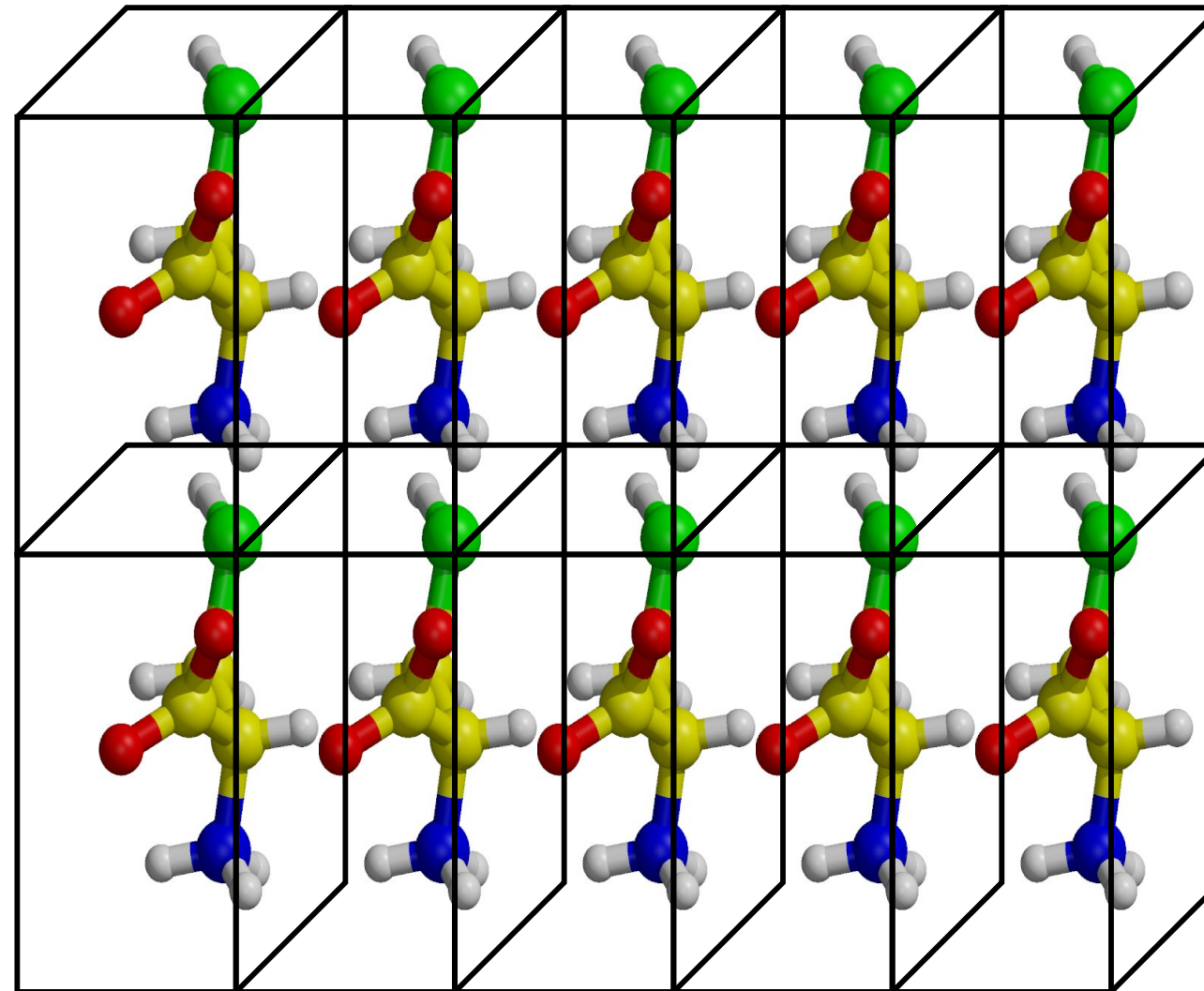
**F** face centred (centred at each face)

**I** body centred: at the centre of the cell (German: innenzentriert)

**R** rhomboedral

## Crystal system $\neq$ Space group

Do not draw conclusions on the space group from the shape of the unit cell: the unit cell **also** depends on the cell content.



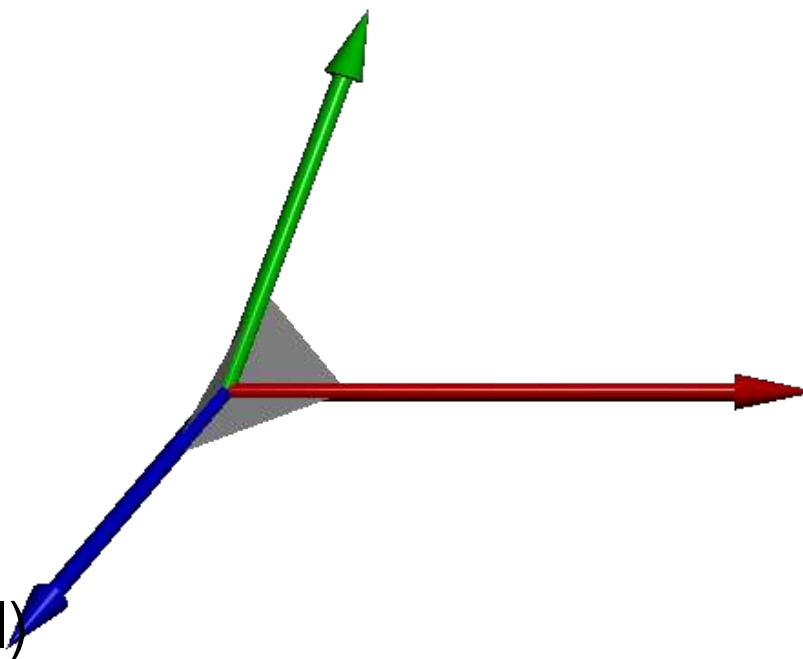
orthorhombic box, non-symmetric space group



## Positions and naming of unit cell axes: Conventions

- The origin (0,0,0) is placed at a position of high symmetry. If present, it is placed at a centre of inversion
- There are  $6 \times 4 \times 2 = 48$  possibilities to name the axes as  $\vec{a}$ ,  $\vec{b}$ , und  $\vec{c}$
- Conventions:
  1. right-handed coordinate system
  2. highest possible symmetry
  3. small as possible volume of unit cell
  4.  $a \leq b \leq c$

(see e.g. <http://xrayweb.chem.ou.edu/notes/symmetry.html>)



## Axis settings and Re-indexing

- Despite these conventions, some space groups still have several possible axis settings
- when two data sets or more are collected, care must be taken to index both consistently
- Example: trigonal space group P3

!!! WARNING !!! SOLUTION MAY NOT BE UNIQUE.

UNIT\_CELL\_A-AXIS= -140.027 -180.486 -28.163

UNIT\_CELL\_B-AXIS= 188.097 21.258 -130.933

UNIT\_CELL\_C-AXIS= 123.664 -120.609 158.073

UNIT\_CELL\_A-AXIS= 188.097 21.258 -130.933

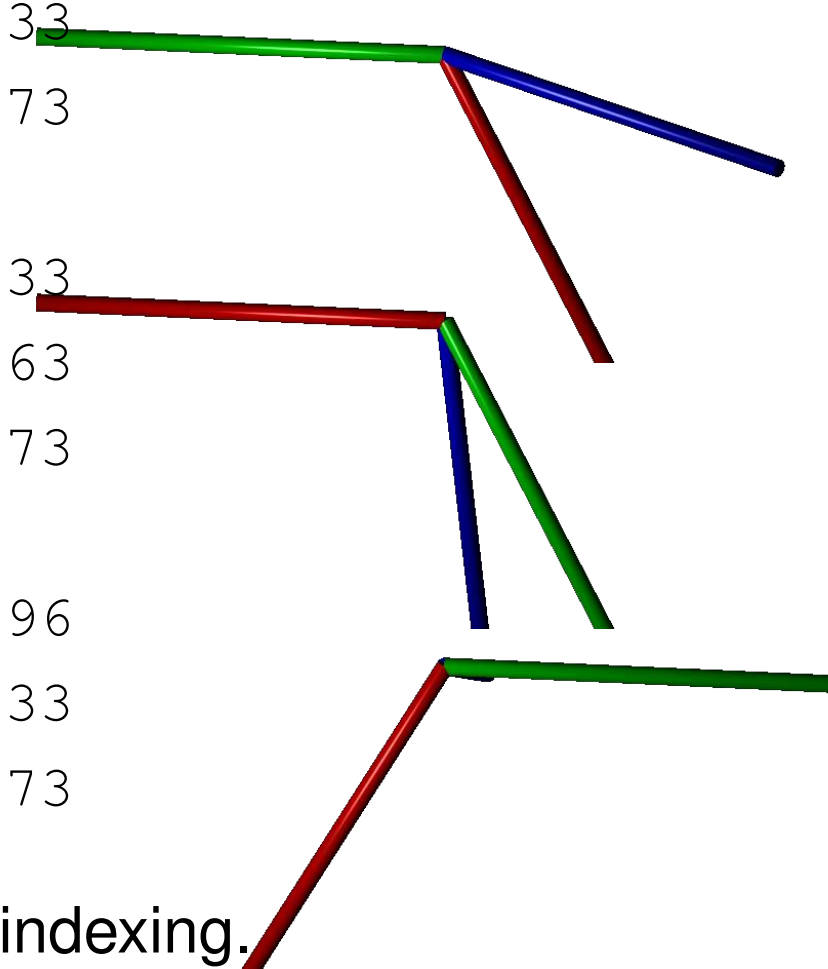
UNIT\_CELL\_B-AXIS= -140.027 -180.486 -28.163

UNIT\_CELL\_C-AXIS= -123.664 120.609 -158.073

UNIT\_CELL\_A-AXIS= 48.070 -159.228 -159.096

UNIT\_CELL\_B-AXIS= -188.097 -21.258 130.933

UNIT\_CELL\_C-AXIS= -123.664 120.609 -158.073



- Modern programs automatically take care of consistent indexing.

## Axis settings and Re-indexing

- Single data set: choice of axis settings is irrelevant, each one is equally good
- Several data sets: with “wrong” settings, intensities do not match weil unterschiedlich indiziert
- either from the same crystal or different crystal
- re-indexing of second data set required in order to match intensities of the first one → **Ums-tellung der Achsen notwendig.**
- Worst case: testing of all possibilities
- Already mentioned: automated in modern software

# Symmetry and X-ray data

## Overview

- Effect of symmetry on X-ray data
- Friedel's law
- Laue groups: point groups in reciprocal space

## Note: Calculation of reflex intensities

Once the chemical composition *i.e. atom types and their positions*, of the asymmetric unit is known, one can calculate the electron density  $\rho(x, y, z)$ .

The intensity of every reflection can be calculated from the electron density  $\rho(x, y, z)^2$

$$I(hkl) = \left| \int_{V(\text{u.c.})} \rho(x, y, z) e^{2\pi i(hx+ky+lz)} d^3x \right|^2$$

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<sup>2</sup>International Tables Volume B, Ch. 1.2

## Symmetry in reciprocal space

Reminder: A symmetry operation  $(R, \vec{t})$  leaves the entire crystal, and in particular the unit cell, unchanged, *i.e.* for every point in the unit cell:

$$\rho(R\vec{x} + \vec{t}) = \rho(\vec{x}) \text{ "u.c."} = R \cdot \text{ "u.c."} + \vec{t}$$

This translates towards the intensities:

$$\begin{aligned} \Rightarrow I(hkl) &= \left| \int_{V(\text{u.c.})} \rho(x, y, z) e^{2\pi i(hx + ky + lz)} d^3x \right|^2 \\ &= \left| \int_{V(\text{u.c.})} \rho(R\vec{x} + \vec{t}) e^{2\pi i(\vec{h}^T (R\vec{x} + \vec{t}))} d^3(R\vec{x} + \vec{t}) \right|^2 \\ &= I(R^T \vec{h}) \end{aligned}$$

(The last step include quite some calculations)

This means: The intensities of the two reflections  $(h, k, l)$  and  $R(h, k, l)$  are identical.

## Symmetry in reciprocal space

For every symmetry operation  $(R, \vec{t})$  of the space group of a crystal:

$$I(\vec{h}) = I(R^T \vec{h}) = I(R^T R^T \vec{h}) = \dots$$

- Crystal symmetry also means symmetry for the reflections
- Translational symmetry is “dropped” in reciprocal space

## Friedel's Law

Even without any symmetry, *i.e.* in all space groups including  $P1$ :

$$I(h, k, l) = I(\bar{h}, \bar{k}, \bar{l})$$

Reciprocal space **always** has a centre of inversion. This is called Friedel's law<sup>3</sup>

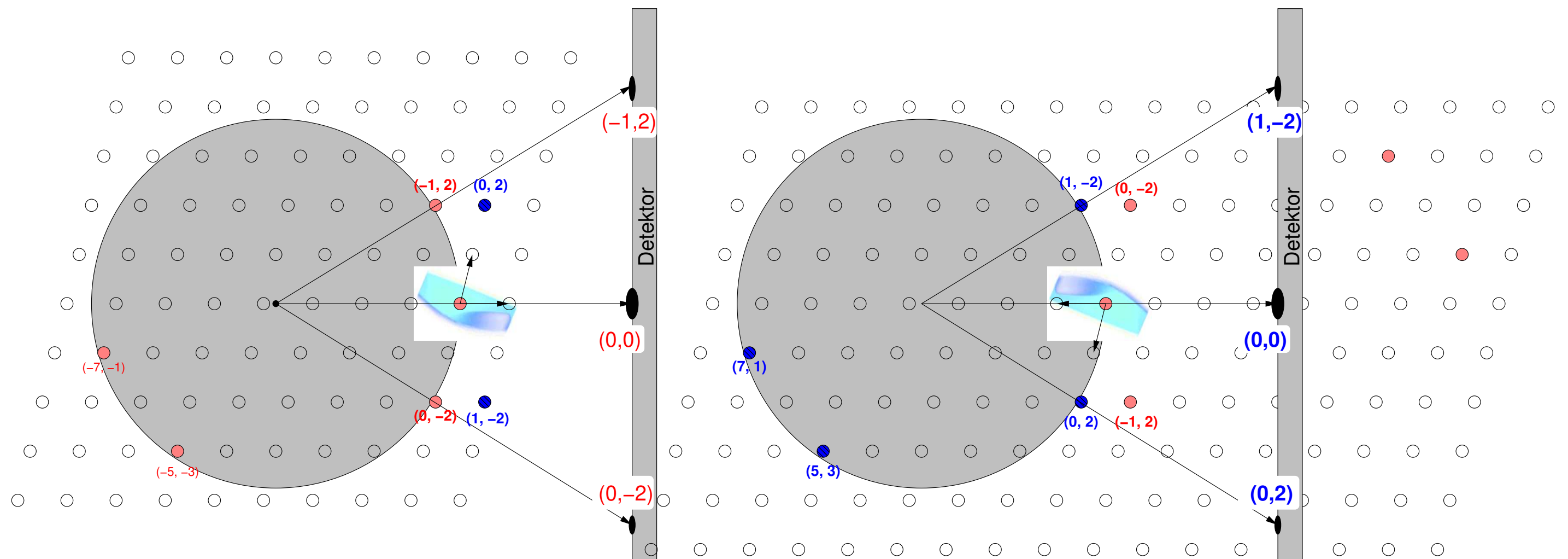
$$\begin{aligned}
 I(\bar{h}\bar{k}\bar{l}) &= \left| \int_{V(\text{E.Z.})} \rho(x, y, z) e^{2\pi i(\bar{h}x + \bar{k}y + \bar{l}z)} d^3x \right|^2 \\
 &= \left| \int_{V(\text{E.Z.})} \rho(x, y, z) e^{-2\pi i(hx + ky + lz)} d^3x \right|^2 \\
 &= \int_{V(\text{E.Z.})} \rho(x, y, z) e^{-2\pi i(hx + ky + lz)} d^3x * \left( \int_{V(\text{E.Z.})} \rho(x, y, z) e^{-2\pi i(hx + ky + lz)} d^3x \right)^* \\
 &= \int_{V(\text{E.Z.})} \rho(x, y, z) e^{-2\pi i(hx + ky + lz)} d^3x * \int_{V(\text{E.Z.})} \rho(x, y, z) e^{2\pi i(hx + ky + lz)} d^3x \\
 &= \left| \int_{V(\text{E.Z.})} \rho(x, y, z) e^{2\pi i(hx + ky + lz)} d^3x \right|^2 \\
 &= I(hkl)
 \end{aligned}$$

<sup>3</sup>Georges Friedel, 1865–1933

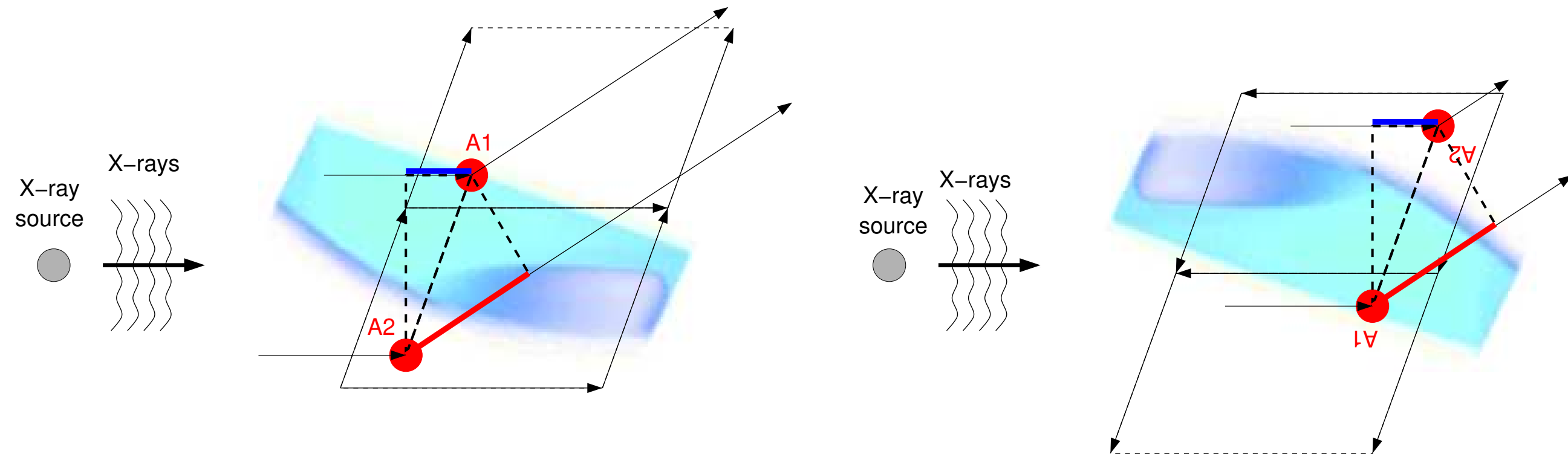


# Measurement of Friedel pairs

Two reflections  $I(hkl)$  and  $I(\bar{h}\bar{k}\bar{l})$  form a **Friedel pair**. They can be measured e.g. by rotation the crystal by  $180^\circ$



# Phase difference of Friedel pairs



$$\Delta_{\text{left}} = -\Delta_{\text{right}}$$

$$\Rightarrow \delta_{\text{left}} = -\delta_{\text{right}}$$

( $\delta = 2\pi\Delta/\lambda$  :) negative phase, same path difference

since cos symmetric:

$$\cos(\delta_{\text{left}}) = \cos(-\delta_{\text{right}}) = \cos(\delta_{\text{right}})$$

no difference in total intensity

## Laue groups

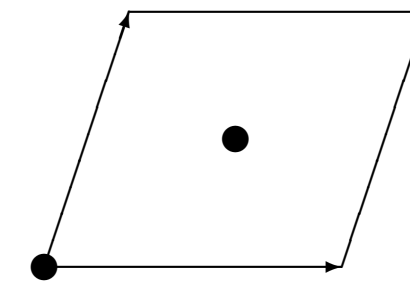
- Crystals belong to one of 230 space groups
- The diffraction pattern contains the symmetry of the space group, but:
  1. no translational component
  2. always centre of inversion (Friedel's law)
- This results in a subset of groups: the 11 **Laue groups**.

# 11 Laue groups

Crystal system	Laue group	point group
Triclinic	$\bar{1}$	1, $\bar{1}$
Monoclinic	$2/m$	2, m, $2/m$
Orthorhombic	$mmm$	222, $mm2$ , $mmm$
Tetragonal	$4/m$	4, $\bar{4}$ , $4/m$
	$4/mmm$	422, $4mm$ , $\bar{4}2m$ , $4/mmm$
Trigonal	$\bar{3}$	3, $\bar{3}$
	$\bar{3}m$	32, $3m$ , $\bar{3}m$
Hexagonal	$6/m$	6, $\bar{6}$ , $6/m$
	$6/mmm$	622, $6mm$ , $\bar{6}m2$ , $6/mmm$
Cubic	$m\bar{3}$	23, $m\bar{3}$
	$m\bar{3}m$	432, $\bar{4}3m$ , $m\bar{3}m$

<http://de.wikipedia.org/wiki/Lauegruppe>

# Extinctions



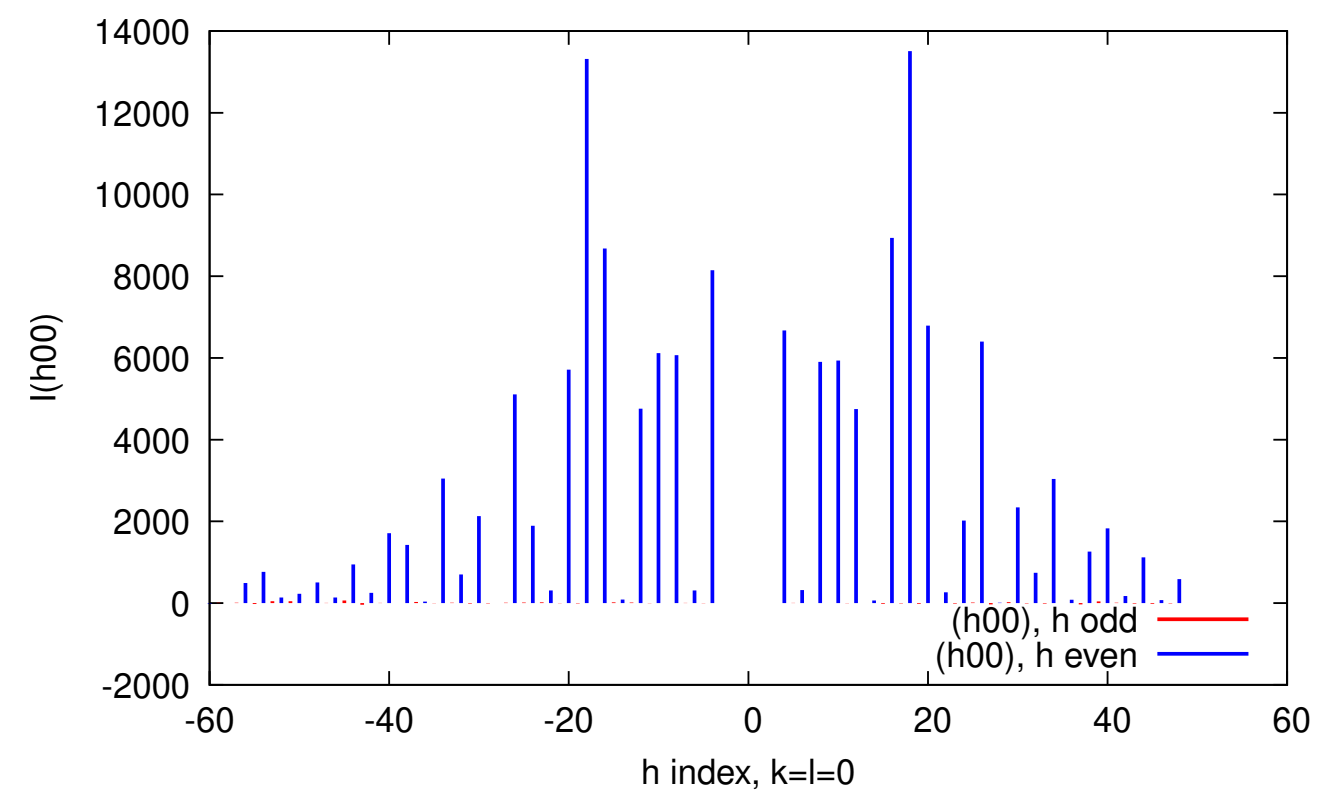
- Extinctions are reflections with systematically zero intensity.
- Extinctions occur in non-primitive Bravais lattices or in the presence of symmetry elements with translational part, *i.e.* glide planes and screw axes.
- Extinctions are important for space group determination, *e.g.* to differentiate between  $P4$  and  $P4_3$ .
- The “Int. Tabl. Vol. A” list the “general reflection conditions”, *i.e.* those reflections with non-zero intensity:

$P3_1$  (No. #144)  $00l : l = 3n$

- only if  $(hkl) = \dots(00 - 6), (00 - 3), (003), \dots$ : Intensities  $\neq 0$ ;
- reflections  $(001), (002), (004), (005), \dots$ , should have zero intensity

## Example: Extinctions in $P4_32_12$

- Reflection condition:  $h00 : h = 2n$  and  $00l : l = 4n$
- Only reflections with  $k = 0, l = 0$  and  $h$  even should have non-zero intensity
- All reflections with  $k = 0, l = 0$  and  $h$  odd should have zero intensity
- Example: Lysozyme data set



## Example: Extinctions in $P4_32_12$

Output from the program `xprep` for Lysozyme data:

Systematic absence exceptions:

41/43	42	n--	-b-	-c-	-n-	-21-	--c		
N	5	3	3490	2365	2359	2358	89	1549	
N I>3s	0	0	2188	1256	1361	1275	0	931	
<I>	0.9	0.9	97.0	64.6	80.7	65.4	0.8	85.0	
<I/s>	0.2	0.2	8.2	6.7	7.3	6.6	0.4	7.5	

Identical indices and Friedel opposites combined before calculating R(sym)

Option	Space Group	No.	Type	Axes	CSD	R(sym)	N(eq)	Syst. Abs.	CFOM
[A]	P4(1)2(1)2	# 92	chiral	1	245	0.067	140065	0.4 / 6.6	1.99
[B]	P4(3)2(1)2	# 96	chiral	1	245	0.067	140065	0.4 / 6.6	1.99

Based on the data alone, we cannot distinguish between  $P4_12_12$  and  $P4_32_12$  (due to Friedel's law). One has to solve the structure and see which one makes sense. For protein structures: the right space group will consist of L-amino acids, the wrong one of D-amino acids.

## Summary: Space group determination

- Crystal symmetry is present in Reflection data intensities
- No translational symmetry in reciprocal space
- Only one of the 11 Laue groups can be determined from symmetry in intensities
- Systematic absences are important to distinguish between space groups within a Laue group



## Summary today's lecture

- Space groups and crystallographic point groups
- Choice of unit cell
- 7 Crystal systems and 14 Bravais lattices
- Symmetry in reciprocal space
- Space group determination

Next lecture: April 23<sup>rd</sup>