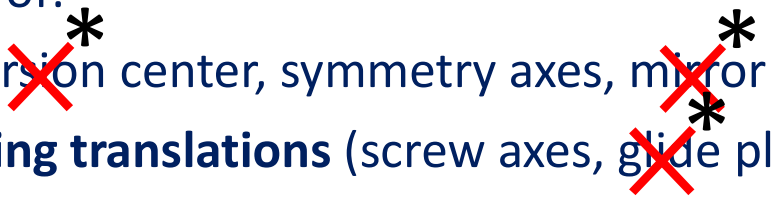
# Space groups

Space groups are a combination of:

- **point group operations** (inversion center, symmetry axes, mirror planes),
- **symmetry operations involving translations** (screw axes, glide planes),
- **centering translations** (base-, face-, body-centering),
- **lattice translations**.



A space group:

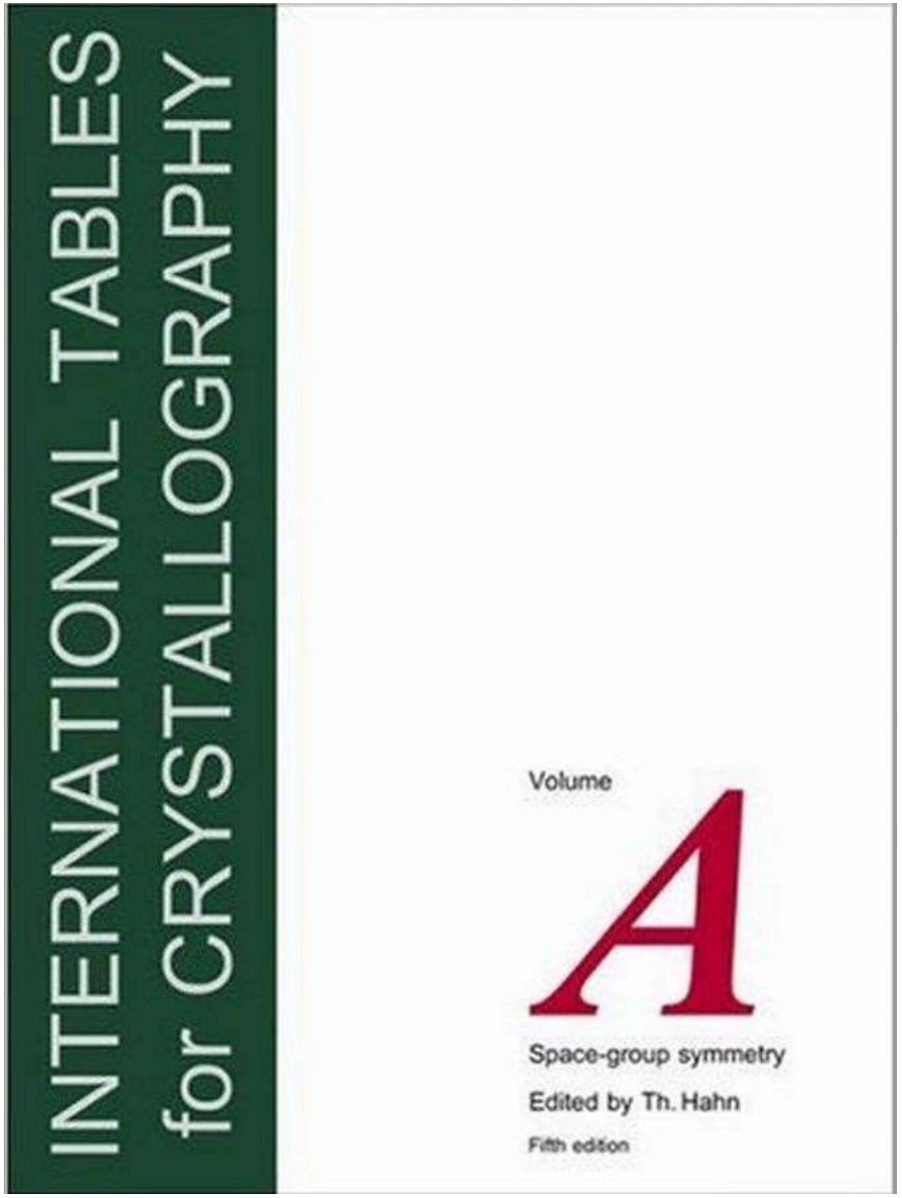
(1) is a **closed** group (combinations of its elements yield the identity transformation),

(2) contains the **identity** transformation,

(3) contains inverse transformations of its elements (**inversion** property),

(4) contains combinations of its elements (**associativity** property).

In 3D, 230 space groups,
but only 65 for protein structures*




# International Tables of Crystallography Volume A

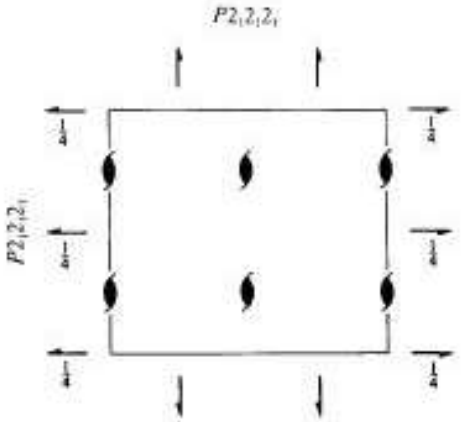
Volume containing information for each of the 230 space groups:

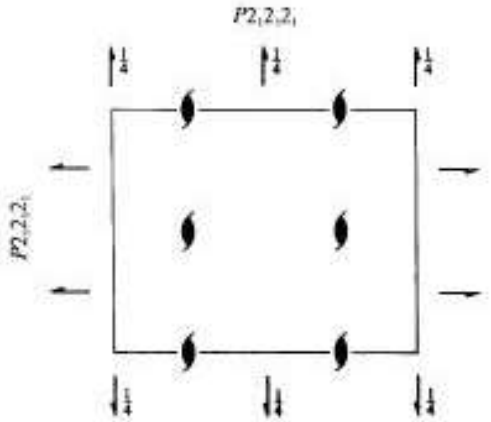
- Symmetry elements and their position
- Origin choice
- General positions and their multiplicity
- Asymmetric unit
- Systematic absences
- ...

$P2_12_12_1$ $D_2^4$ 222 Orthorhombic

No. 19 $P2_12_12_1$ Patterson symmetry $Pmmm$

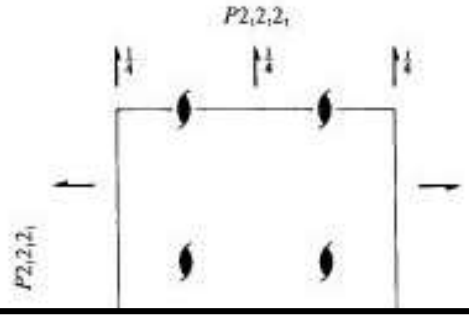
Name: type of lattice (*P*) and symmetry elements along the lattice main axes

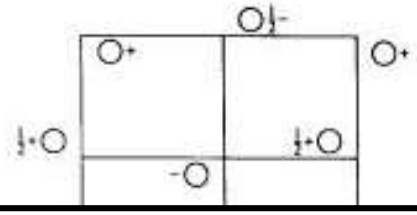




Crystal system and Patterson symmetry

Projections of the unit cell with symmetry elements





**Origin** at midpoint of three non-intersecting pairs of parallel $2_1$ axes

**Asymmetric unit** $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

**Symmetry operations**

(1) 1 (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$

Origin position, asymmetric unit limits in fractional coordinates, symmetry operations

**Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

**Positions**

| Multiplicity, Wyckoff letter, Site symmetry | | Coordinates | | | |
|---|---|---|---|---|---|
| 4 | $a$ 1 | (1) $x,y,z$ | (2) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$ | (3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ | (4) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ |

Symmetry equivalents for a generic point in fractional coordinates

**Reflection conditions**

General:

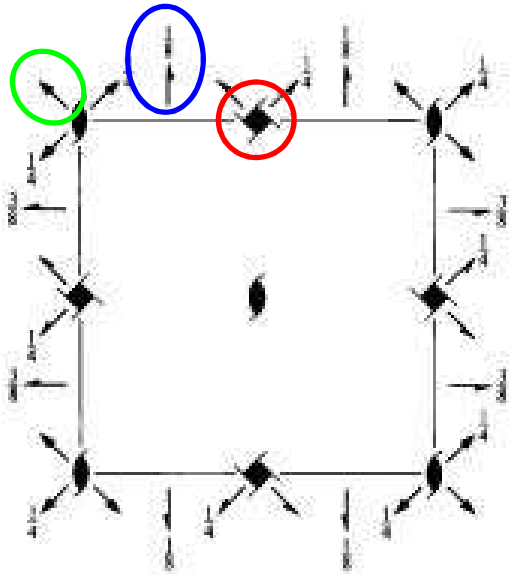
$h00$ : $h = 2n$
$0k0$ : $k = 2n$
$00l$ : $l = 2n$

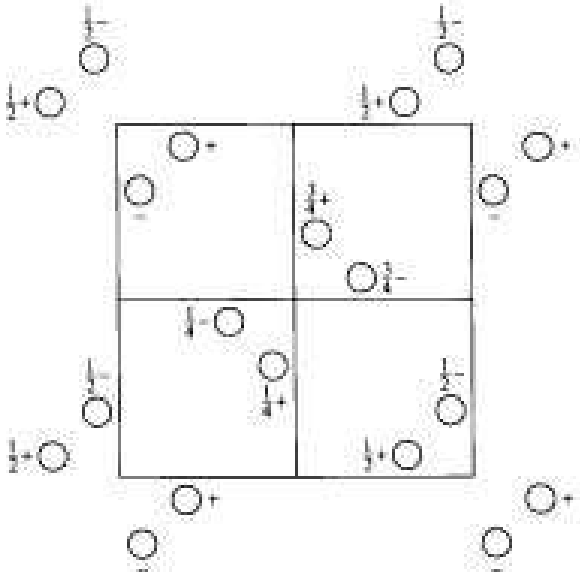
Reflections allowed by systematic absences

*International Tables for Crystallography* (2006). Vol. A, Space group 96, pp. 376–377.

# $P4_32_12$ $D_4^8$ 422 Tetragonal

No. 96 $P4_32_12$ Patterson symmetry $P4/mmm$





**Origin** on $2\,[1\,1\,0]$ at $2_1\,1\,(1,2)$

**Asymmetric unit** $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{8}$

**Symmetry operations**

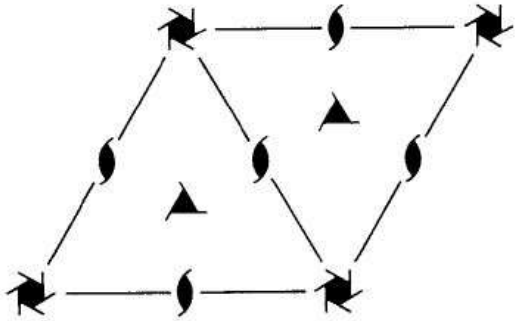
(1) 1
(2) $2(0,0,\frac{1}{2})$ $0,0,z$
(3) $4^+(0,0,\frac{1}{4})$ $0,\frac{1}{2},z$
(4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{8}$
(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{8}$
(7) $2$ $x,x,0$
(8) $2$ $x,x,\frac{1}{4}$

# Enantiomorphic space groups

Enantiomorphic space groups, with screw axis in opposite directions:

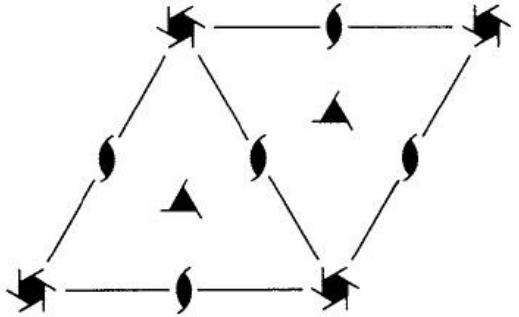
$P6_1$ $C_6^2$

No. 169 $P6_1$



$P6_5$

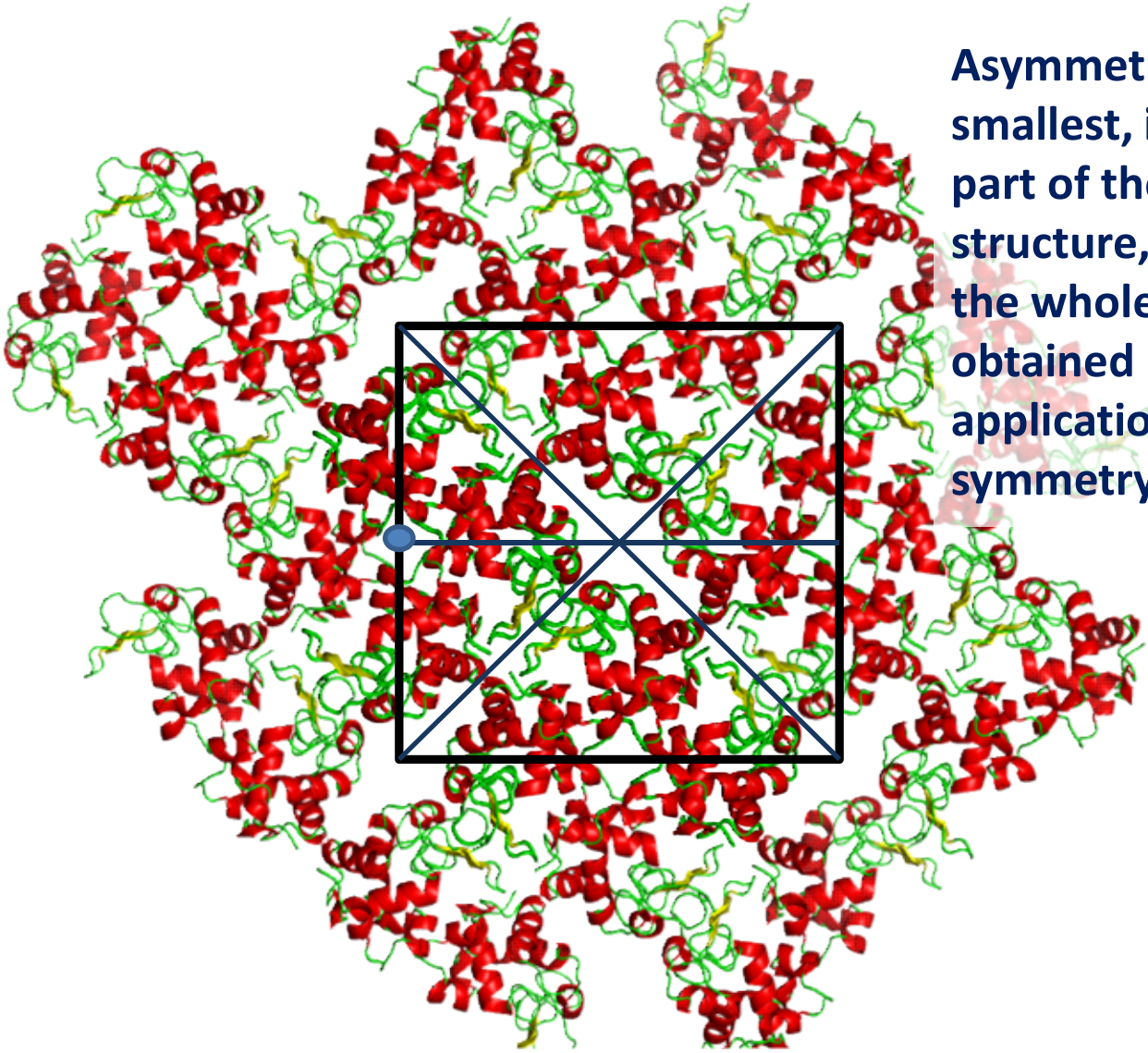
No. 170



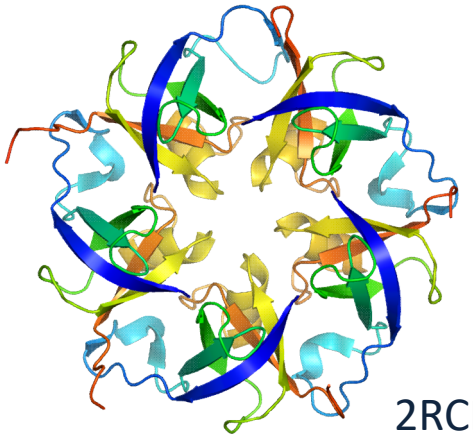
Enantiomorphic pairs:
(tetragonal) *P* $4_1$ and *P* $4_3$, *P* $4_1$ *2 2* and *P* $4_3$ *2 2*, *P* $4_1$ $2_1$ *2* and *P* $4_3$ $2_1$ *2*, *I* $4_3$ *2 2*, ...
(hexagonal) *P* $3_1$ and *P* $3_2$ , *P* $3_1$ *2 1* and *P* $3_2$ *2 1* , *P* $3_1$ *1 2* and *P* $3_2$ *1 2*, *P* $6_1$ and *P* $6_5$ , *P* $6_1$ *2 2* and *P* $6_5$ *2 2* , *P* $6_2$ and *P* $6_4$ , *P* $6_2$ *2 2* and *P* $6_4$ *2 2*
(cubic) *P* $4_1$ *3 2* and *P* $4_3$ *3 2.*

# Asymmetric unit

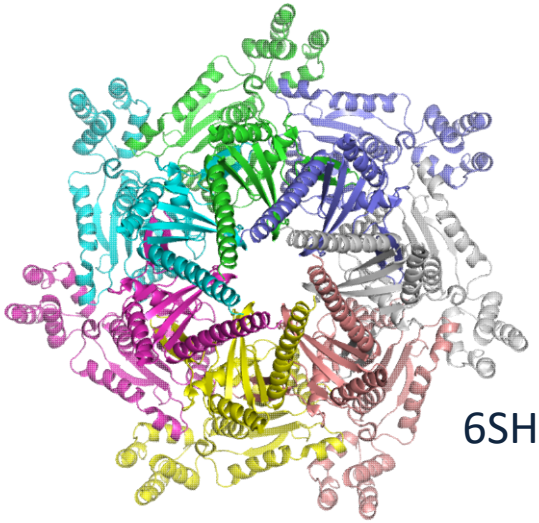
**Lysozyme** (pdb: 193L):
tetragonal lattice, space group $P\,4_3\,2_1\,2$, unit cell $a$ = 78.54 Å, $c$ = 37.77 Å



**Asymmetric units: smallest, independent part of the crystals structure, from which the whole structure is obtained upon application of the symmetry operations**



2RCF



6SH4

# Non-crystallographic symmetry

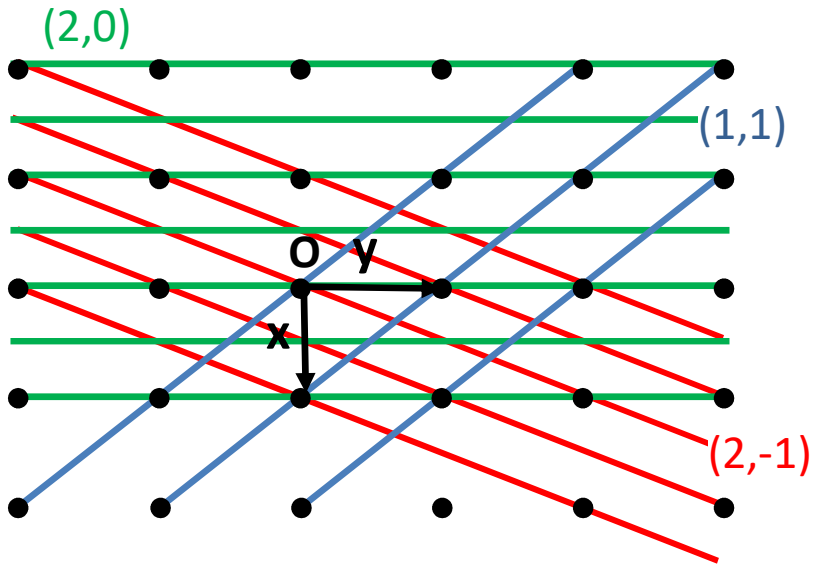
Besides the symmetry elements of the space group, other symmetry elements may occur in a crystal structure, including symmetry elements not allowed by the lattice periodicity (e.g. 5-fold axes, 7-fold axes, ...).

They are called Non-Crystallographic Symmetry (NCS).

Two protein chains related by NCS are crystallographically independent and both belong to the asymmetric unit. Usually, NCS is not perfect.

# Miller indices

Crystal lattice: described in the real space (coordinates *x*,*y*,*z*)




In the real space of the crystal lattice, we can define **families of parallel planes**.

To identify this planes, we can use the **Miller indices (h,k)**:

starting from the origin of the lattice and moving in a lattice direction, we can count the number of planes until the next node.

For the blue set of planes: the first Miller index (in *x* direction) is 1, the second is 1.

For the red set of planes: the first Miller index is 2, the second is -1.

For the green set of planes: the first Miller index is 2, the second is 0.

Which of the families has the shorter distance $d$ between planes?

The distance between planes depends on the Miller indices: planes with higher Miller indices have shorter distances.

# From the real to the reciprocal lattice

The **reciprocal lattice** is a mathematical construction, but it is useful to describe diffraction phenomena.

Reciprocal lattice: described in the reciprocal space by the Miller indices (*h*,*k*,*l*).

The origin of the lattice is common to the real lattice.

Direction of the reciprocal lattice base vectors:

$$\boldsymbol{a}^*\boldsymbol{a} = 1,\ \boldsymbol{a}^* \perp \boldsymbol{b},\ \boldsymbol{a}^* \perp \boldsymbol{c}$$

$$\boldsymbol{b}^*\boldsymbol{b} = 1,\ \boldsymbol{b}^* \perp \boldsymbol{a},\ \boldsymbol{b}^* \perp \boldsymbol{c}$$

$$\boldsymbol{c}^*\boldsymbol{c} = 1,\ \boldsymbol{c}^* \perp \boldsymbol{a},\ \boldsymbol{c}^* \perp \boldsymbol{b}$$

A family of planes in real space can be described by a vector $\boldsymbol{d}^*$ in reciprocal space.

The vector $\boldsymbol{d}^*$ is obtained by the combination of the Miller indices and the base vectors of the lattice: $\boldsymbol{d}^* = h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$.

The modulus of $\boldsymbol{d}^*$ is: $d^* = {}^1/_d$ , with $d$ distance between planes of the family in the real space.

***For an orthogonal system (i.e. orthorhombic, tetragonal, cubic):

$$d_{hkl} = \sqrt{\frac{a^2}{h^2} + \frac{b^2}{k^2} + \frac{c^2}{l^2}} \quad \text{and } a^* = {}^1/_a\,, b^* = {}^1/_b\,, c^* = {}^1/_c$$