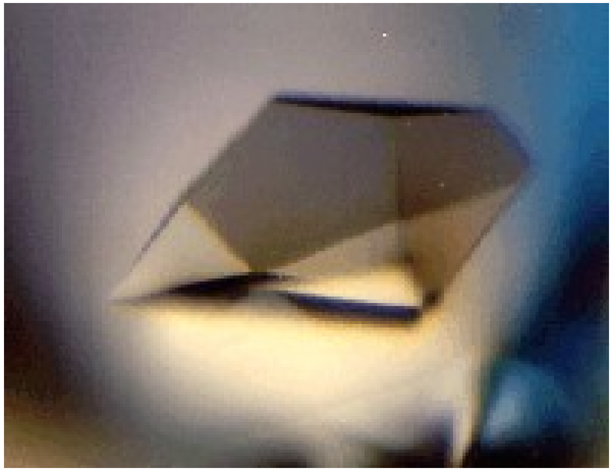
Bioinformatics III

Analysis and prediction of 3D macromolecule structures

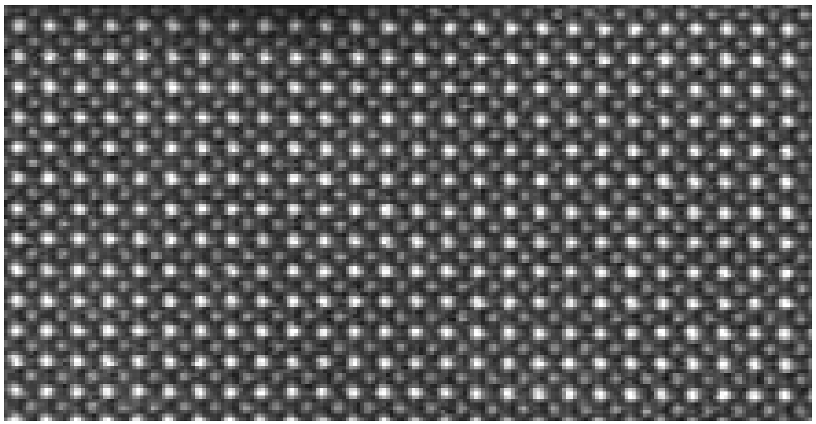
Lecture 8 – symmetry

Saulius Gražulis
2022

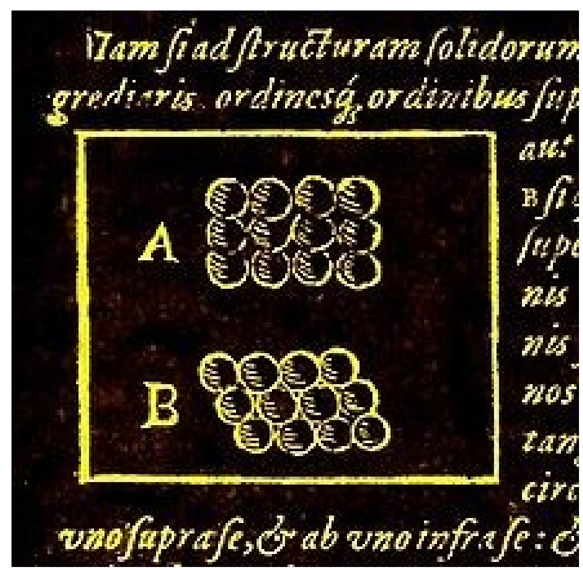
Crystals

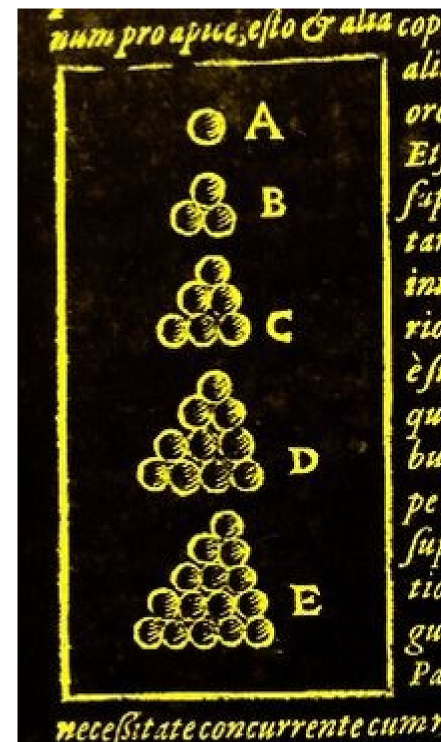


Explanation of crystal shape

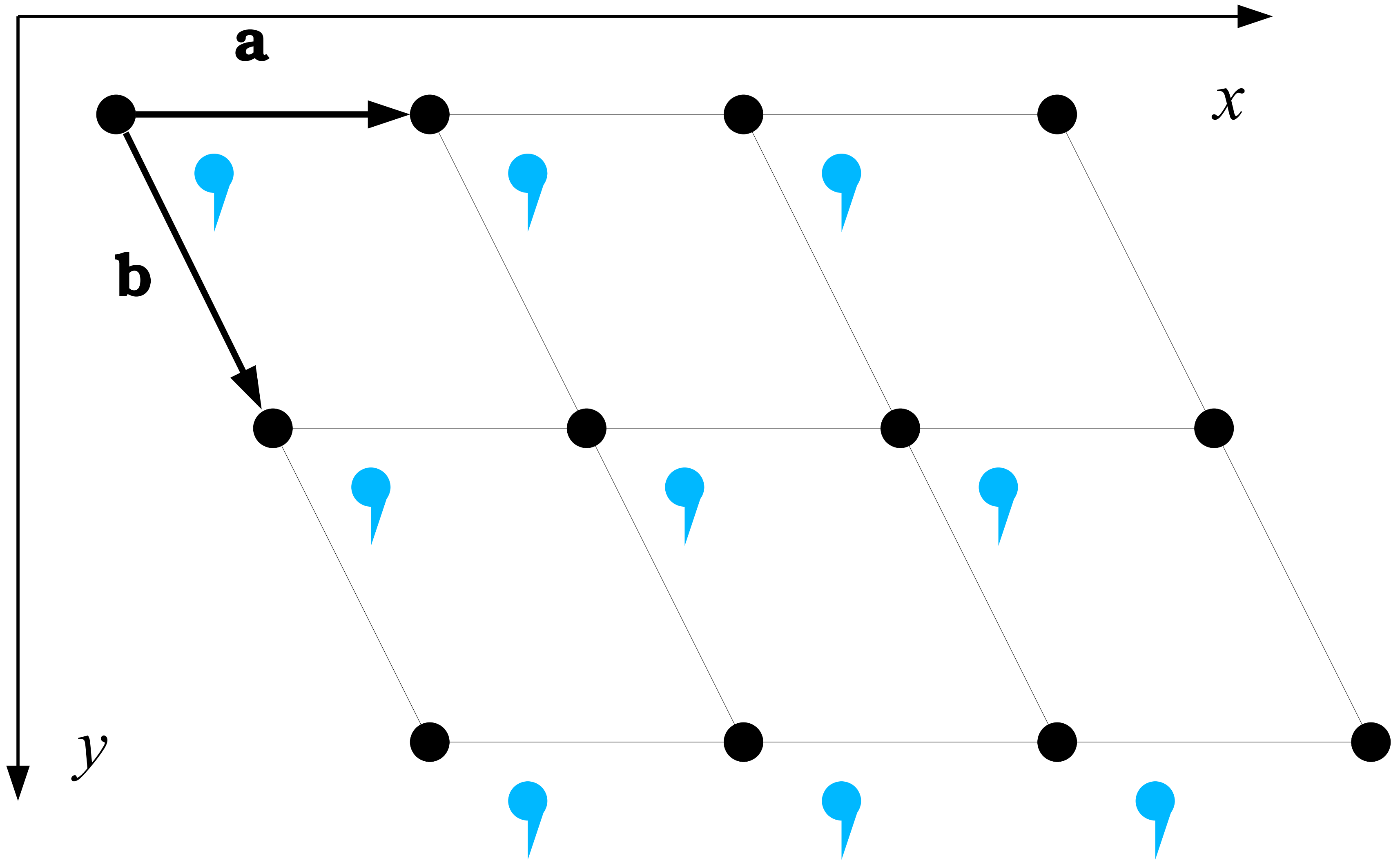


Johannes Kepler 1611 m. „Strena Seu de Nive Sexangula“ (A New Year's Gift of Hexagonal Snow)

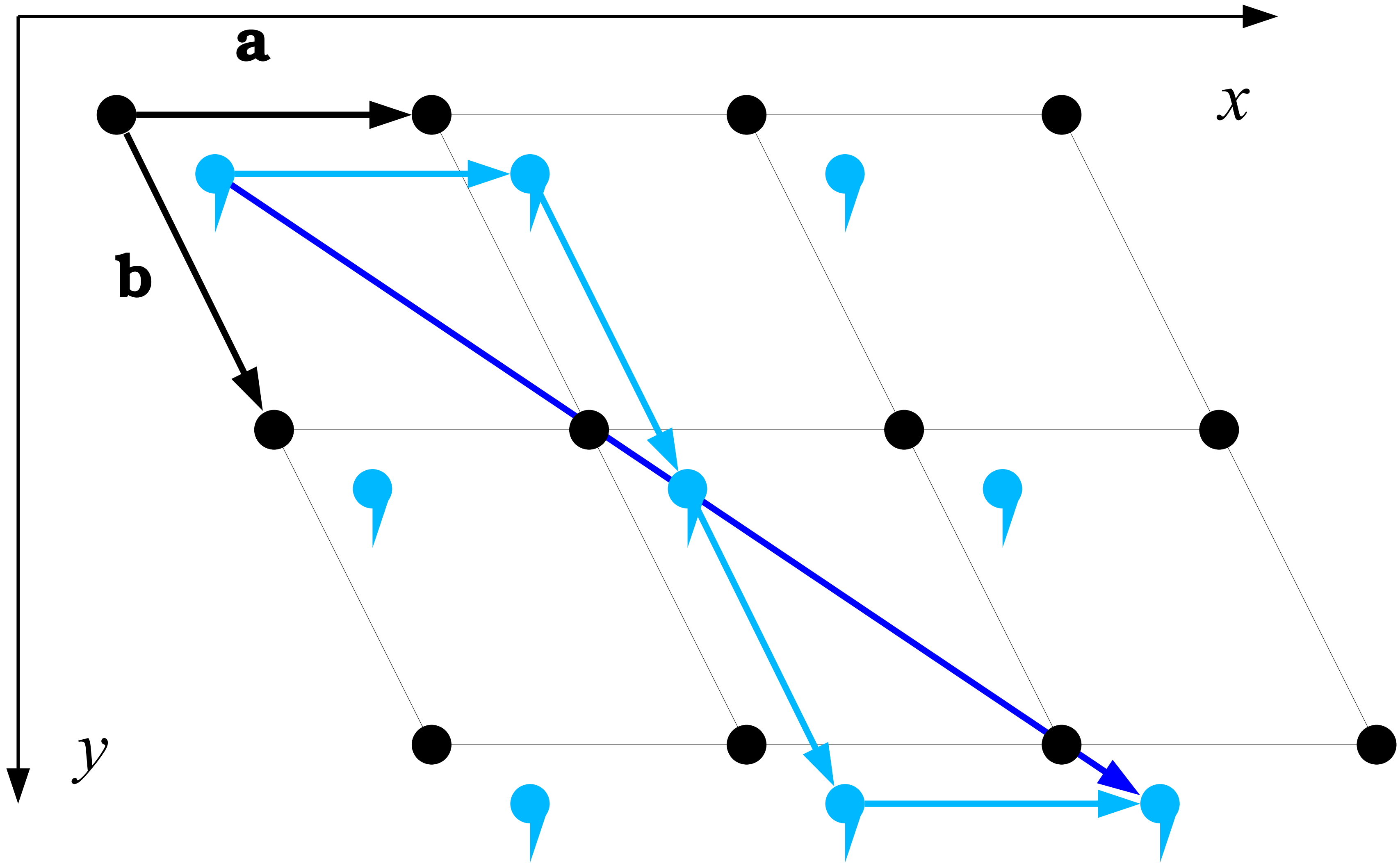




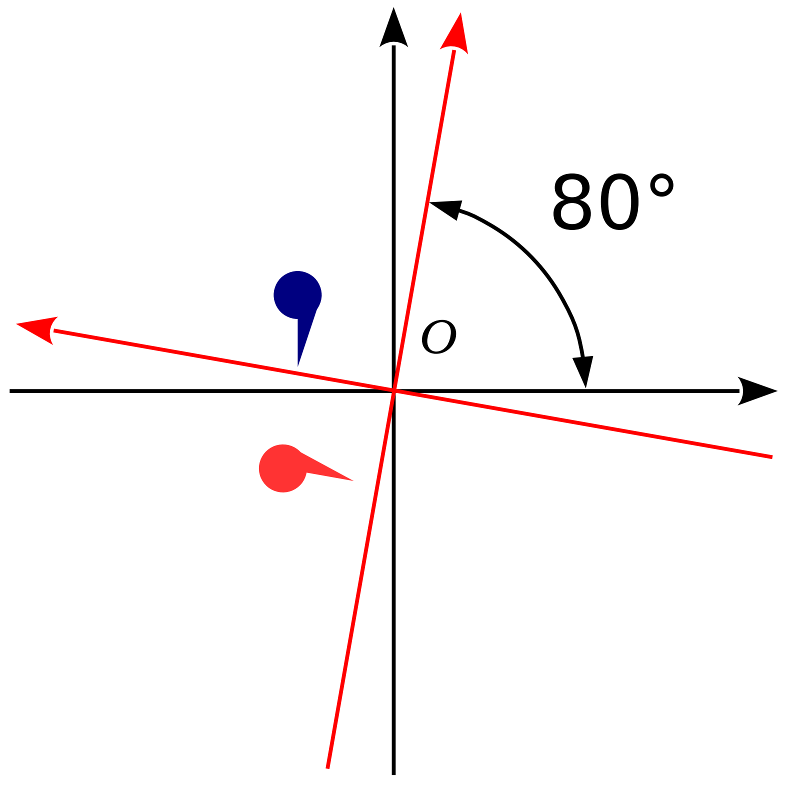
Periodicity and translations



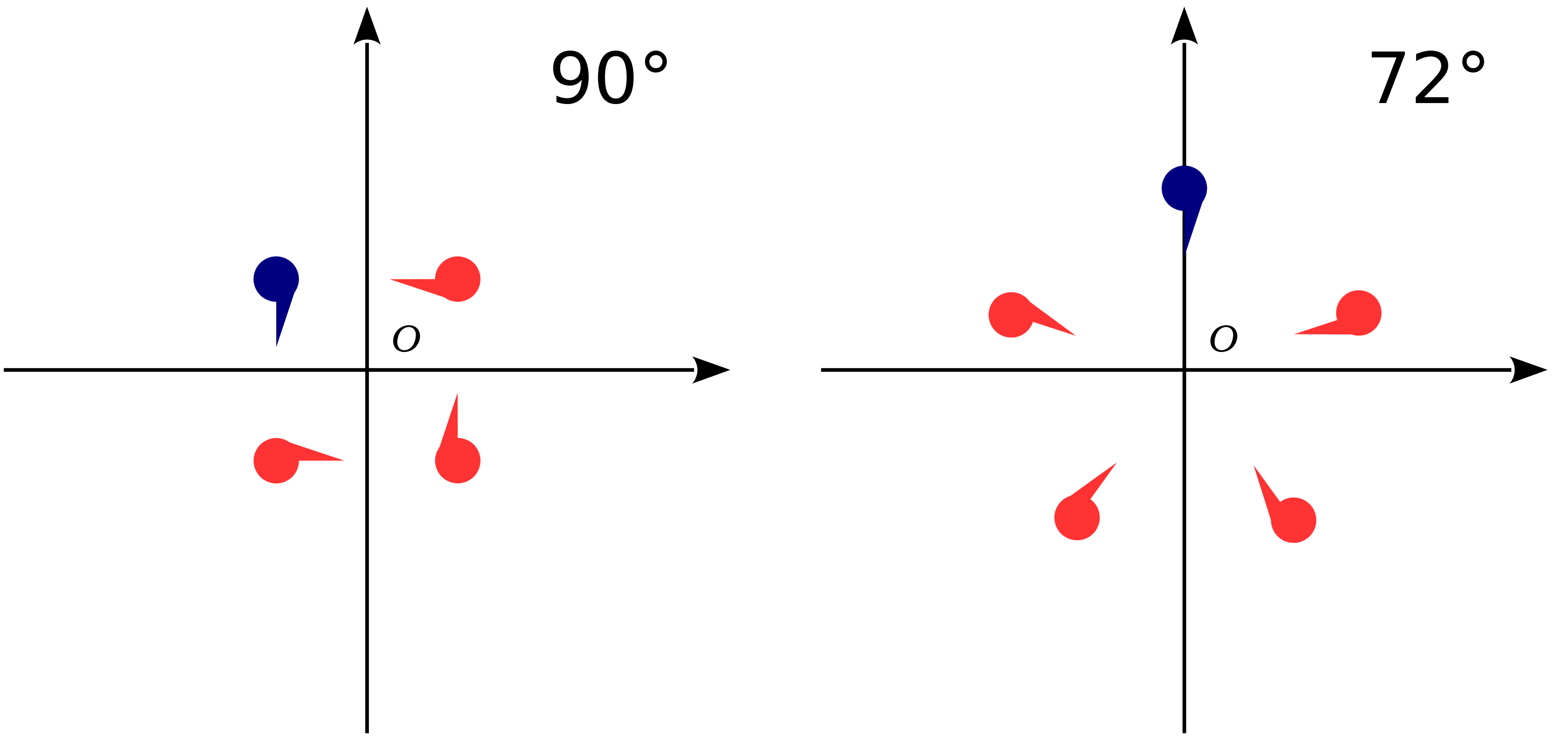
The translation group



Point symmetry elements



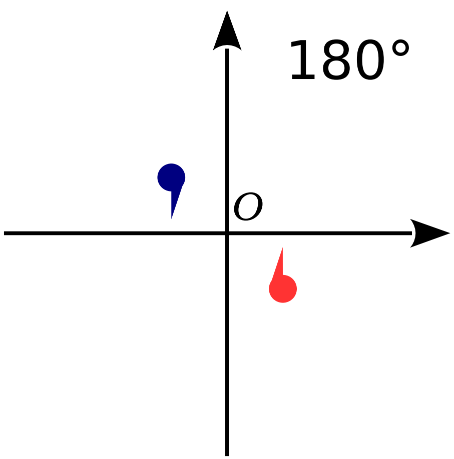
Point groups



Description of symmetry

Coordinates of a general position:

$$-x, -y, z+\frac{1}{2}$$



Rotation matrix + translation

$$\vec{x}' = R\vec{x} + \vec{T}$$

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0.5 \end{bmatrix}$$

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} t_x \\ t_y \\ t_z \end{bmatrix}$$

Combination of symmetry elements

$$\vec{x}' = R\vec{x} + \vec{T}$$

$$\vec{x}'' = R'(R\vec{x} + \vec{T}) + \vec{T}' =$$

$$= R'R\vec{x} + R'\vec{T} + \vec{T}'$$

$$S = R + \vec{T}\,;\, S' = R' + \vec{T}'$$

$$S'S = R'R + (R'\vec{T} + \vec{T}')$$

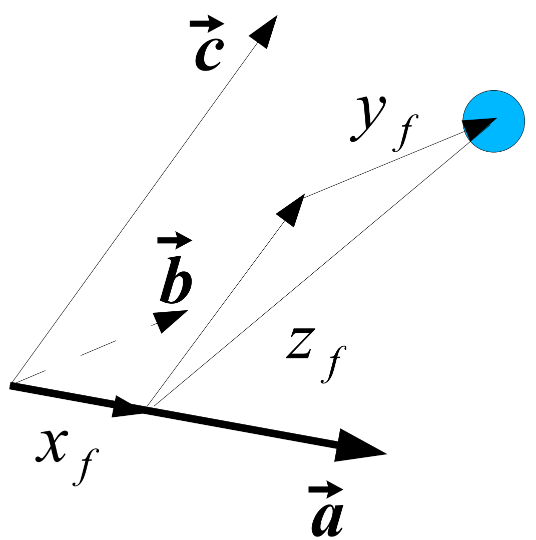
$$R'R = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$-x, -y, z \qquad -x, y, -z \qquad x, -y, -z$$

Coordinates

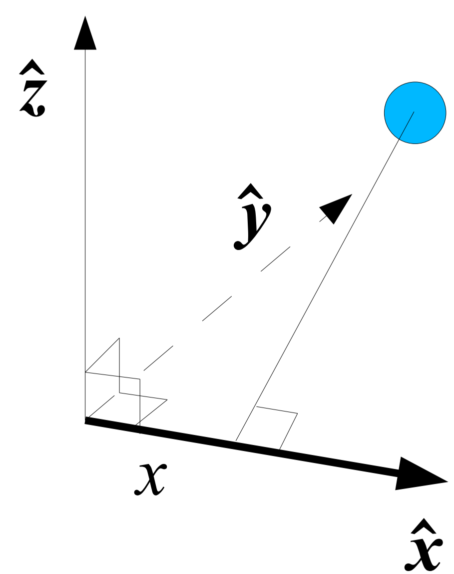
Fractional

(as fractions of unit cell vectors)



Cartesian (orthonormal)

In an orthonormal basis (coordinate system)



Coordinate transformations (Perl)

$$\vec{x}' = R\vec{x} + \vec{T}_o$$

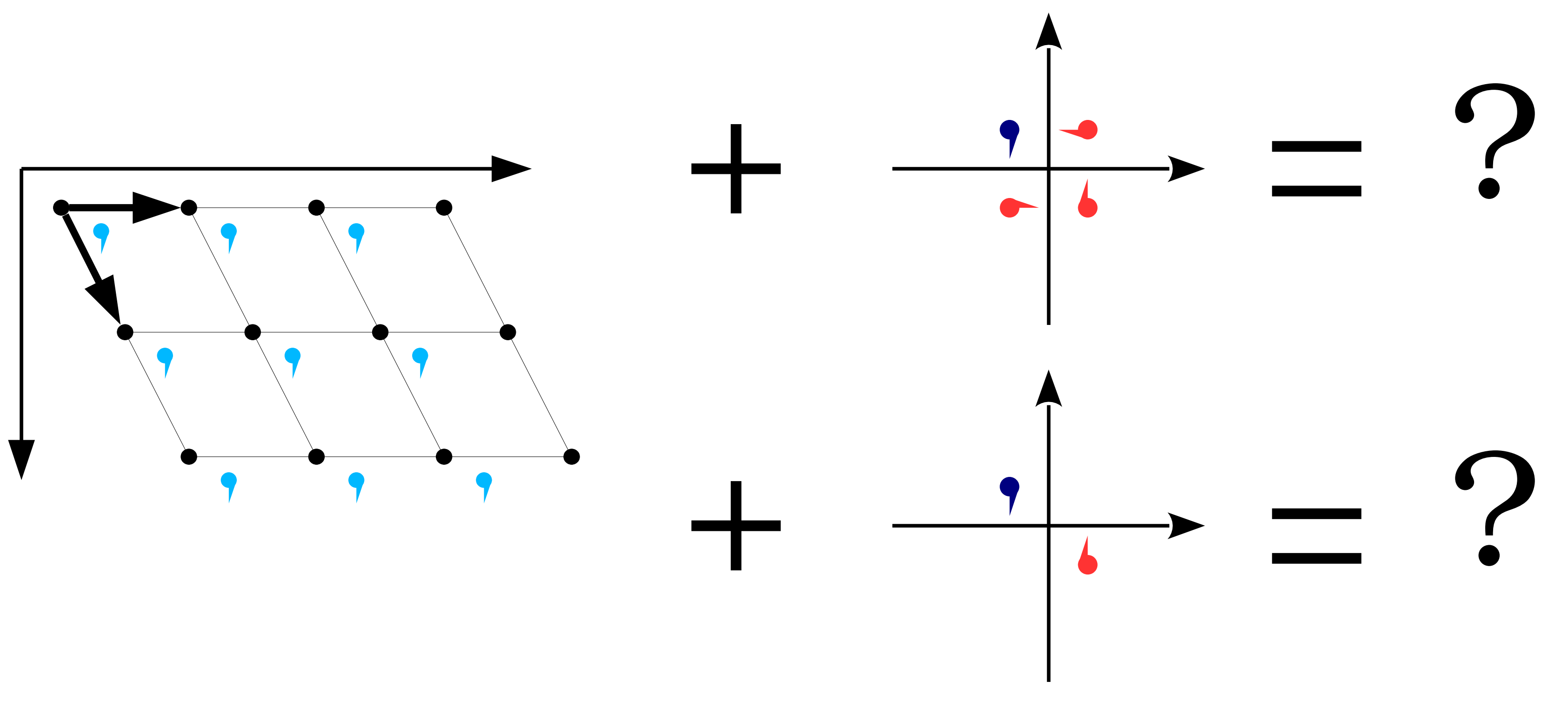
```
sub symop_ortho_from_fract
{
    my @cell = @_;
    my ($a, $b, $c) = @cell[0..2];
    my ($alpha, $beta, $gamma) = map {$Pi * $_ / 180} @cell[3..5];
    my ($ca, $cb, $cg) = map {cos} ($alpha, $beta, $gamma);
    my $sg = sin($gamma);

    return [
        [ $a, $b*$cg, $c*$cb               ],
        [  0, $b*$sg, $c*($ca-$cb*$cg)/$sg ],
        [  0,      0,
              $c*sqrt($sg*$sg-$ca*$ca-$cb*$cb+2*$ca*$cb*$cg)/$sg ]
    ];
}
```

Coordinate transformations (Ada)

$$\vec{x}' = R\vec{x} + \vec{T}_o$$

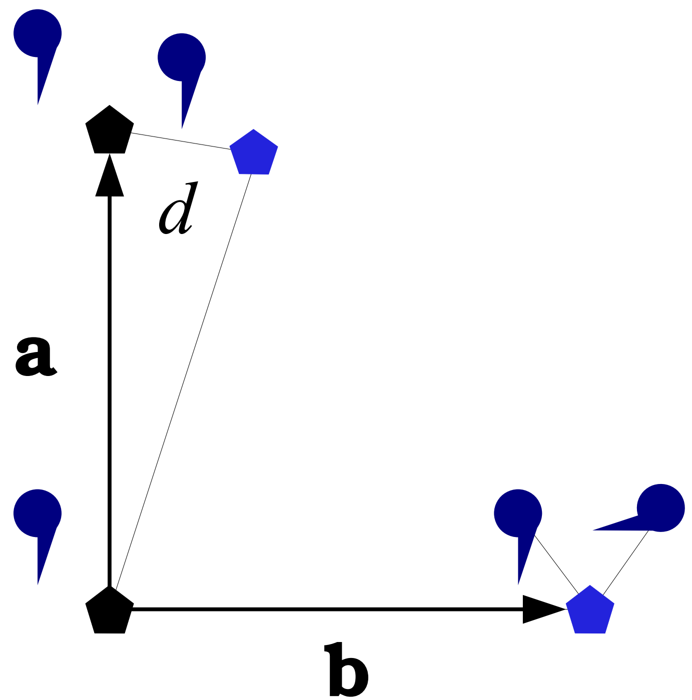
```
function Matrix_Ortho_From_Fract ( Cell : Unit_Cell_Type )
                                   return Matrix3x3
is
   A : Long_Float := Cell(1);
   B : Long_Float := Cell(2);
   C : Long_Float := Cell(3);
   Alpha : Long_Float := Cell(4) * Ada.Numerics.Pi / 180.0; -- in radians;
   Beta  : Long_Float := Cell(5) * Ada.Numerics.Pi / 180.0;
   Gamma : Long_Float := Cell(6) * Ada.Numerics.Pi / 180.0;
   CA : Long_Float := Cos(Alpha);
   CB : Long_Float := Cos(Beta);
   CG : Long_Float := Cos(Gamma);
   SG : Long_Float := Sin(Gamma);
begin
   return (
            (   A, B * CG, C * CB                ),
            ( 0.0, B * SG, C * (CA - CB*CG) / SG ),
            ( 0.0,    0.0,
              C * Sqrt (SG*SG - CA*CA - CB*CB + 2.0*CA*CB*CG)/SG)
          );
end;
```

Translations with point groups
= space groups



Symmetry elements compatible with lattices

Why don't you see five-sided snowflakes?



Symmetry elements compatible with lattices

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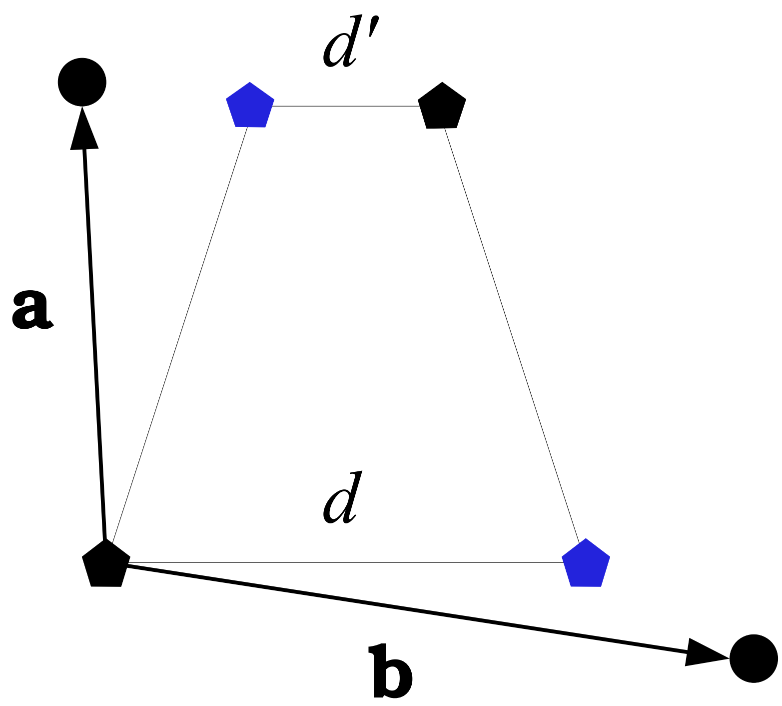
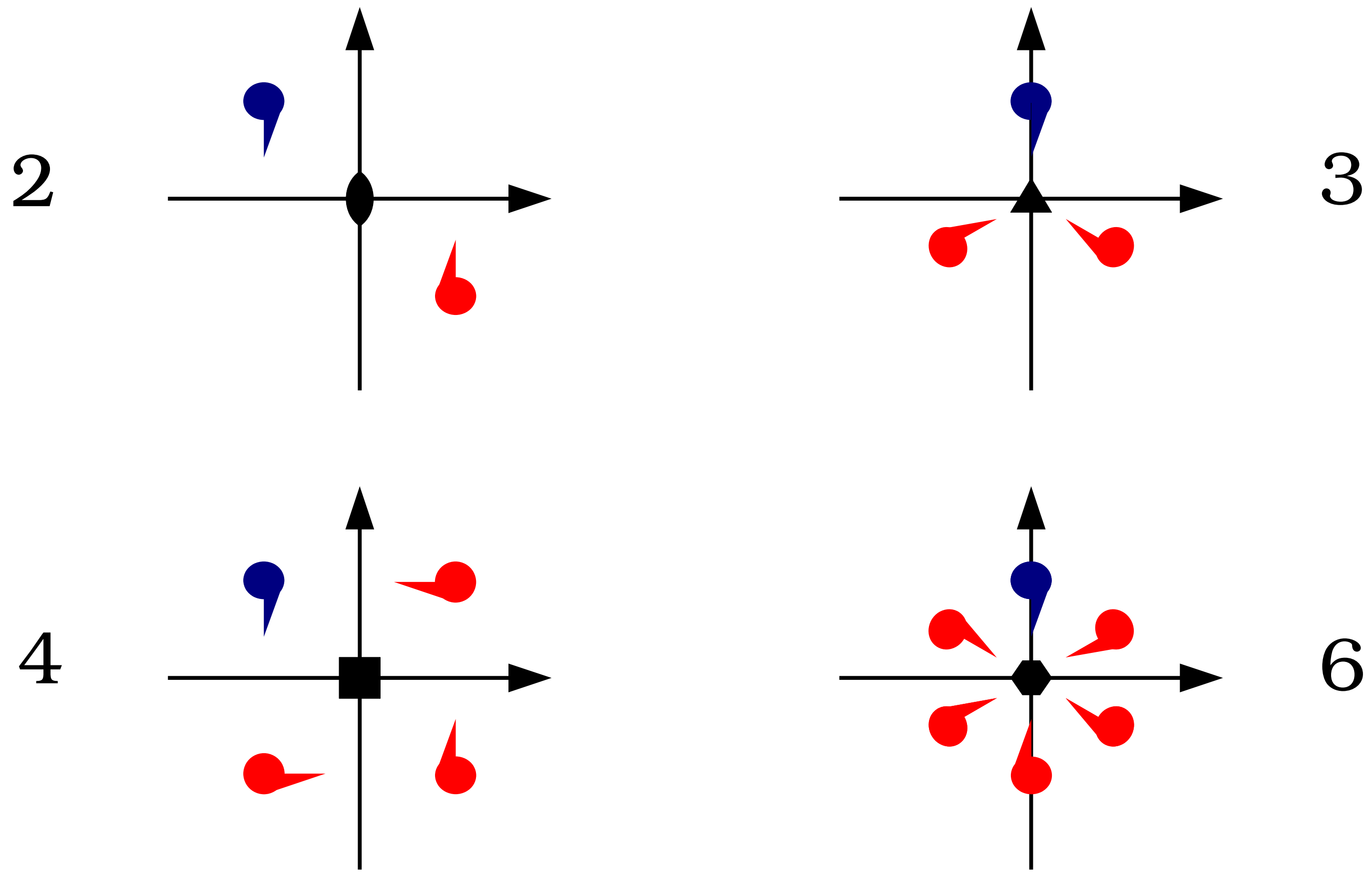
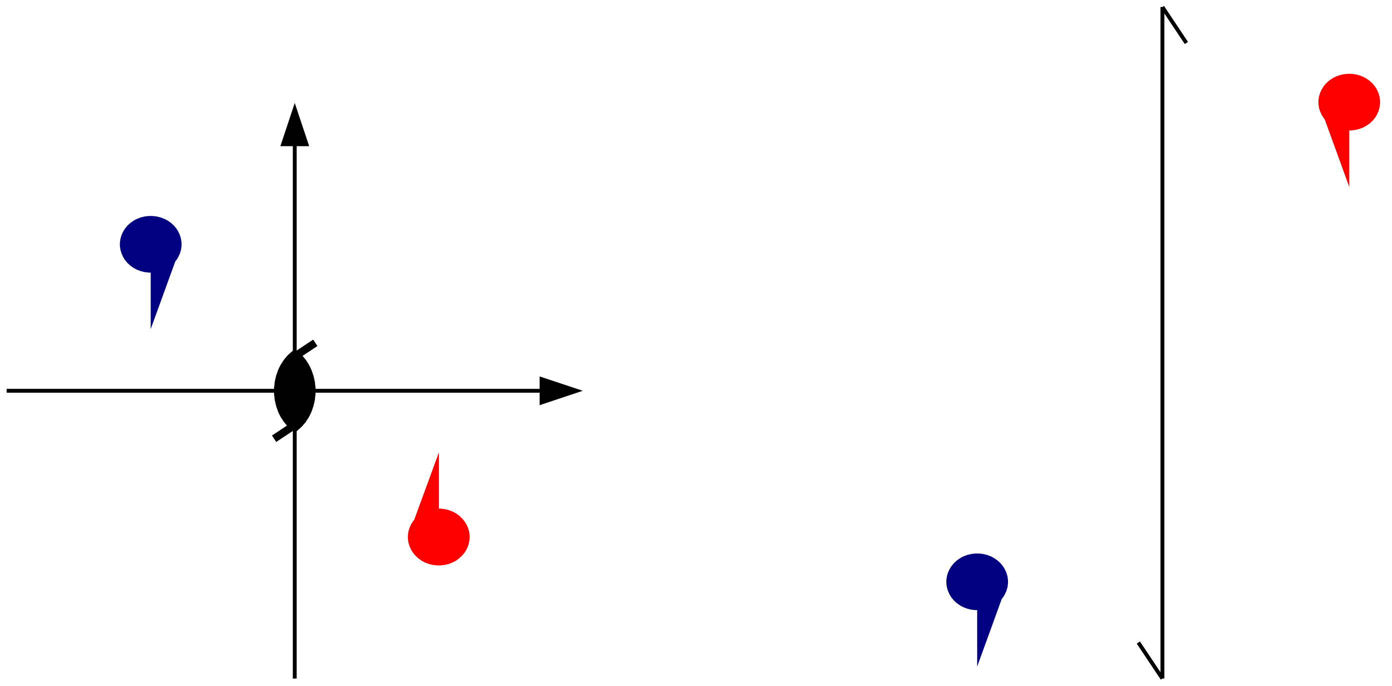


Symmetry elements: rotation axes



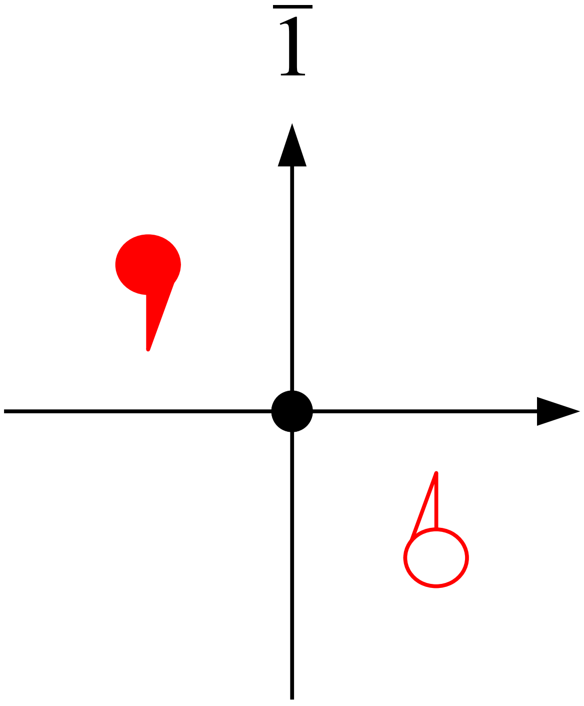
Symmetry elements: screw axes



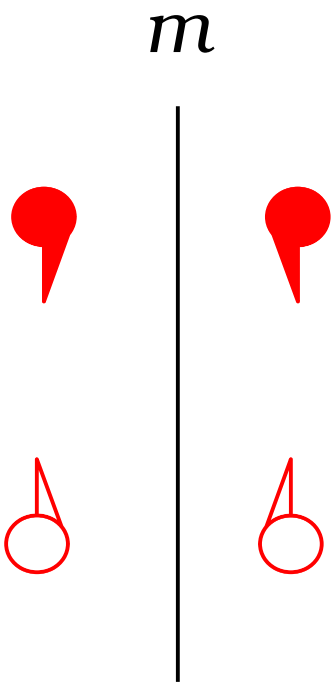
Sraigtinės ašys: 2_1

Kitos galimybės: 3_1, 3_2, 4_1, 4_2, 4_3, 6_1, 6_2, 6_3, 6_4, 6_5

Inversion centres and mirror planes

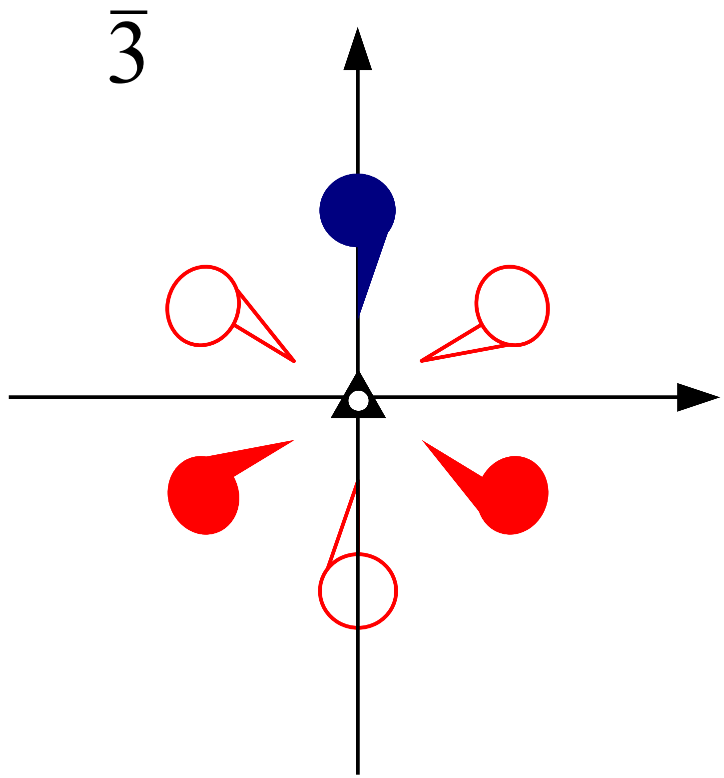


Inversion centre

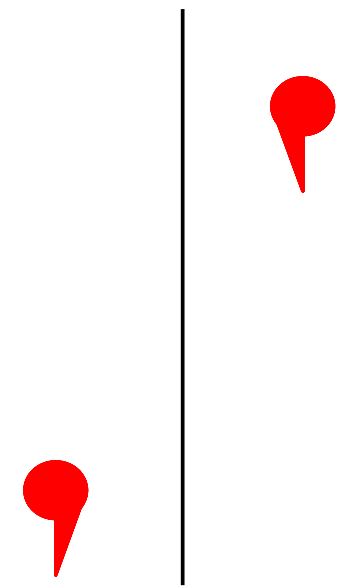


Mirror plane

Rotoinversion axes; glide planes



Rotoinversion axis



Glide plane

Nomenclature of space groups

Hermann–Mauguin symbols

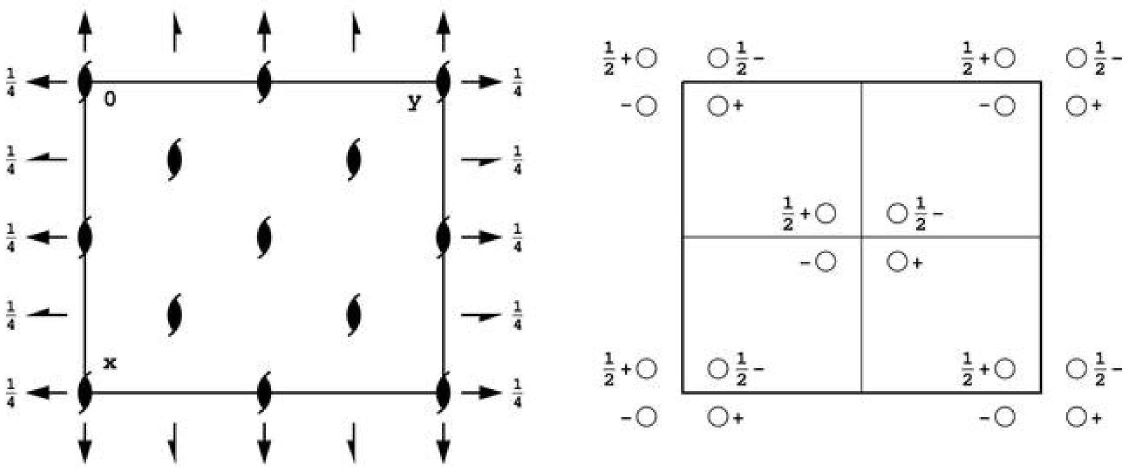
e.g.: $P2_12_12_1$ C2 F432

- 230 space groups
- 65 Sohncke groups (preserve chirality; available for biomolecules ;)

Other nomenclatures:
Schönflies symbols, Hall symbols

International Tables for Crystallography

$C222_1$



(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (4) $x,\bar{y},\bar{z}$

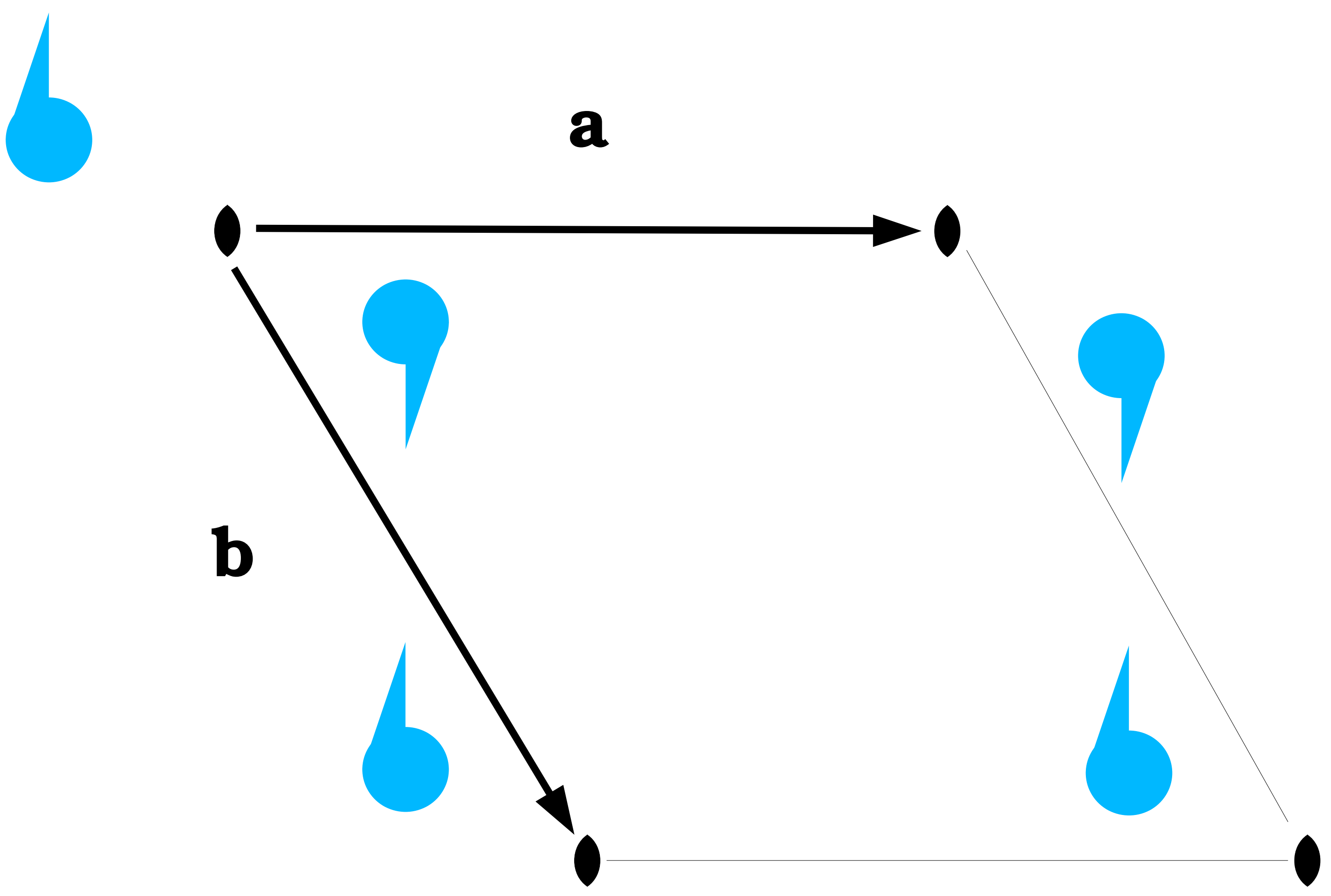
(5) $x+\frac{1}{2},y+\frac{1}{2},z$ (6) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (7) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$

Space group $C222_1$:

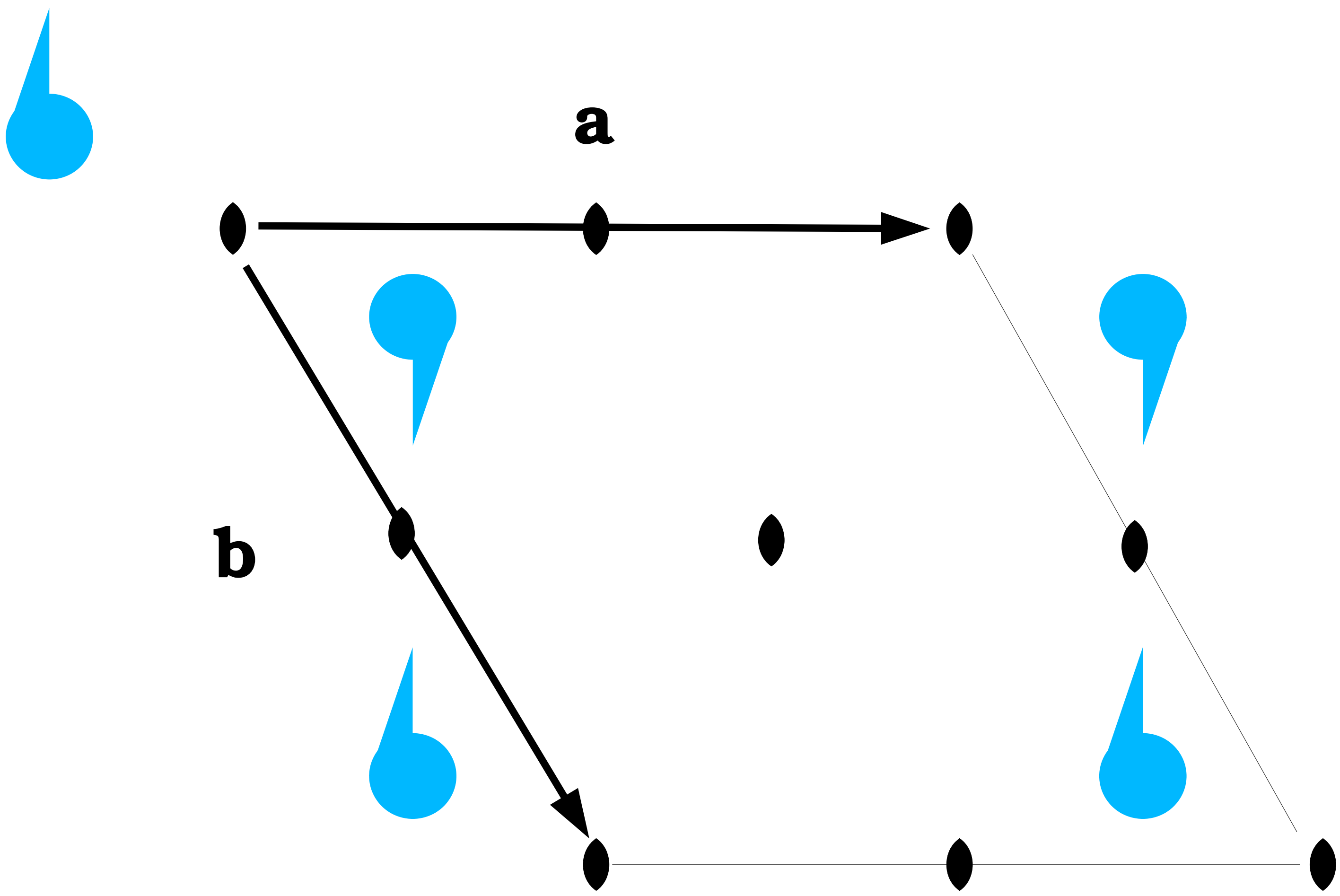
Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
				$(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},0)+$		
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$
4	b	. 2 .	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$		
4	a	2 . .	$x,0,0$	$\bar{x},0,\frac{1}{2}$		

Zbigniew Dauter; Mariusz Jaskolski *How to read (and understand) Volume A of International Tables for Crystallography...*, JAC 43(5) 2010
http://journals.iucr.org/j/issues/2010/05/02/kk5061/index.html
http://journals.iucr.org/j/issues/2010/05/02/isscontsbdy.html

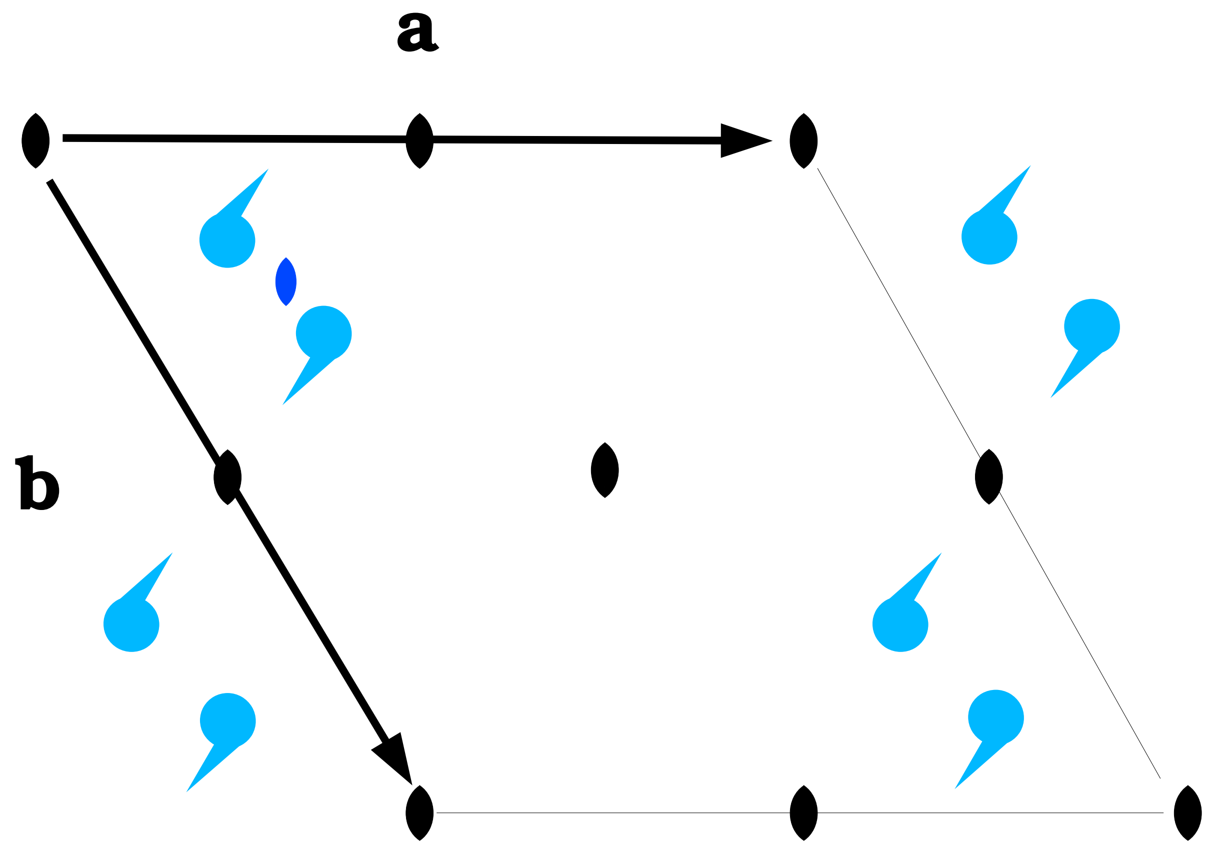
Filling the lattice



Asymmetric unit



Non-crystallographic symmetry



Relation of asymmetric and biological unit

- Asymmetric unit contains one or several protein/NA chains
- Biological unit can have various relations to the asymmetric unit (1/2, 2, 1 1/2, and so forth)