

# Crystallographic Groups: Enumeration and Classification

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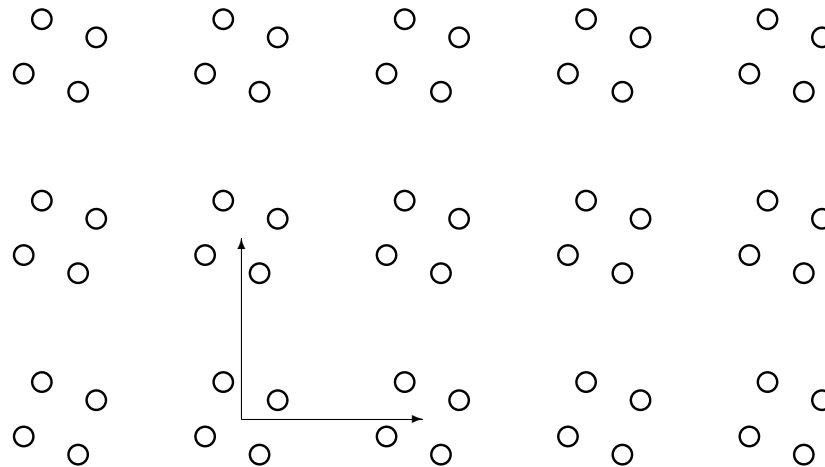
# Overview

- Crystal patterns and their isometries
- Analysis of crystallographic space groups
- Construction
- Classification

# Crystal patterns

Official definition from the *International Tables for Crystallography, Vol. A (Space-group symmetry)*:

**Definition:** A **crystal pattern** is a set of points in  $\mathbb{R}^n$  such that the translations leaving it invariant form a (full) lattice in  $\mathbb{R}^n$ .



# Diffraction

If the points of a crystal structure with translation lattice  $L$  are taken as **diffraction gratings**, the amplitude  $F(x)$  of the diffraction pattern at the point  $x$  is proportional to

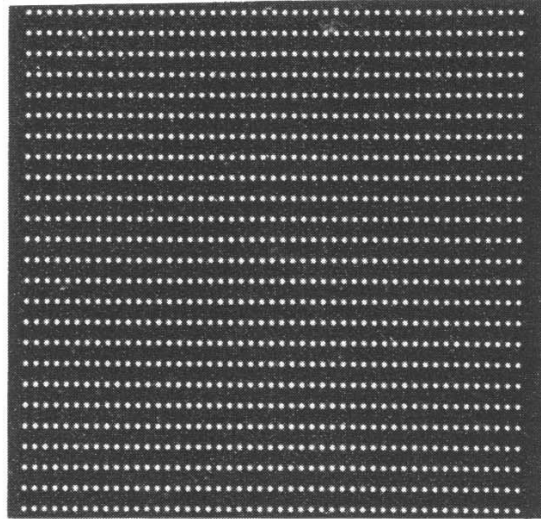
$$F(x) \sim \sum_{v \in L} e^{-ix \cdot v}$$

i.e. the diffraction pattern can be seen as a **Fourier transform** of the crystal pattern.

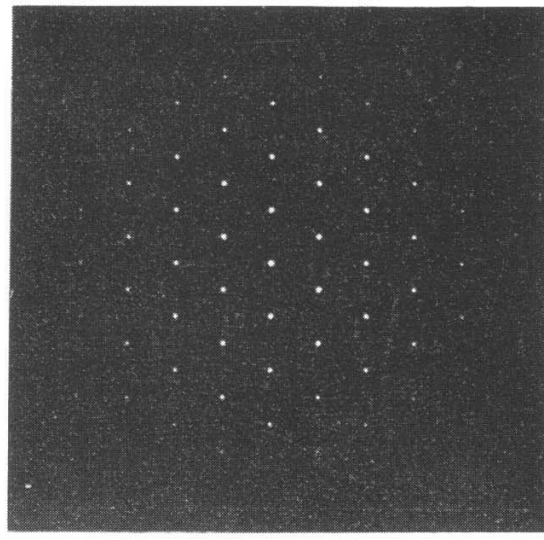
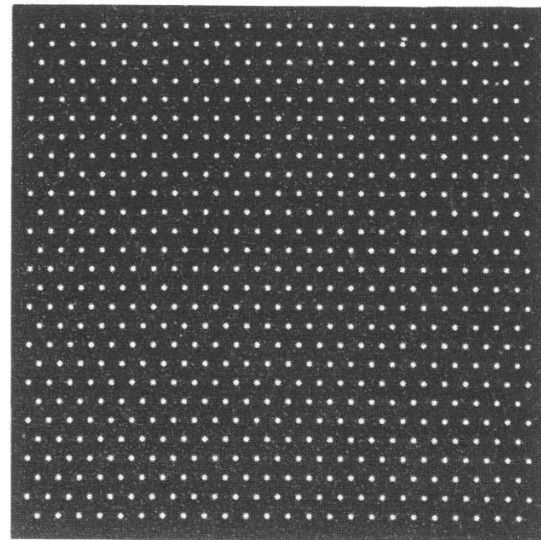
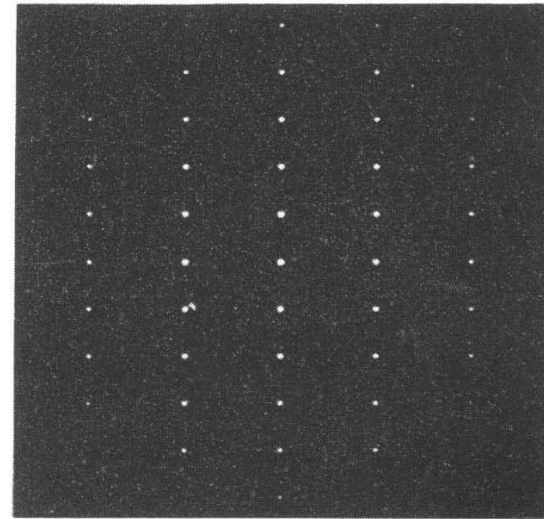
Thus, the diffraction pattern shows sharp **Bragg peaks** at the points of the dual lattice  $L^\#$  (rescaled by  $2\pi$ )

$$L^\# := \{x \in \mathbb{R}^n \mid x \cdot v \in \mathbb{Z} \text{ for all } v \in L\}.$$

lattice



diffraction pattern



# Space groups

**Idea:** Classify crystal structures according to their **symmetry properties**.

Note that this carries over to diffraction patterns, since a lattice  $L$  and its dual lattice  $L^\#$  have the same symmetry group.

Another definition from the *International Tables*:

**Definition:** A (crystallographic) **space group** is a group of isometries of  $\mathbb{R}^n$  which leaves some crystal pattern invariant.

## Affine mappings

**Fact (exercise):** Every mapping on  $\mathbb{R}^n$  that preserves the (Euclidean) distances between points and has a fixed point is a linear mapping.

**Consequence:** Isometries are compositions of invertible linear mappings and translations, i.e. [affine mappings](#).

An affine mapping  $\varphi : v \mapsto gv + t$  is denoted by  $\{g \mid t\}$  (Seitz notation),  $g$  is called the [linear part](#) of  $\varphi$ ,  $t$  is called its [translation part](#).

Composition of affine mappings:

$$\{g \mid t\} \cdot \{h \mid u\} = \{gh \mid gu + t\}.$$

## Augmented matrices

**Definition:** The **augmented matrix** of an affine mapping  $\{g \mid t\}$  on  $\mathbb{R}^n$  is the  $(n + 1) \times (n + 1)$  matrix

$$\left( \begin{array}{c|c} g & t \\ \hline 0 \dots 0 & 1 \end{array} \right).$$

An augmented matrix is applied to a vector  $v \in \mathbb{R}^n$  by left-multiplication with the augmented vector having an additional component of value 1:

$$\left( \begin{array}{c|c} g & t \\ \hline 0 & 1 \end{array} \right) \cdot \left( \begin{array}{c} v \\ 1 \end{array} \right) = \left( \begin{array}{c} g \cdot v + t \\ 1 \end{array} \right).$$

**Example:** The matrix  $\left( \begin{array}{ccc|c} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{4} \\ \hline 0 & 0 & 0 & 1 \end{array} \right)$  describes a **4-fold screw rotation** along the  $z$ -axis (in  $\mathbb{R}^3$ ).

## A useful homomorphism

Let  $\Pi$  be the mapping  $\Pi : \mathcal{A}_n \longrightarrow GL_n(\mathbb{R}) : \{g \mid t\} \mapsto g$  which forgets about the translation part of an affine mapping.

In terms of augmented matrices,  $\Pi$  simply picks out the upper left  $n \times n$  submatrix.

- The mapping  $\Pi$  is a group homomorphism from  $\mathcal{A}_n$  onto  $GL_n(\mathbb{R})$ .  
The kernel of  $\Pi$  is  $\mathcal{T} := \{\{id \mid t\} \mid t \in \mathbb{R}^n\}$  and its image is  $GL_n(\mathbb{R})$ .
- $\mathcal{A}_n$  contains a subgroup isomorphic to the image  $GL_n(\mathbb{R})$  of  $\Pi$ , namely the group  $\mathcal{G} = \{\{g \mid 0\} \mid g \in GL_n(\mathbb{R})\}$  of elements with trivial translation part.
- Since  $\mathcal{G}$  is a complement of  $\mathcal{T}$ ,  $\mathcal{A}_n$  is a **semidirect product**  $\mathcal{T} \rtimes GL_n(\mathbb{R})$  of  $\mathcal{T}$  and  $GL_n(\mathbb{R})$ .

# Space group analysis

The projection  $\Pi$  can be restricted to any space group  $G \leq \mathcal{A}_n$ .

- The subgroup  $T := \{\{id \mid t\} \in G\} = \mathcal{T} \cap G$  is the kernel of the restriction of  $\Pi$  to  $G$  and is called the **translation subgroup** of  $G$ .
- The group  $P := \Pi(G)$  of linear parts in  $G$  is called the **point group** of  $G$ . It is isomorphic to the factor group  $G/T$ .
- In general,  $G$  does not contain a subgroup isomorphic to its point group  $P$ . If this happens to be the case, the group  $G$  is called a **symmorphic** group.

# Translation lattices

For a space group  $G$  we call the lattice

$$L := \{t \in \mathbb{R}^n \mid \{id \mid t\} \in G\}$$

of translation vectors in  $G$  the **translation lattice** of  $G$ .

The fact that the translation subgroup  $T = \ker \Pi$  is a normal subgroup of  $G$  implies that the **point group**  $P = \Pi(G)$  actually **acts on**  $L$ .

**Consequence:** The point group  $P$  is a subgroup of the full symmetry group

$$Aut(L) := \{g \in O_n(\mathbb{R}) \mid g(L) = L\}$$

of  $L$ . In particular,  **$P$  is finite**.

## Chicken and egg *opportunity*

Given an **interesting lattice**  $L$ , the subgroups of  $Aut(L)$  may serve as point groups of space groups having  $L$  as translation lattice.

Given an **interesting finite matrix group**  $P \leq GL_n(\mathbb{Q})$ , the lattices  $L \subset \mathbb{R}^n$  invariant under  $P$  may serve as translation lattices of space groups having  $P$  as point group.

Fortunately, computing with lattices and finite matrix groups is by now a standard task for computer algebra systems (at least for reasonable  $n$ ).

## Standard form for space groups

If we choose a lattice basis  $B = (b_1, \dots, b_n)$  for the translation lattice  $L$  of  $G$  and write the augmented matrices with respect to this basis, the linear parts of the elements of  $G$  become **integral matrices**.

Moreover, elements with the same linear part differ only by a **translation in  $\mathbb{Z}^n$** . Thus, with respect to  $B$ , the space group  $G$  can be written as:

$$G = \left\{ \left( \begin{array}{c|c} g & t_g + t \\ \hline 0 & 1 \end{array} \right) \mid g \in P, t \in \mathbb{Z}^n \right\}$$

where  $P \leq GL_n(\mathbb{Z})$  is finite.

The metric properties of  $L$  are captured in the **metric tensor** (Gram matrix)  
 $F := (b_i \cdot b_j)_{1 \leq i, j \leq n}$ .

The point group elements fix the metric tensor, i.e.  $g^{tr} F g = F$  for all  $g \in P$ .

## Intermezzo

In crystallography, transforming to a lattice basis of  $L$  is **not** the standard approach. Instead, **conventional bases** are used which have nice and simple metric properties.

If the conventional basis is a lattice basis,  $L$  is called a **primitive lattice**. For a **centered lattice**  $L$ , in addition to the integral linear combinations of the basis, one or more centering vectors are required (which are coset representatives in  $L$  of the sublattice spanned by the basis).

**Example:** All lattices belonging to the cubic crystal family are written with respect to an orthonormal basis.

For the body-centered cubic (bcc) lattice, the centering vector  $\left(\frac{1}{2} \ \frac{1}{2} \ \frac{1}{2}\right)^{tr}$  is required.

For the face-centered cubic (fcc) lattice, the centering vectors  $\left(\frac{1}{2} \ \frac{1}{2} \ 0\right)^{tr}$ ,  $\left(\frac{1}{2} \ 0 \ \frac{1}{2}\right)^{tr}$ ,  $\left(0 \ \frac{1}{2} \ \frac{1}{2}\right)^{tr}$  are required.

## Intermezzo (contd.)

In dimensions 2 and 3, the primitive lattices always have symmetry groups which are the same or larger than those of their centerings.

Thus, the symmetry groups for the centered lattices remain integral when written with respect to a lattice basis of the corresponding primitive lattice.

In dimension 4, the standard lattice  $\mathbb{Z}^4$  has a symmetry group of order 384. It contains the root lattice of type  $D_4$  as a sublattice of index 2 which has a symmetry group of order 1152, i.e. larger by a factor of 3.

The root lattice of type  $E_8$  can be regarded as a centering of the 8-dimensional checkerboard lattice  $D_8$ , which in turn is a sublattice of the standard lattice  $\mathbb{Z}^8$ . Since  $Aut(D_8) = Aut(\mathbb{Z}^8) \not\subseteq Aut(E_8)$ , there is no basis with respect to which both  $Aut(D_8)$  and  $Aut(E_8)$  could be written as integral matrix groups.

## Intermezzo - A problem

**Conclusion:** There is no obvious concept of distinguishing between primitive and centered lattices that generalizes to arbitrary  $n$ -dimensional space.

Research questions (for your spare time):

**Problem 1:** For the lattices belonging to the same crystal family, find a criterion that distinguishes one from the others.

**Problem 2:** For the distinguished lattice, define a canonical basis.

## Constructing space groups

Let  $P$  be a prospective point group, acting on a lattice  $L$ . Then a space group  $G$  with point group  $P$  and translation subgroup  $T$  (corresponding to  $L$ ) is determined by the vectors  $t_g \in \mathbb{R}^n$  in a transversal  $\{\{g \mid t_g\} \mid g \in P\}$  of  $T$  in  $G$ .

**Definition:** The set  $\{t_g \mid g \in P\}$  is called a **vector system** or system of nonprimitive translations (SNoT).

Due to  $\{g \mid t_g\} \cdot \{h \mid t_h\} = \{gh \mid g \cdot t_h + t_g\}$ , the elements of a vector system conform with the **cocycle condition**

$$t_{gh} \equiv g t_h + t_g \pmod{L}.$$

## Inner derivations

A **shift of the origin** by  $v \in \mathbb{R}^n$  corresponds to conjugating with the affine mapping  $\{id \mid v\}$ .

Such a shift of origin alters the elements of a vector system according to:

$$t_g \mapsto t_g + (g - id)v$$

**Definition:** A vector system of the form  $\{(g - id)v \mid g \in P\}$  for some  $v \in \mathbb{R}^n$  is called an **inner derivation** or coboundary.

Space groups for which the vector systems only differ by a coboundary, i.e. which are transformed into each other by a shift of origin are (clearly) regarded as equivalent.

## Frobenius congruences

To find the possible vector systems for a point group  $P = \langle g_1, \dots, g_s \rangle$ , we use a **presentation**

$$\langle x_1, \dots, x_s \mid r_1, \dots, r_t \rangle$$

of  $P$ .

Regard the components of the translation parts  $t_i$  of the space group generators  $\{g_i \mid t_i\}$  as **indeterminates**.

Evaluating the relators  $r_j$  of the presentation on these elements has to give translations, hence one obtains a system of linear congruences for the indeterminates modulo  $\mathbb{Z}$ , called **Frobenius congruences**.

The solutions of the Frobenius congruences yield the possible vector systems. The trivial solution (all  $t_i = 0$ ) gives the **symmorphic** space group with point group  $P$ .

## Intermezzo - Extension theory

Abstractly seen, a space group  $G$  is an extensions of the translation subgroup  $T$  by the point group  $P$ . These extensions are determined by the **second cohomology group**  $H^2(P, T)$ .

Via the **snake lemma** one obtains the exact sequence

$$H^1_{=0}(P, \mathbb{R}^n) \longrightarrow H^1(P, \mathbb{R}^n/T) \longrightarrow H^2(P, T) \longrightarrow H^2_{=0}(P, \mathbb{R}^n),$$

(note that  $\mathbb{R}^n$  is a free  $P$ -module) which implies that

$$H^2(P, T) \cong H^1(P, \mathbb{R}^n/T) = C^1(P, \mathbb{R}^n/T)/B^1(P, \mathbb{R}^n/T).$$

$C^1(P, \mathbb{R}^n/T)$ : solutions to the Frobenius congruences

$B^1(P, \mathbb{R}^n/T)$ : inner derivations

**Conclusion:** The different extensions of  $T$  by  $P$  correspond to the solutions of the Frobenius congruences modulo inner derivations.

## Isomorphism classes of space groups

**Theorem** ( Bieberbach, 1911): Space groups are isomorphic if and only if they are conjugate in the affine group.

For fixed point group  $P$  and lattice  $\mathbb{Z}^n$ , the linear part of the affine mapping inducing an isomorphism has to lie in the **normalizer**  $N := N_{GL_n(\mathbb{Z})}(P)$ . Since translations are dealt with by the inner derivations, we can assume mappings of the form  $\{a \mid 0\}$  with  $a \in N$ .

Such a mapping transforms the vector system by  $t_g \mapsto a^{-1} t_{aga^{-1}}$ .

**Theorem:** For a given point group and lattice, the different space groups correspond to the **orbits** of the action **of the normalizer**  $N := N_{GL_n(\mathbb{Z})}(P)$  on the vector systems modulo inner derivations.

## A rectangular example

Consider the point group  $2mm = \left\langle g = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, h = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \right\rangle$   
with presentation  $\langle x, y \mid x^2, y^2, (xy)^2 \rangle$ .

Evaluating the relators on generators with translation parts  
 $t_g = \begin{pmatrix} a \\ b \end{pmatrix}$  and  $t_h = \begin{pmatrix} c \\ d \end{pmatrix}$  gives the Frobenius congruences

$$2a \equiv 0 \pmod{\mathbb{Z}} \quad \text{and} \quad 2b \equiv 2d \pmod{\mathbb{Z}}.$$

The solutions with  $a = 0$  and  $b = d$  correspond to translations of the origin,  
thus  $t_h$  can be chosen to be trivial.

This gives  $a, b \in \{0, \frac{1}{2}\}$  and the four different vector systems are given by

$$t_g^{(0)} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad t_g^{(1)} = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}, \quad t_g^{(2)} = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}, \quad t_g^{(3)} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}.$$

The normalizer  $N := N_{GL_2(\mathbb{Z})}(2\text{mm})$  contains the matrix  $a := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$  interchanging the two basis vectors. This element interchanges the vector systems  $t_g^{(1)} = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}$  and  $t_g^{(2)} = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$ .

Both vector systems  $t_g^{(1)}$  and  $t_g^{(2)}$  give rise to a space group in which both reflections  $g$  and  $gh$  in the point group give rise to glide reflections along one of the basis vectors.

The underlying lattice is a rectangular lattice. But from the group, we can not tell which of the basis vectors is the shorter one, hence the two groups are [geometrically indistinguishable](#).

**To remember:** The normalizer is the [symmetry of the symmetries](#).

## Some historical notes

- The original enumeration of 3-dimensional space groups by Fedorov and Schoenflies (1891) used purely geometric methods.
- Niggli, Speiser and Burckhardt (the Zürich school) developed the algebraic approach in the 1920's.
- Zassenhaus described the complete method including normalizer action in 1948.
- In 1965/68, Ascher and Janner introduced the extension theoretic point of view to the crystallography community (without too much impact).
- Plesken et al. developed a computer package (CARAT,  $\sim$  2000, also incorporated in GAP) that allows to compute with space groups up to degree  $n = 6$  (many of the algorithms even for  $n > 6$ ).

## Examples for permutation groups

In 1937, Burckhardt gave results for the cyclic, symmetric and alternating groups  $C_n$ ,  $S_n$ ,  $A_n$  (at least partially).

For  $S_n$  and  $A_n$  the presentations as Coxeter groups are used.

Natural permutation action on  $\mathbb{R}^n$ :

- $C_n$  only gives the symmorphic space group;
- $S_n$  gives two space groups for  $n \geq 3$ ;
- $A_n$  gives three space groups for  $n = 4, 5$  and one for  $n \geq 6$ .

Reduced action on  $\mathbb{R}^{n-1}$ :

- $S_n$  gives two space groups for  $n = 4$  and one for  $n = 3$  and  $n \geq 5$ ;
- $A_n$  gives two space groups for  $n = 4$ , three for  $n = 5, 6$  and one for  $n \geq 7$ .

## Enumeration in higher dimensions???

Let  $P \leq GL_n(\mathbb{Z})$  be the group of diagonal matrices, i.e.  $P \cong C_2^n$ .

One has  $H^1(P, \mathbb{R}^n/\mathbb{Z}^n) \cong C_2^{n(n-1)}$  and the action of  $N_{GL_n(\mathbb{Z})}(P)$  on  $H^1(P, \mathbb{R}^n/\mathbb{Z}^n)$  gives  $N \cong S_n$ .

The number of orbits can be determined by Burnside's lemma

$$\#orbits = \frac{1}{|N|} \sum_{g \in N} |Fix(g)|.$$

The dominant term is that for  $g = id$ , hence we can estimate the number  $o_n$  of orbits by  $2^{n(n-1)}/n!$  (for  $n = 6$ , the error is 3%).

Since  $o_{n+1}/o_n = 2^{2n}/(n+1)$ , the number of space groups in this class grows exponentially with  $n$ .

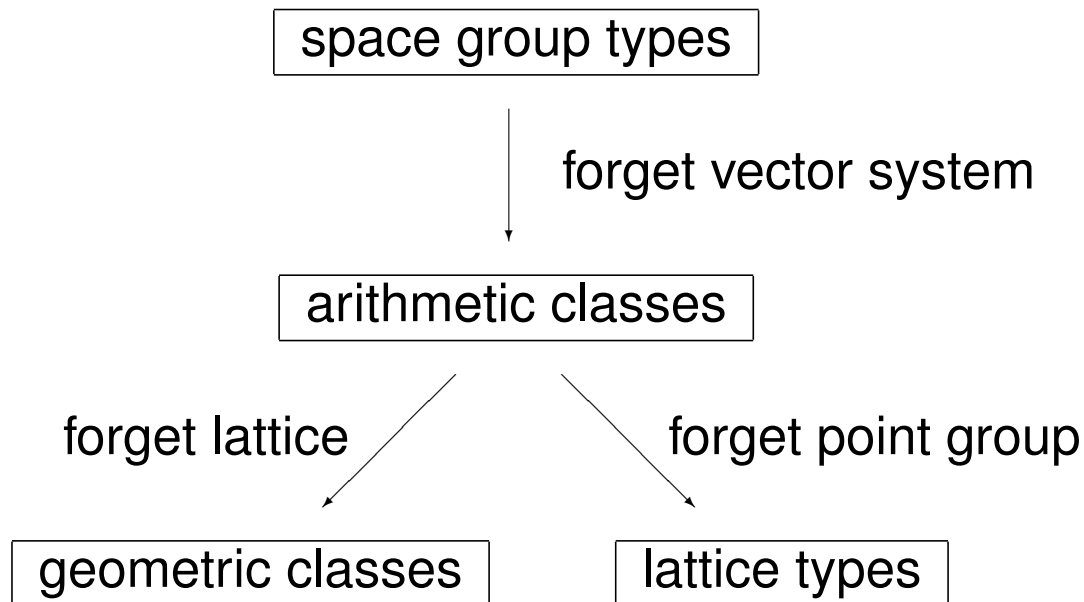
$n$	2	3	4	5	6
$o_n$	2	11	171	8739	1491309
$s_n$	17	219	4783	222018	$2.9 \cdot 10^7$
$o_n/s_n$	0.118	0.050	0.036	0.039	0.052

$s_n$ : total number of space group types in dimension  $n$

# Classification of space groups

The finest level on which space groups are classified are the **space group types**, i.e. the isomorphism classes of space groups.

A space group type is characterized by a **point group**, a **lattice** and a **vector system**. Forgetting one or two of these pieces of information results in coarser classifications:



## Arithmetic classes

**Definition:** Two space groups belong to the same **arithmetic class** if their point groups  $P$  and  $P'$  differ only by a lattice basis transformation.

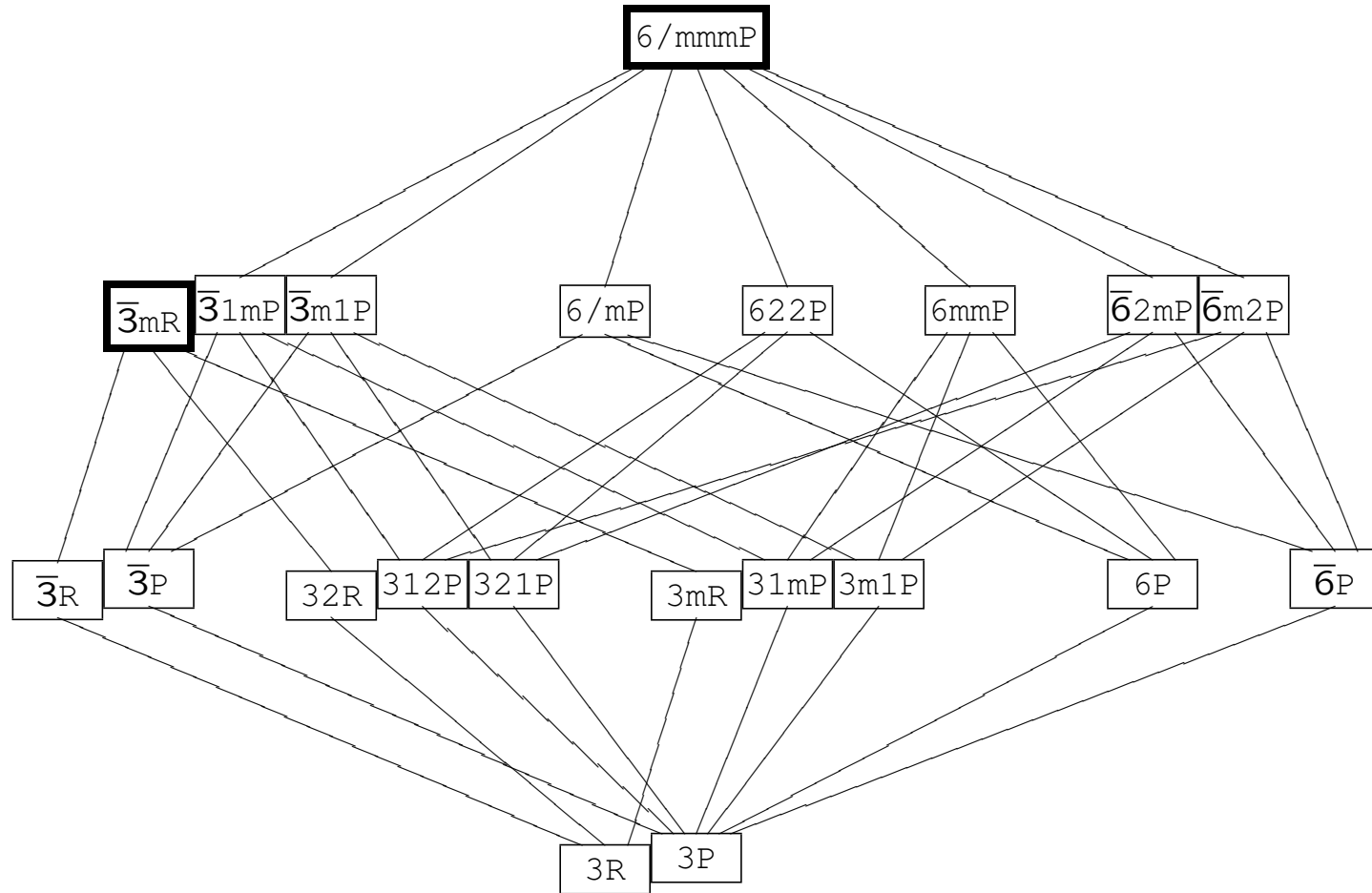
Also, point groups  $P, P' \leq GL_n(\mathbb{Z})$  are said to lie in the same arithmetic class if  $P' = X^{-1}PX$  for some  $X \in GL_n(\mathbb{Z})$ .

Since space groups in the same arithmetic class differ only by their vector systems, the arithmetic classes are in 1-1 correspondence with the symmetric space group types.

**Definition:** A point group  $P$  acting on a lattice  $L$  is called a **Bravais group** if  $P = \text{Aut}(L)$ .

The arithmetic class containing  $P$  is called a **Bravais class**.

## A diagram of arithmetic classes



Boxes directly joined: Same group acting on a different lattice (centering)

Boxes joined by a line: Subgroup acting on the same lattice

Thick boxes: Bravais class

## Geometric classes

**Definition:** Two space groups belong to the same **geometric class** (or **point group type**) if their point groups  $P$  and  $P'$  differ only by a basis transformation of  $\mathbb{R}^n$ .

Also, point groups  $P, P' \leq GL_n(\mathbb{Z})$  are said to lie in the same geometric class or to have the same type if  $P' = X^{-1}PX$  for some  $X \in GL_n(\mathbb{R})$ .

Point groups in the same geometric class are the actions of a point group on different lattices.

Historically, the **geometric classes** in dimension 3 were determined much **earlier** than the space groups. They were obtained as the symmetry groups for the set of **normal vectors of crystal faces** which describe the **morphological symmetry** of macroscopic crystals (Frankenheim, 1826 and Hessel, 1830).

## Lattice types

**Definition:** Two lattices  $L$  and  $L'$  belong to the same **lattice type** if  $Aut(L)$  and  $Aut(L')$  lie in the same arithmetic class.

The lattice types are in 1-1 correspondence with the Bravais classes.

A Bravais group together with its subgroups which genuinely act on the same lattice, i.e. not on a more general lattice, form a **Bravais flock**.

A subgroup  $Q \leq P$  of a Bravais group  $P$  acts on a more general lattice if  $\dim \mathcal{F}(Q) > \dim \mathcal{F}(P)$ , where

$$\mathcal{F}(P') := \{F \in \mathbb{R}^{n \times n} \mid F = F^{tr}, g^{tr} F g = F \text{ for all } g \in P'\}$$

is the **space of metric tensors** of  $P'$ .

## Number of parameters

For  $P$  acting genuinely on  $L$ ,  $\dim \mathcal{F}(P)$  is called the **number of parameters** of  $L$  (or of its metric tensor).

**Example:** Lattice types in  $\mathbb{R}^2$

- square, hexagonal: 1 parameter (length of shortest vector)
- rectangular: 2 parameters (lengths of 2 basis vectors)
- centered rectangular (rhombic): 2 parameters (length of 1 basis vector, angle)
- oblique: 3 parameters: (lengths of 2 basis vectors, angle)

Note that  $\dim \mathcal{F}(P)$  can be read off the decomposition of the natural character of  $P$  into absolutely irreducible characters.

# Crystal families

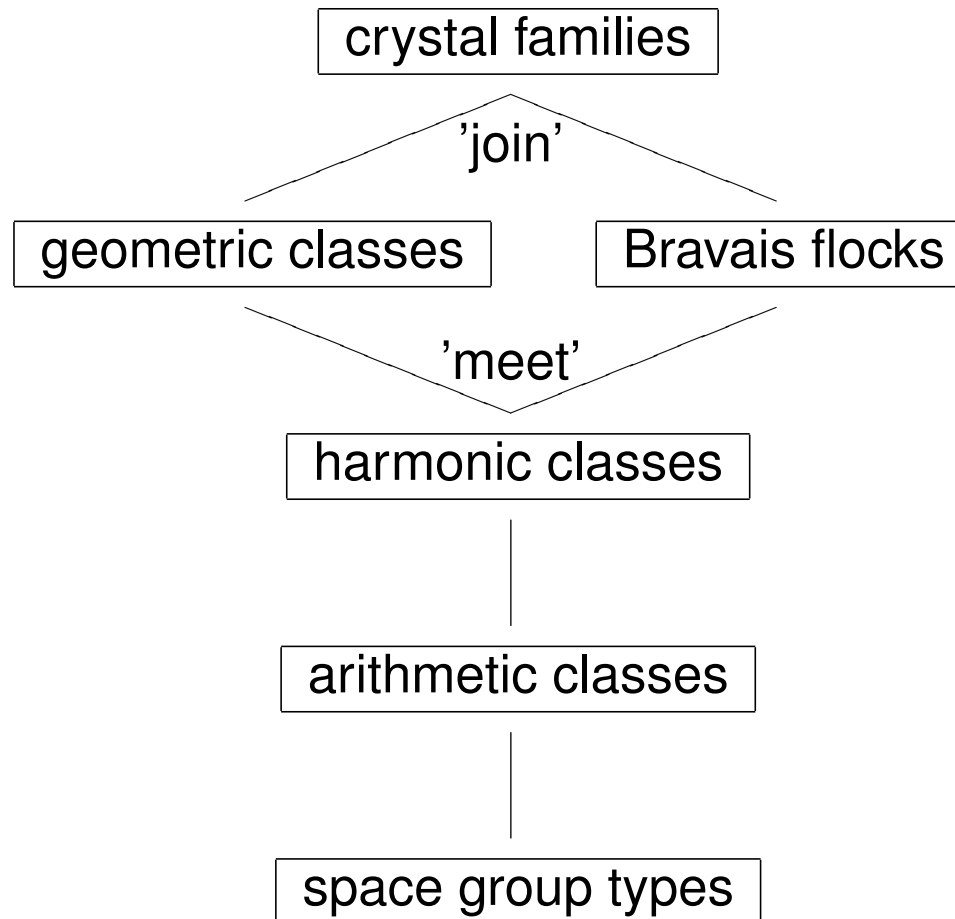
**Definition:** The **crystal family** of a space group  $G$  is the smallest set of arithmetic classes containing  $G$  which contains **full geometric classes** and **full Bravais flocks**.

In terms of the diagram of arithmetic classes, the crystal families are the **connected components** if we regard boxes **joined by lines** or directly **joined horizontally** as being linked.

All point groups in a crystal family are thus reached by an iteration of the following moves:

- move to a subgroup or supergroup with the same number of parameters;
- move to a conjugate group (acting on a different lattice).

## Classification lattice (tralie [NL], Verband [D])



Harmonic classes are (so far) of little significance in crystallography.

## Harmonic classes

Let  $P$  and  $P'$  be point groups in the same harmonic class (but not in the same arithmetic class).

Since  $P$  and  $P'$  belong to the same geometric class, they are actions of the same group (e.g.  $P$ ) on **different lattices**  $L$  and  $L'$ .

Since  $P$  and  $P'$  belong to the same Bravais flock, the lattices  $L$  and  $L'$  are **of the same type**.

If the natural character of  $P$  is  $\mathbb{R}$ -irreducible, this means that  $L$  and  $L'$  are similar, i.e. **isometric up to scaling**.

This shows that  $L$  displays **self-similarity** in a non-trivial way, i.e. allows a scaling that is not induced by an endomorphism of  $P$ .

## Harmonic class for the hexagonal lattice

The group  $31m \cong S_3$  acts on the hexagonal lattice with basis  $(b_1, b_2)$ .

The group  $3m1$  is the action of  $31m$  on the sublattice with basis  $(b'_1, b'_2)$  (black points) which is also hexagonal.

The groups belong to **different arithmetic classes** due to the different position of the reflection axes with respect to the lattice.

