Group-subgroup relations

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Overview

- Finite subgroups
  - Site-symmetry groups
  - Wyckoff positions

- Subgroups of finite index
  - Maximal subgroups
  - Colour groups
  - Splitting of Wyckoff positions

Where are the atoms?

Depending on

chemical composition,

the kind of chemical bonding,

electron configuration of the atoms,

relative sizes of the atoms,

pressure, temperature etc.,

there often exists one energetically most favourable surrounding for atoms of a given kind which all of these atoms strive to attain (Brunner).

Consequence: The arrangement of atoms reveals a pronounced tendency towards the highest possible symmetry.

Site-symmetry groups

Definition: For an n-dimensional space group G and $x \in \mathbb{R}^n$, the stabilizer $\mathcal{S}_G(x) := \{g \in G \mid g \cdot x = x\}$ is called the site-symmetry group of x.

Facts:

- Site-symmetry groups are finite (they do not contain translations).
- The projection Π from G to its point group P induces an isomorphism from $\mathcal{S}_G(x)$ to a subgroup of P.
- G contains a site-symmetry group isomorphic with P iff G is symmorphic.

Corollary: The unit cell of the lattice L of G contains $|P|/|\mathcal{S}_G(x)|$ points of the orbit x^G of x under G.

Thus, to avoid crowding, atoms better take positions of high symmetry.

Wyckoff positions

Idea: Classify points of $\mathbb{R}^n$ according to their site-symmetry groups.

Definition: A point $x \in \mathbb{R}^n$ is called a point in general position (with respect to a space group G) if $\mathcal{S}_G(x) = \{1\}$, otherwise x is called a point in special position.

Points in the same orbit under G are regarded as equivalent, they have site-symmetry groups which are conjugate in G.

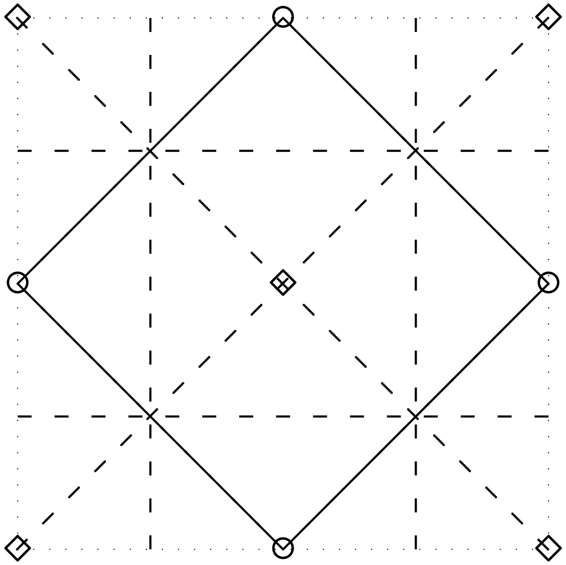
Definition: Two points $x, y \in \mathbb{R}^n$ belong to the same Wyckoff position of G if their site-symmetry groups $\mathcal{S}_G(x)$ and $\mathcal{S}_G(y)$ are conjugate in G.

Note that in general Wyckoff positions are unions of G-orbits.

Example of Wyckoff positions

The space group `p4gm` is generated by a 4-fold rotation and a glide reflection along the axis $x = y$. Representatives of the special positions are:

$$\begin{array}{ll} x = (0,0)^{tr}, & \mathcal{S}_G(x) \cong C_4 \\ x = (\frac{1}{2},0)^{tr}, & \mathcal{S}_G(x) \cong V_4 \\ x = (a, a+\frac{1}{2})^{tr},\ a \neq 0, \frac{1}{2}, & \mathcal{S}_G(x) \cong C_2 \end{array}$$



Computing Wyckoff positions

Theorem: Let $H \leq G$ be generated by $\{g_1|t_1\}, \ldots, \{g_s|t_s\}$.
Then $x \in \mathbb{R}^n$ has a site-symmetry group $\mathcal{S}_G(x)$ with $\Pi(\mathcal{S}_G(x)) = \Pi(H)$ iff $(g_i - id)x \equiv -t_i \bmod \mathbb{Z}^n$ for all i.

Idea: Run over the subgroups of $\Pi(G)$ and solve the congruences.
Take care that a solution x may actually have a larger site-symmetry group than the group $\Pi(H)$ for which it was obtained.

Algorithm: Stack $g_1, \ldots, g_s$ vertically in a $ns \times n$ matrix A and the vectors $-t_1, \ldots, -t_s$ in a vector $b \in \mathbb{R}^{ns}$.

Compute the Smith normal form of A, i.e. find $P \in GL_{ns}(\mathbb{Z})$ and $Q \in GL_n(\mathbb{Z})$ such that $PAQ = D$ is a diagonal matrix $diag(d_1, ..., d_r, 0, ..., 0)$.
Then $Ax \equiv b \bmod \mathbb{Z}^n \Leftrightarrow D(Q^{-1}x) \equiv Pb \bmod \mathbb{Z}^n$.

This is solvable iff only the first r components of Pb are nonzero (mod $\mathbb{Z}$) and in this case a solution is easily read off.

Subgroups of finite index

Definition: Let $H \leq G$ be a subgroup of the space group G.

(i) H is called a lattice-equal (translationengleiche) subgroup of G (t-subgroup), if $T(H) = T(G)$, i.e. if $T(G) \leq H$.

(ii) H is called a class-equal (klassengleiche) subgroup of G (k-subgroup), if $\Pi(H) = \Pi(G)$.

Theorem (Hermann, 1929): Every subgroup $H \leq G$ is a lattice-equal subgroup of a uniquely determined class-equal subgroup $M \leq G$, namely of $M := \langle H, T(G) \rangle$.

Corollary: Every maximal subgroup of a space group is either class-equal or lattice-equal.

Lattice-equal subgroups

Theorem: The lattice-equal subgroups of G are the full preimages $\Pi^{-1}(Q)$ of the subgroups $Q \leq \Pi(G)$.

Some remarks:

- For small n (e.g. $n \leq 7$), the full subgroup lattice of the point groups can be computed.
- For soluble groups, especially efficient methods are available.
- A subgroup $Q \leq P$ is maximal if the permutation action on the cosets of Q is primitive.

Class-equal subgroups

Theorem: Let G be a space group with point group $P := \Pi(G)$. Let $H \leq G$ be a class-equal subgroup and denote the translation lattices of G and H by L_G and L_H, respectively.

(i) P acts on L_G/L_H.

(ii) Let $L_H \leq L \leq L_G$ be a P-invariant lattice, then $\langle H, L \rangle$ is a class-equal subgroup of G containing H.

Corollary: If $H < G$ is a maximal class-equal subgroup of G, then L_H is a maximal P-invariant sublattice of L_G.
In particular, L_G/L_H is an irreducible $\mathbb{F}_p P$-module for some prime p.

Thus, find L_H as the kernel of an $\mathbb{F}_p P$-epimorphism from L_G to an irreducible constituent of L_G/pL_G. Use (e.g.) the MeatAxe!

Complements

If $H \leq G$ is a maximal class-equal subgroup of G, then $H/T(H)$ is a complement of $T(G)/T(H)$ in $G/T(H)$.
However, not for every P-invariant sublattice $T(H)$ of $T(G)$, there exists a complement of $T(G)/T(H)$ in $G/T(H)$.

- If $\gcd(|P|, [T(G) : T(H)]) = 1$ then there exists a complement and all complements are conjugate (Schur-Zassenhaus).

- The problem of finding complements boils down to adjusting the vector system $\{t_g \mid g \in \Pi(G)\}$ to a vector system $\{t'_g \mid g \in \Pi(G)\}$ such that $t'_g - t_g \in L_G$ and such that with the new vector system the relations of $\Pi(G)$ evaluate to translations in L_H.
  This is not difficult, but somewhat technical.

Examples of class-equal subgroups

Example 1: The space group `p2mm` generated by

$$g := \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \text{ and } h := \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right)$$

has a maximal P-invariant sublattice with basis $(2e_1, e_2)$.
The translation parts of g and h can independently be changed to $(1,0)^{tr}$, giving rise to four maximal class-equal subgroups for this lattice.

Example 2: The space group `pg` generated by $g := \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right)$ has a maximal P-invariant sublattice with basis $(e_1, 2e_2)$. Since

$$\left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & \frac{1}{2} + y \\ \hline 0 & 0 & 1 \end{array}\right)^2 = \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & \frac{1}{2} + 2y \\ \hline 0 & 0 & 1 \end{array}\right)$$

and $\frac{1}{2} + 2y \notin \mathbb{Z}$ for $y \in \mathbb{Z}$, there is no class-equal subgroup for this lattice.

Minimal supergroups

In some situations, one is interested in space groups G such that a given space group H is a maximal subgroup of G. In this case G is called a minimal supergroup of H.

- Class-equal minimal supergroups are easy to determine:
  For $P := \Pi(H) = \Pi(G)$, find the minimal P-invariant superlattices L of L_H (for which again L/L_H is an irreducible $\mathbb{F}_p P$-module) and form $G := \langle H, L \rangle$.
- Lattice-equal minimal supergroups can be tricky, e.g. when $\Pi(H) = \{1\}$. In this case the orientation of an additional symmetry element is undetermined.
  However, in many cases additional information is available which allows to obtain the possible point groups of G.
- Given $\Pi(G)$ such that $\Pi(H)$ is a maximal subgroup of $\Pi(G)$, one has to determine the vector systems for $\Pi(G)$ which restrict to the vector system of H (on $\Pi(H)$).

Colour groups

Let G be a transformation group acting on a system of points (areas, vectors, etc.). Every point is supposed to have a certain property, e.g. a colour, which takes only finitely many values.
Each transformation $g \in G$ is assumed to induce a permutation π_g of the colours.

Definition (Belov, Tarhova): A colour-symmetry group is given by the combined product

$$(g, \pi_g) \cdot (h, \pi_h) = (gh, \pi_g \pi_h).$$

Crucial observation: The mapping $\rho : g \longrightarrow \pi_g$ is a permutation representation of G.
In particular, $\rho(G)$ is a factor group of G and the colour-symmetry group is a subdirect product of G and $\rho(G)$, amalgamated over $\rho(G)$.

Transitive permutation actions

Assume that the colour group acts transitive on the colours, i.e. that for any pair of colours there is a transformation mapping a point of the one colour to a point of the other colour.

Theorem: Every transitive permutation representation of G is obtained as the permutation of the cosets of a subgroup.
Two such representations are equivalent if the subgroups are conjugate.

Consequence: The transitive colour groups with transformation group G correspond uniquely to the conjugacy classes of subgroups of G.
For colourings with k colours, only the subgroups of index k have to be considered.

If $H \leq G$ is the stabilizer of colour c_1 and if g maps colour c_1 to c_i, then the coset gH is the set of *all* elements mapping c_1 to c_i.

Starting with the colour c_i instead of c_1, H is replaced by gHg^{-1}.

Colour groups vs. colourings

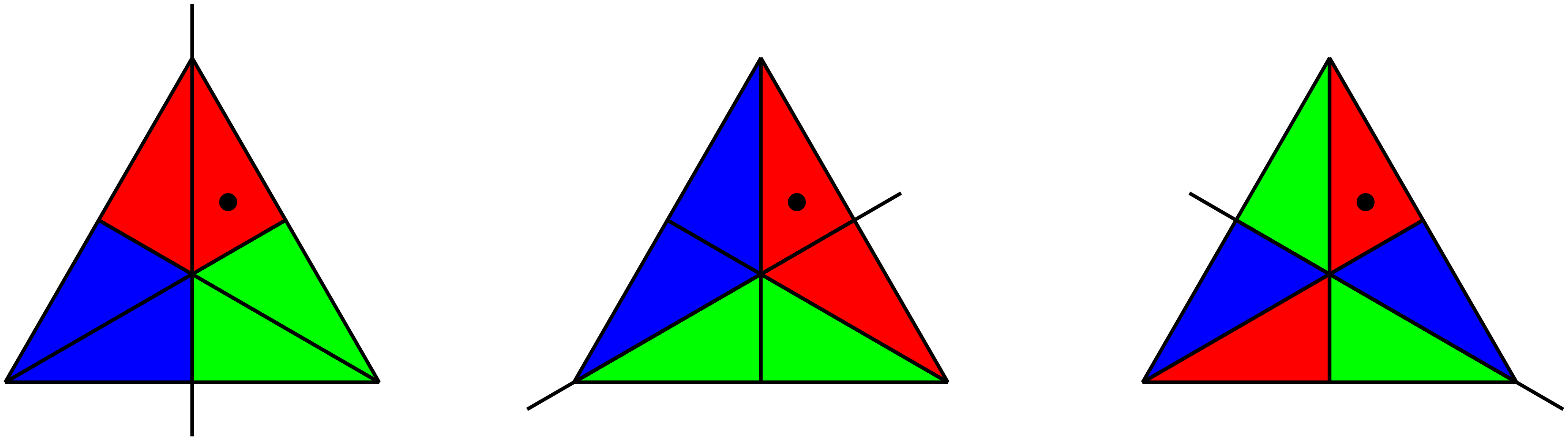
A group-subgroup pair (G, H) can be interpreted as a colour-symmetry group by applying the elements of the different cosets $g_1 H, \ldots, g_k H$ to a point x in general position and giving $g_i H \cdot x$ colour c_i.

However, different choices of the location of the point x with respect to the subgroup may give rise to different colourings.

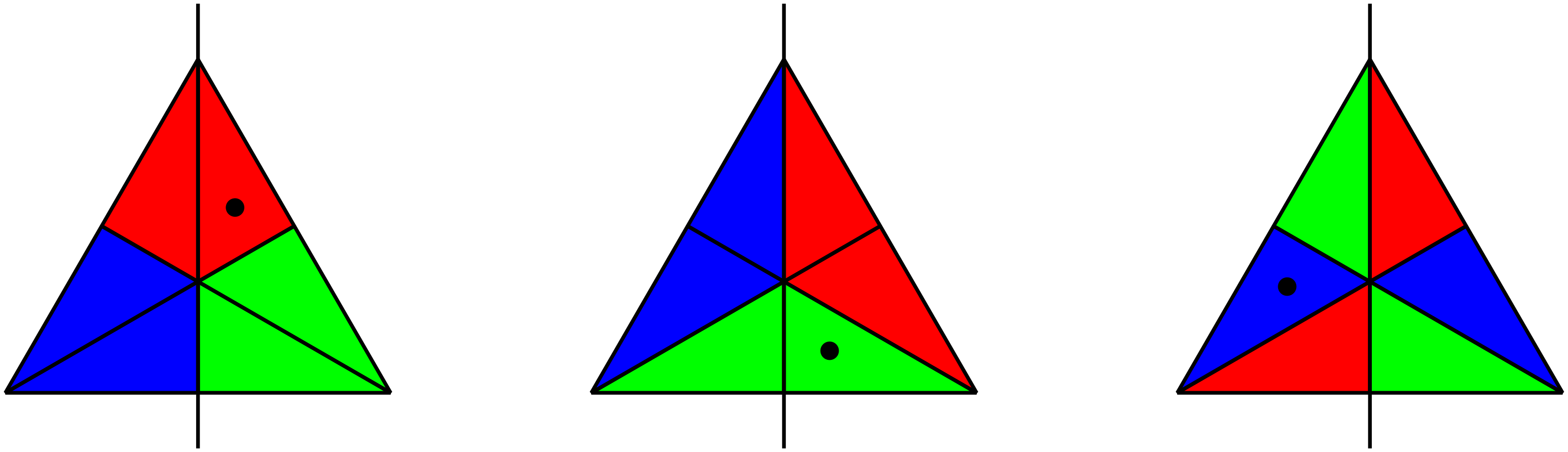
There are two perspectives from which this can be interpreted:

- If the point in general position is kept, the different conjugate subgroups correspond to the different colourings.
- If the subgroup is kept, the different points in the orbit (under G) of the point in general position give the different colourings.

Fixed point position, conjugate subgroups

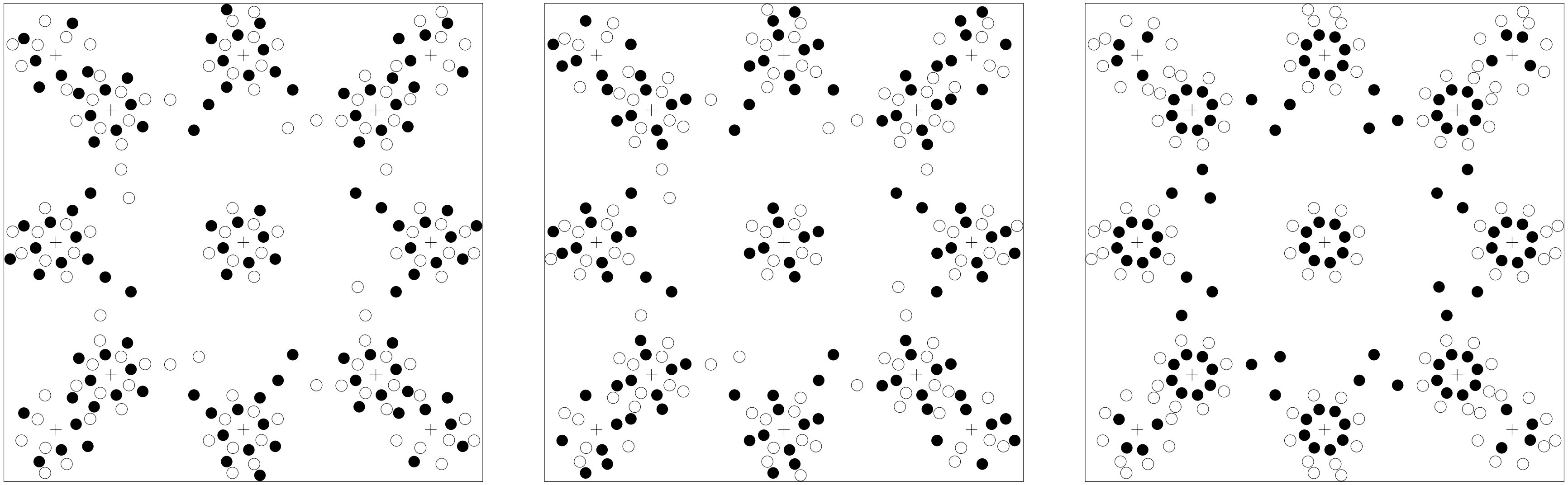


Fixed subgroup, different point positions



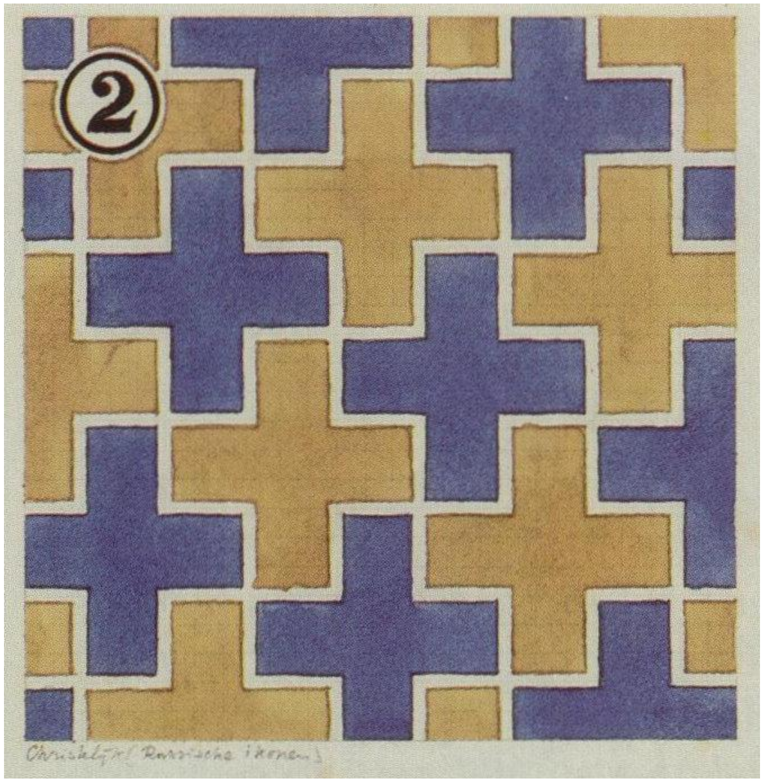
Group-subgroup relations as colourings

Coulor groups are an excellent way to illustrate group-subgroup relations.



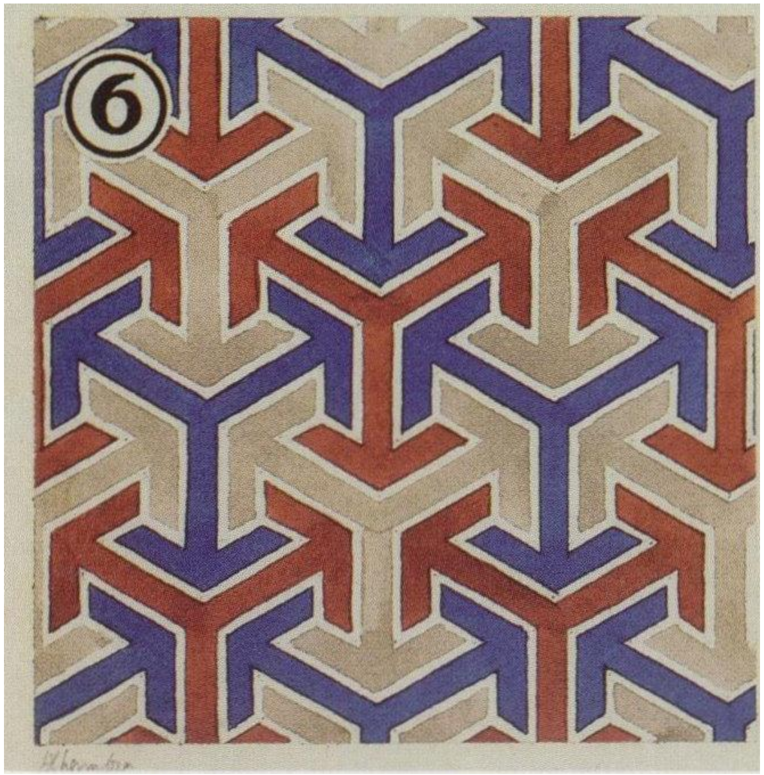
Three different class-equal subgroups of index 2 in a 4-dimensional space group containing an 8-fold rotation.

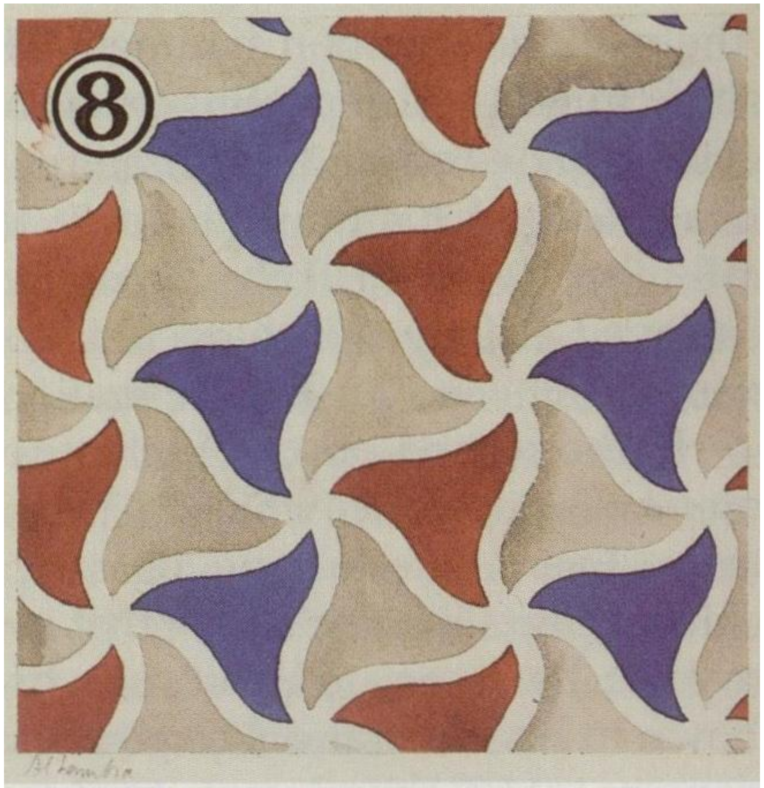
Examples collected by M.C. Escher



(2): Russian icon: class-equal subgroup

(3): Mesquita, Cordoba: lattice-equal subgroup (4-fold rotation not in the subgroup)





(6): Alhambra, Granada: class-equal subgroup

(8): Alhambra, Granada: not a colour-group (only after disregarding 3-fold rotations)

Splitting of Wyckoff positions

The transition from G to a subgroup $H \leq G$ has one or both of the following effects on a Wyckoff position x of G:

- The site-symmetry of x in H is reduced.
- The orbit x^G under G splits into several orbits $x_1^H, \ldots, x_s^H$ under H.

Theorem: $\sum_{i=1}^{s} [\mathcal{S}_G(x) : \mathcal{S}_H(x_i)] = [G : H]$.

Extreme cases:

- $\mathcal{S}_H(x_i) = \mathcal{S}_G(x) \Rightarrow$ splitting into $[G : H]$ orbits (e.g. for general position).
- $x^H = x^G \Rightarrow [\mathcal{S}_G(x) : \mathcal{S}_H(x)] = [G : H]$ (requires H to be a lattice-equal subgroup).

Phase transition

The alloy $CuZn$ (β-brass) has a disorder-order transition at 741 K.
In the high-temperature form, Cu and Zn atoms randomly occupy the points of the orbit of $(0,0,0)^{tr}$ under the space group `Im3m`, i.e. the points

$$\begin{pmatrix}0\\0\\0\end{pmatrix} + \mathbb{Z}^3 \bigcup \begin{pmatrix}1/2\\1/2\\1/2\end{pmatrix} + \mathbb{Z}^3$$

of the body-centered cubic lattice.

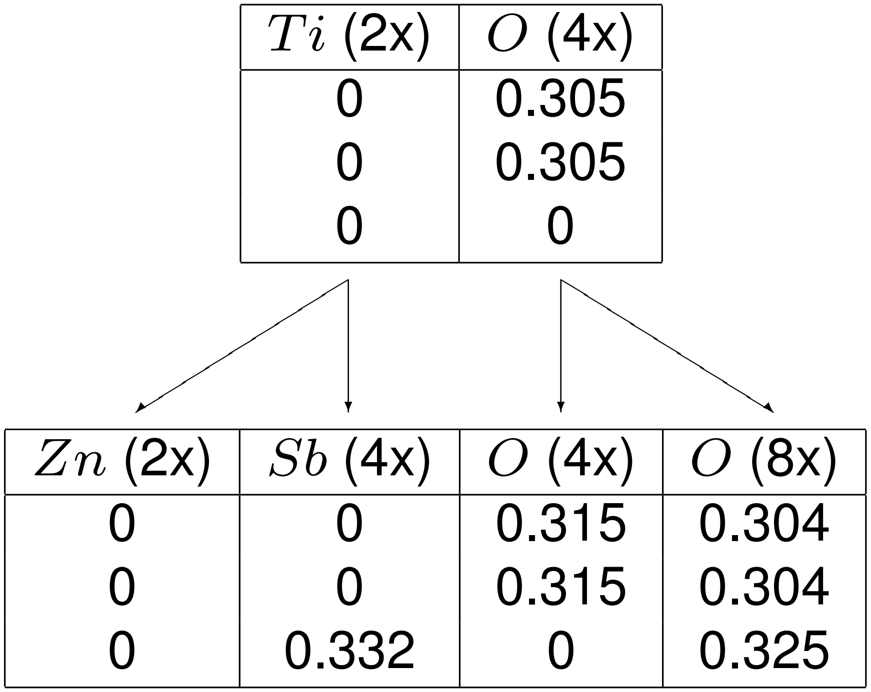
In the ordered state, both kinds of atoms form a (primitive) cubic lattice, and each kind occupies the centers of the cubes of the other kind.

The corresponding space group of type $\mathtt{Pm\overline{3}m}$ is a class-equal subgroup of index 2 of the space group $\mathtt{Im\overline{3}m}$.

Isomorphic subgroup example

$Ti\,O_2$ (rutile) has space group $\mathtt{P4_2/mnm}$ (with point group $\cong D_4 \times C_2$). This group has a class-equal subgroup of index 3, upon scaling the translation lattice by 3 along the axis of the 4-fold rotation (z-axis).

This subgroup allows to replace the Ti-atoms by two different kinds of atoms in the ratio 1:2, to obtain e.g. $Zn\,Sb_2\,O_6$ (trirutile).



Ti (2x)	O (4x)
0	0.305
0	0.305
0	0

Zn (2x)	Sb (4x)	O (4x)	O (8x)
0	0	0.315	0.304
0	0	0.315	0.304
0	0.332	0	0.325

Prediction of new structures

A crystal is called ferroelectric if it has an electric dipole moment the direction of which can be changed by an electric field.

An electric dipole moment can only exist in polar structures, i.e. in structures that have an axis which has no symmetrically equivalent directions, e.g. a unique rotation axis.

Good candidates for displacive ferroelectric materials are polar structures whose atomic positions deviate only slightly from a hypothetical non-polar configuration (of higher symmetry), since a phase transition between these configurations at higher temperatures is very likely.

Idea: Given the space group H of a polar structure $\mathcal{S}$, look at the minimal supergroups G which are non-polar.

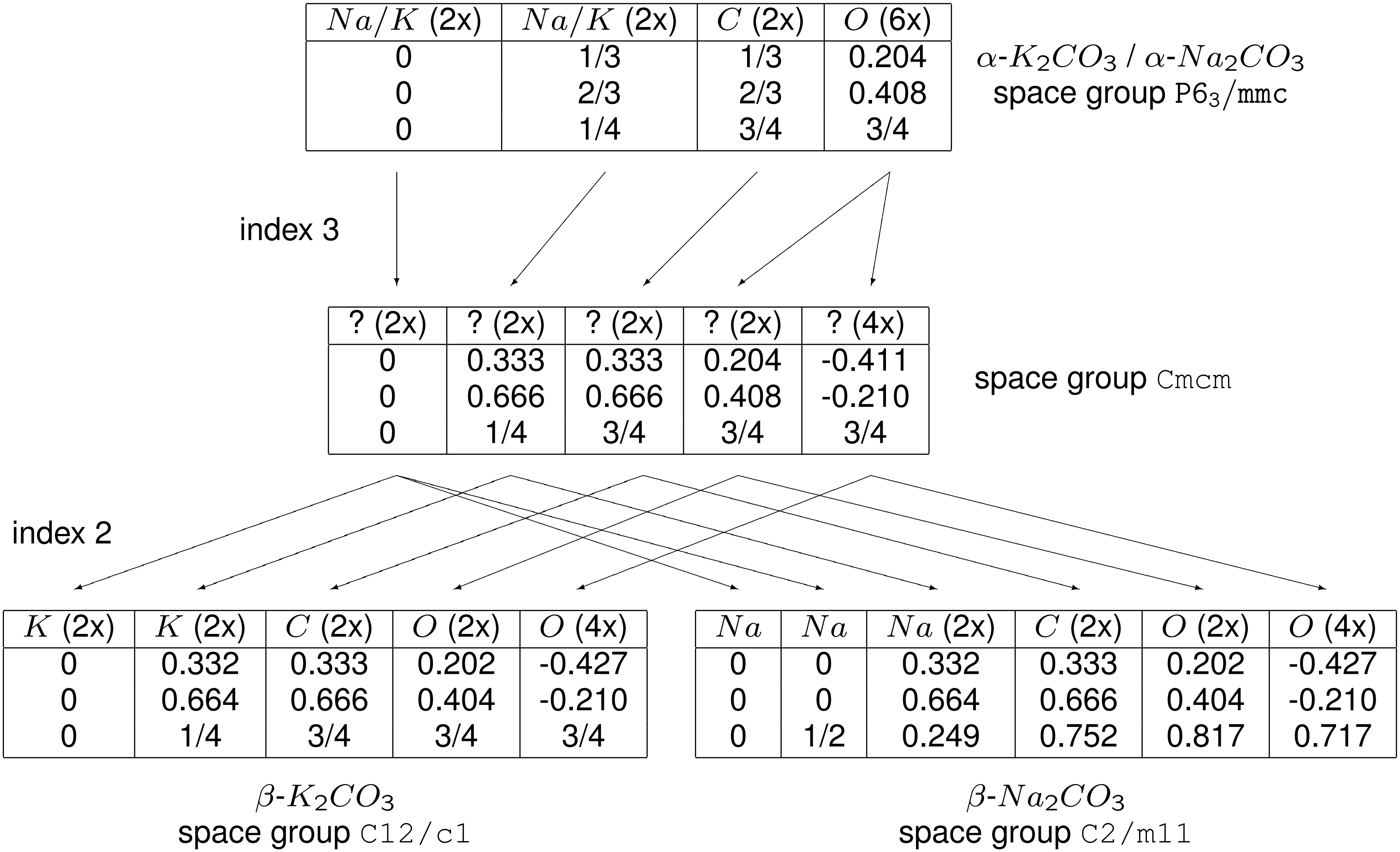
Check for coset representatives $g_1, \ldots, g_k$ of H in G whether they are pseudosymmetries of $\mathcal{S}$, i.e. whether $g_i\mathcal{S}$ can be matched with $\mathcal{S}$ with small deviations only.

Hypothetical structure

The alkali metal carbonates β-K_2CO_3 and β-Na_2CO_3 have similar structures and unit cells, but their space groups `C12/c1` and `C2/m11` (with point group of order 4) are not in a group-subgroup relation.

The only candidate for a common minimal supergroup is `Cmcm` (point group of order 8), but no structure with this group can be related to the given carbonate structures.

However, `Cmcm` has a minimal supergroup $\mathtt{P6_3/mmc}$ (point group of order 24) and the high-temperature modifications α-K_2CO_3 and α-Na_2CO_3 crystallize in a structure with this space group.



Na/K (2x)	Na/K (2x)	C (2x)	O (6x)
0	1/3	1/3	0.204
0	2/3	2/3	0.408
0	1/4	3/4	3/4

α-K_2CO_3 / α-Na_2CO_3
space group $P6_3/mmc$

index 3

? (2x)	? (2x)	? (2x)	? (2x)	? (4x)
0	0.333	0.333	0.204	-0.411
0	0.666	0.666	0.408	-0.210
0	1/4	3/4	3/4	3/4

space group `Cmcm`

index 2

K (2x)	K (2x)	C (2x)	O (2x)	O (4x)
0	0.332	0.333	0.202	-0.427
0	0.664	0.666	0.404	-0.210
0	1/4	3/4	3/4	3/4

β-K_2CO_3
space group `C12/c1`

Na	Na	Na (2x)	C (2x)	O (2x)	O (4x)
0	0	0.332	0.333	0.202	-0.427
0	0	0.664	0.666	0.404	-0.210
0	1/2	0.249	0.752	0.817	0.717

β-Na_2CO_3
space group `C2/m11`