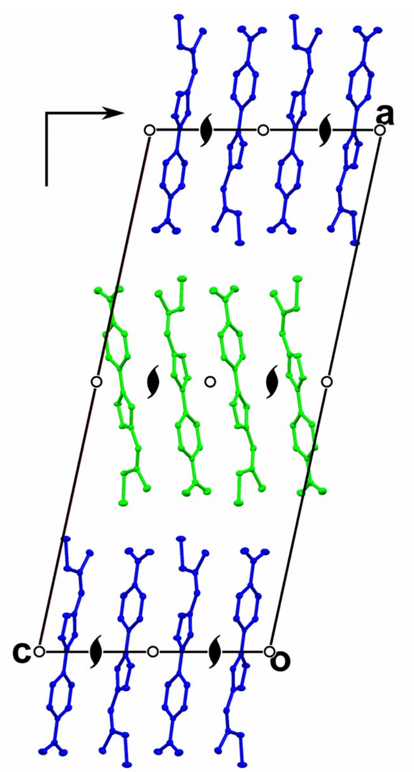
Exercises on OD structures

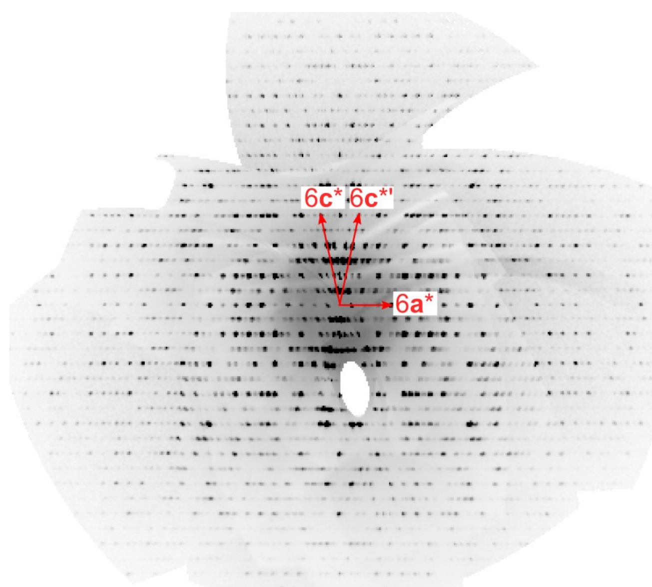
Exercise 1: OD layers

Locate OD layers, determine their (idealized) layer symmetry and one kind of PO relating adjacent layers (if any) explaining the observed stacking faults. The solutions are not necessarily unique. OD layers do not necessarily correspond to chemical layers. The solutions should not allow for more stacking possibilities than given.

Exercise 1a

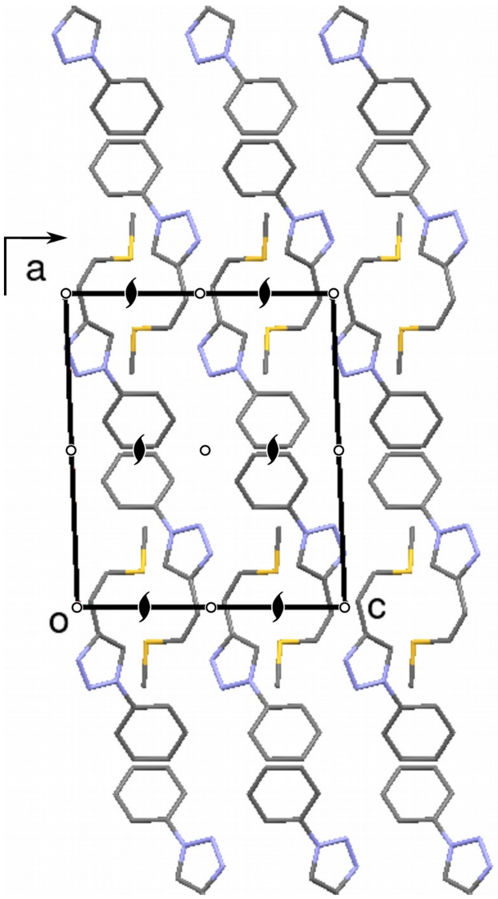
An organic molecule crystallizing with $P2_1/c$ symmetry. Molecules are colored according to space group symmetry. All crystals were systematically twinned by reflection at (001). The diffraction pattern is shown for information only and does not help with the solution. Hint: locate non-space group symmetry that maps blue onto green molecules.

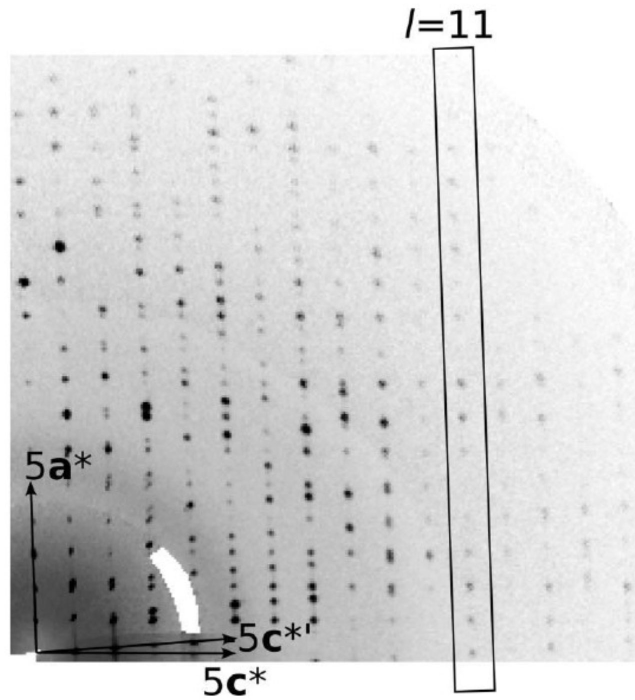




Exercise 1b

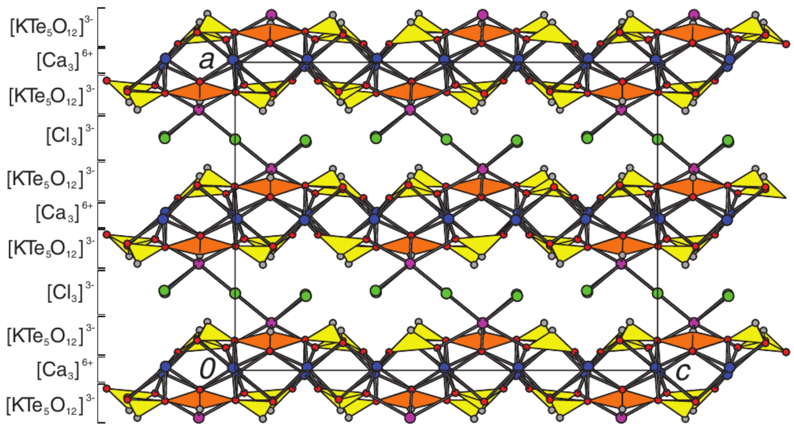
An organic molecule crystallizing in $P2_1/c$ symmetry. All crystals were systematically twinned by $m_{[001]}$. The diffraction pattern is shown for information only and does not help with the solution.



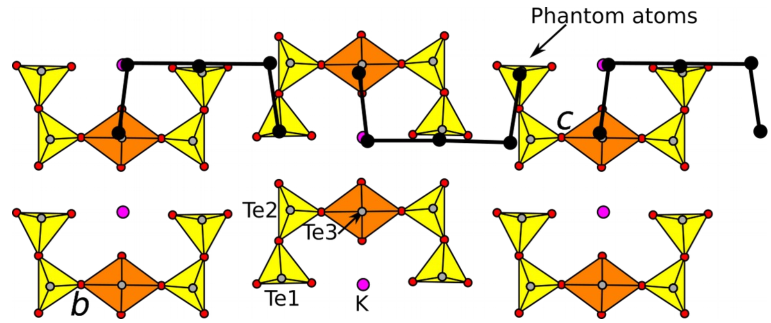


Exercise 1c

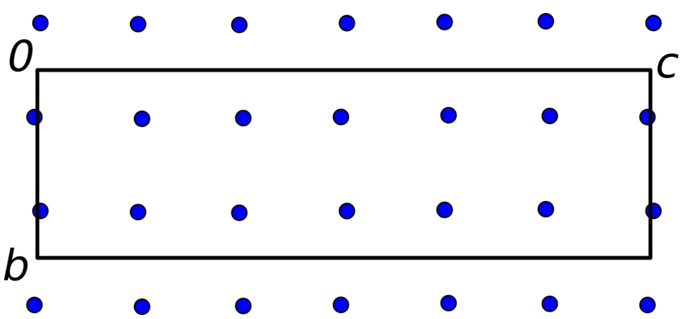
A potassium chloride tellurate (IV) crystallizing as allotwins (two polytypes with *C*2/*c* and *I*2/*a* symmetry, each in two orientations). When only reflections of one domain are used for refinement, distinct phantom atoms of the other polytype appear in difference Fourier maps. Hint: Te is the heaviest atom in the structure, therefore the phantom atoms correspond most likely to Te.



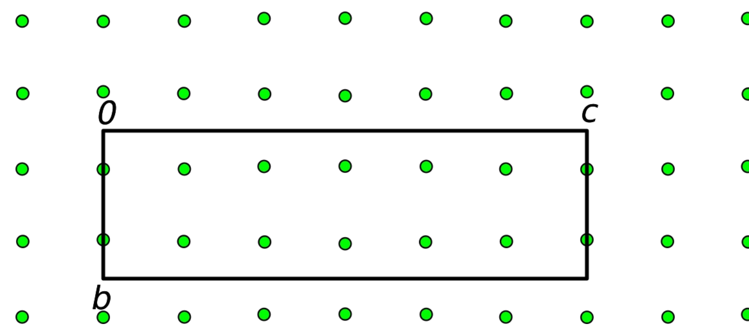
I2/a polytype viewed down [010]



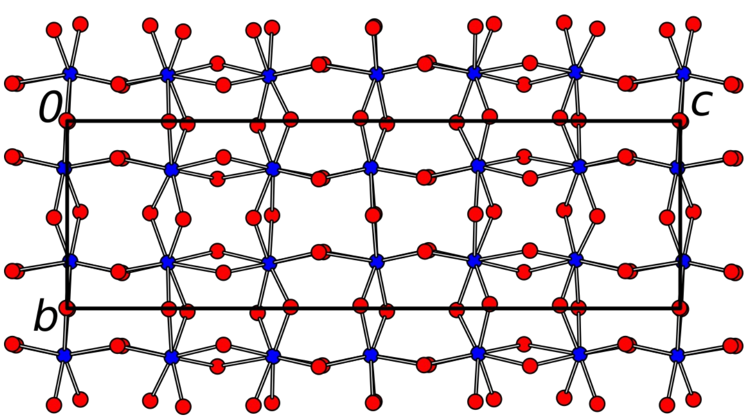
Te/K/O atoms. Phantom atoms in black. Black lines for visual guide only.



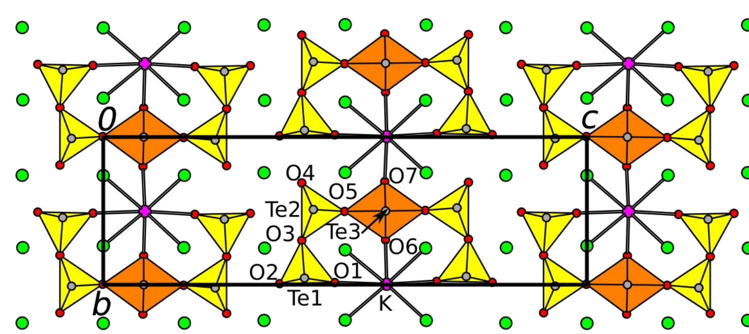
Only Ca atoms



Only Cl atoms



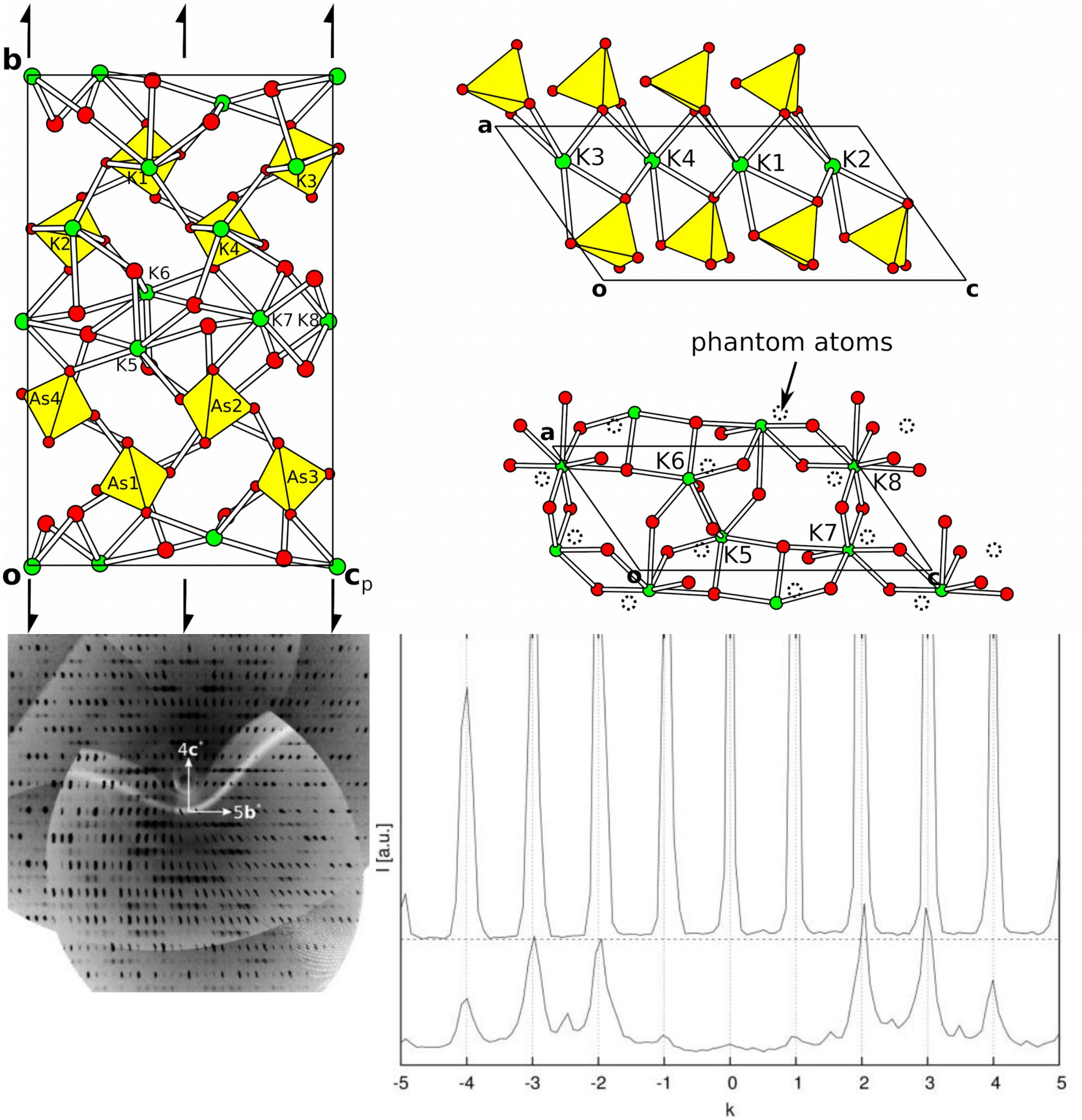
Ca atoms and adjacent O atoms



K/Te/O and adjacent Cl atoms

Exercise 1d

A potassium arsenate hydrate crystallizing with $P2_1$ symmetry. The crystals are systematically twinned by inversion. Additional reflections and distinct phantom atoms are observed. The diffraction pattern is given for information only. Hint: there are two solutions, one more obvious than the other.

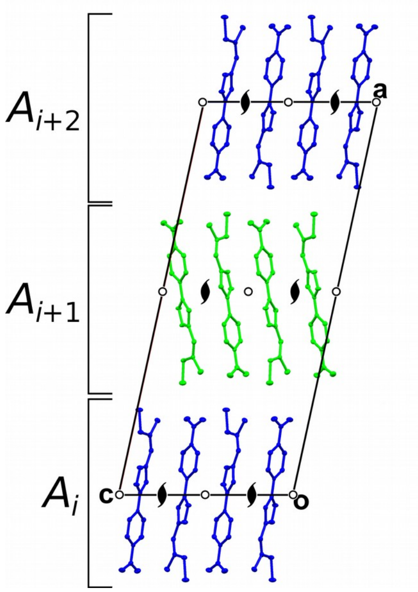


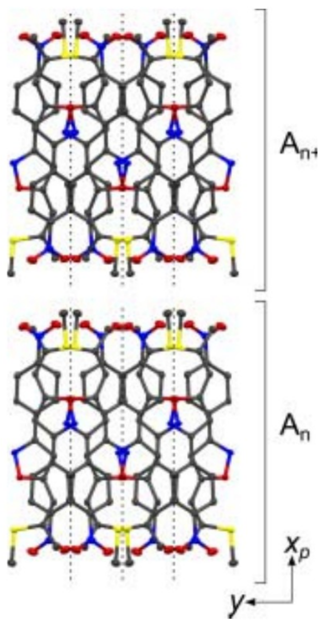
Exercise 2: POs

List all σ-POs relating adjacent layers up to the common lattice of the layers using generalized Hermann-Mauguin symbols and give the direction. To indicate intrinsic translations use variables *r*, *s* or actual values if they are fixed for structural reasons.

Exercise 2a

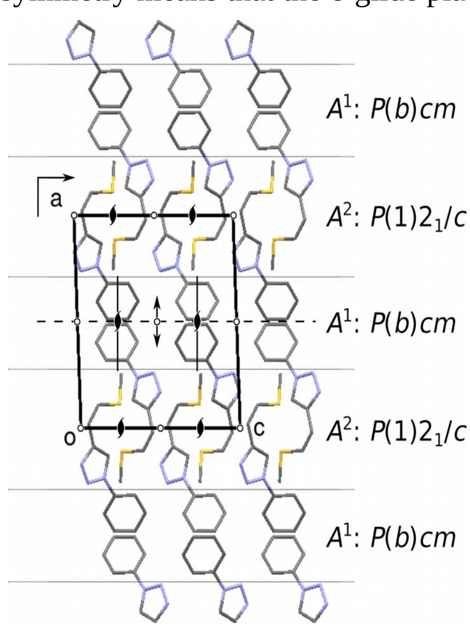
Organic molecule, layer symmetry $P(1)2_1/c1$, space group symmetry $P2_1/c$. Hint: note that the *c*-glide planes of all layers overlap perfectly. Hint: When factoring out the translation subgroup of $P(1)2_1/c$, a group with four elements is obtained. Representative elements in this group: { 1, $\bar{1}$, 2_1, c}. Therefore, there should be (up to translation) four σ-POs.





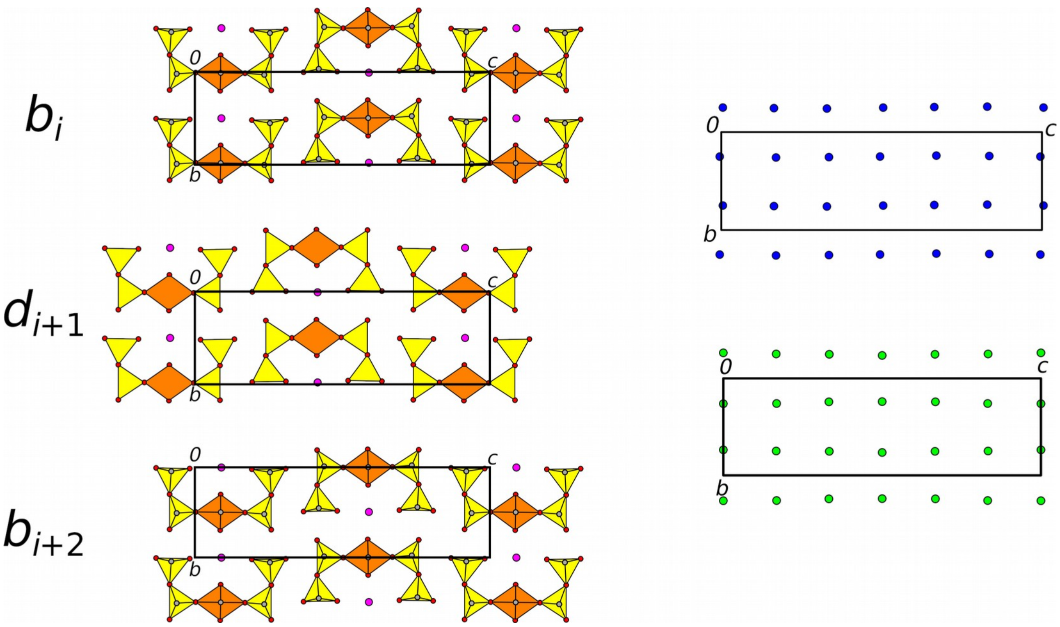
Exercise 2b

Organic molecule crystallizing with $P2_1/c$ symmetry. Two kinds of layers with symmetry $P(b)cm$ and $P(1)2_1/c1$. Hint: the space group symmetry means that the c-glide places of all layers overlap perfectly.



Exercise 2c

A potassium chloride tellurate (IV) with layers of $P(2)cm$ symmetry. There are two kinds of layer contacts and therefore two sets of σ-POs. Hint: The Ca and Cl atoms belong to both adjacent layers. This means that they must be mapped by the σ-POs and therefore the intrinsic translations can only adopt discrete values. Hint: The order of $P(2)cm$ factored by its translation group is 4.

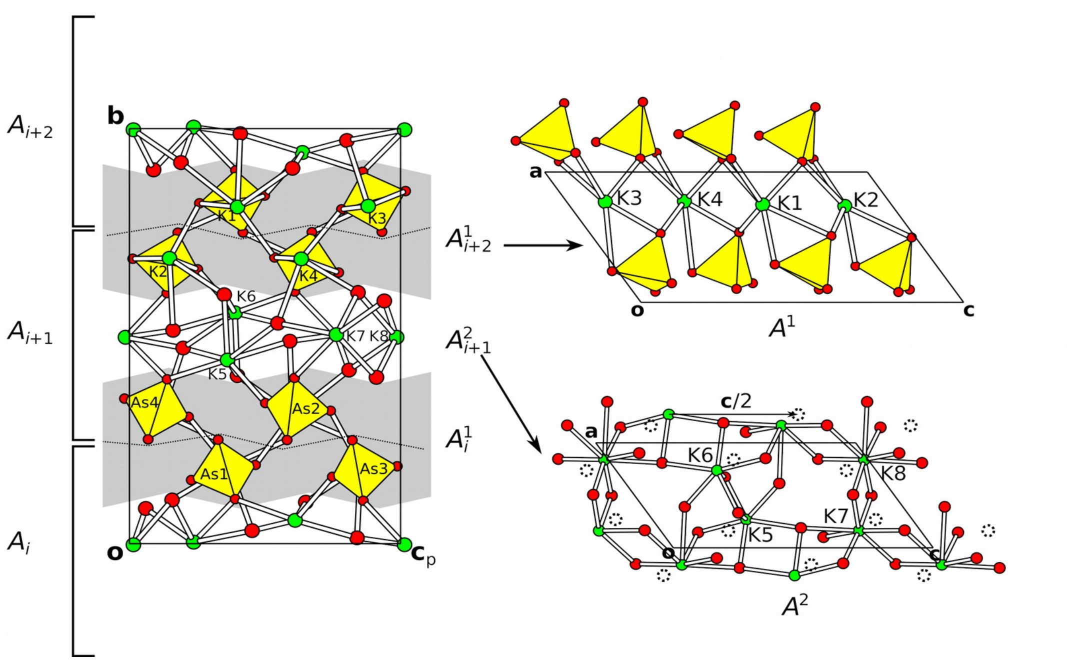


Exercise 2d

A potassium arsenate hydrate crystallizing with $P2_1$ symmetry. Two OD interpretations, one of them trivial.

Interpretation 1: A^1: $X1(c)1$ [centering (00½)], A^2: $P\bar{1}(\bar{1})\bar{1}$

Interpretation 2: A: $P\bar{1}(\bar{1})\bar{1}$

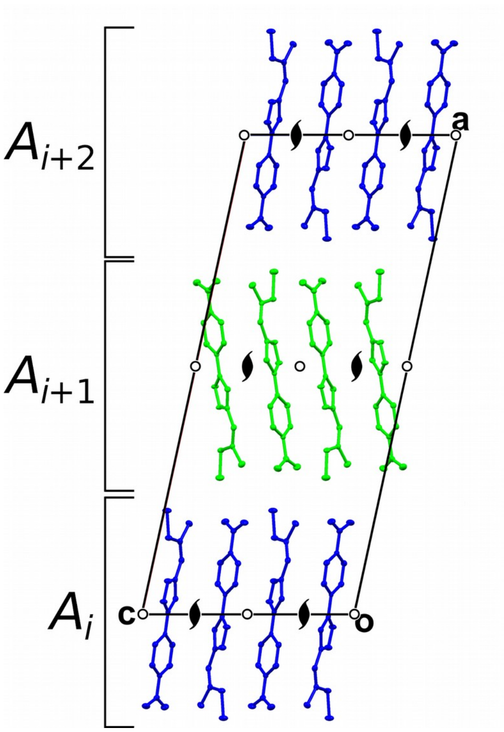


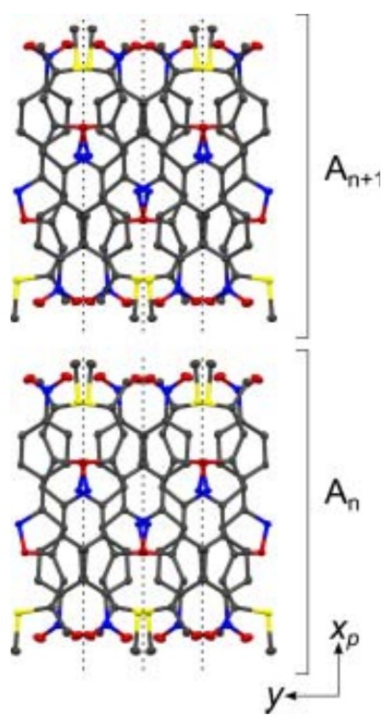
Exercise 3: NFZ relationship

For the given layer contacts: are there σ-ρ-POs but no reverse continuations? What are the groups of operations of λ-τ-POs valid for a single layer and for both layers. How many stacking possibilities are there according to the NFZ relationship, how are they related?

Exercise 3a

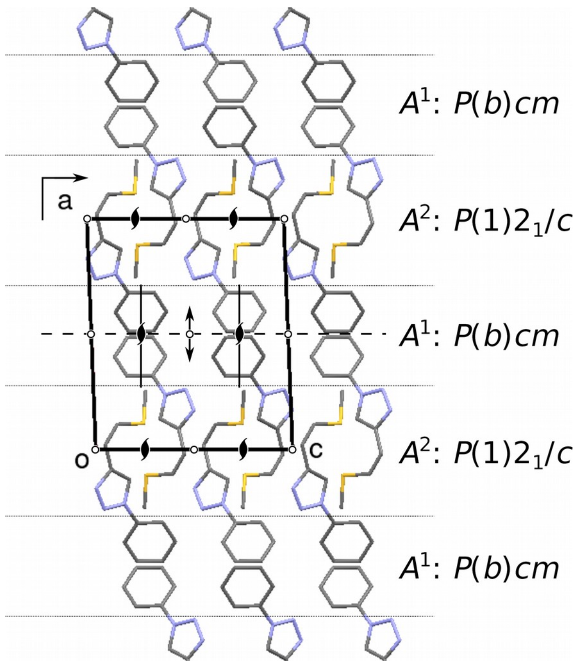
Organic molecule, layer symmetry $P(1)2_1/c$, σ-POs:
[100]: τ: 2_2, ρ: $n_{1,s}$
[001]: ρ: 2_{s+1}, τ: a_2
Hint: reverse continuations can only be σ-ρ-POs.





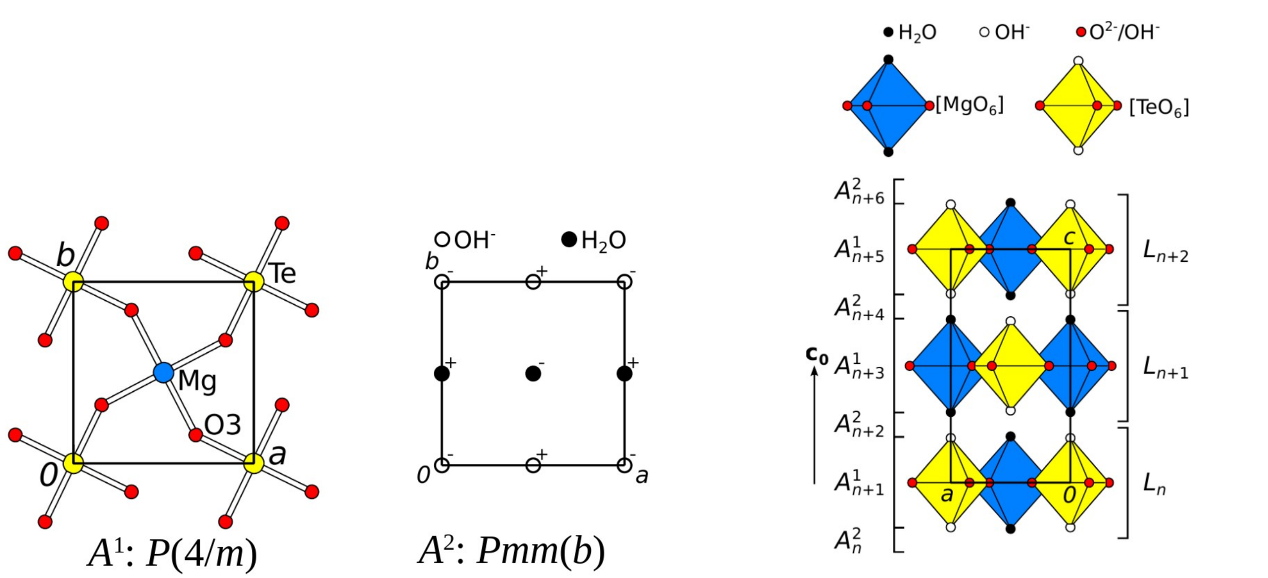
Exercise 3b

Organic molecule, two kinds of layers, space group symmetry $P2_1/c$. Hint: the space group symmetry requires that the *c*-glide planes of all layers overlap perfectly.



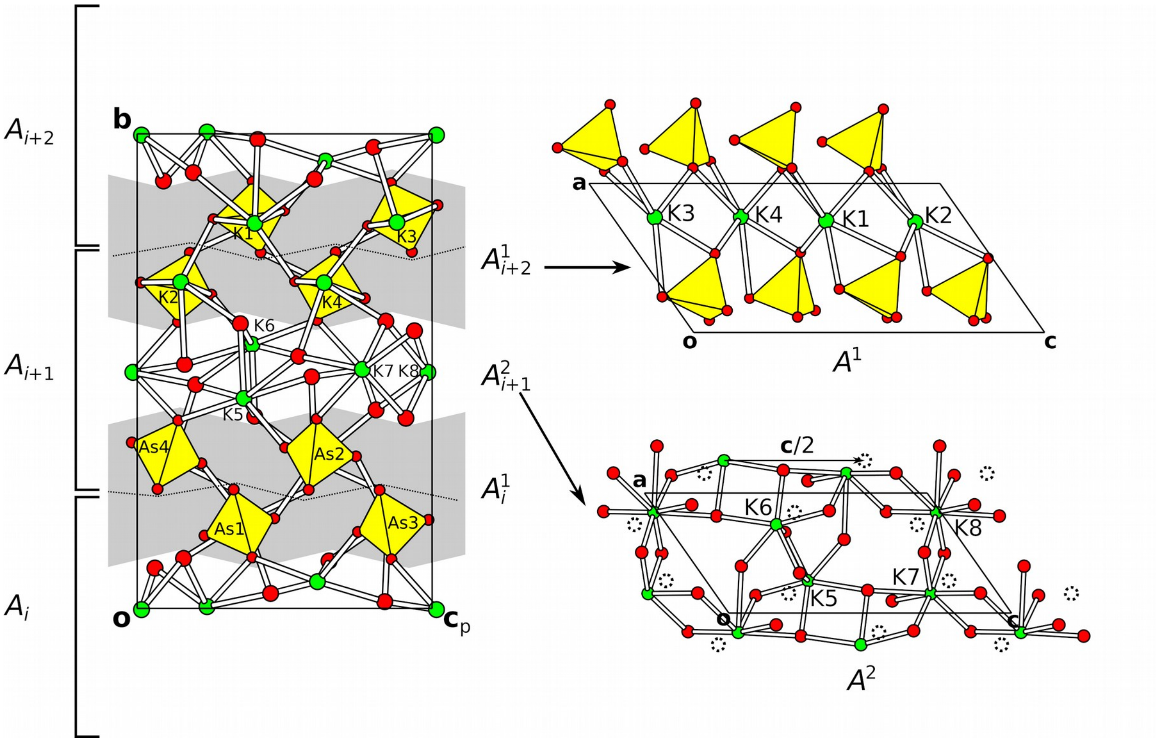
Exercise 3c

$MgTeOH_8$, two kinds of layers with $P(4/m)$ and $Pmm(b)$ [or $Pmm(a)$] symmetry. The four- and twofold axes of the two layers overlap perfectly.



Exercise 3d

A potassium arsenate hydrate crystallizing with $P2_1$ symmetry. Two OD interpretations.
Interpretation 1: A^1: $X1(c)1$ [centering (00½)], A^2: $P\bar{1}(\bar{1})\bar{1}$, no σ-POs
Interpretation 2: A: $P\bar{1}(\bar{1})\bar{1}$, σ-POs: [010]: 2_2, $c_{1/2}$.



Exercise 4: OD categories

Exercise 4a

Derive the categories of OD structures made of layers of 3 kinds.

Exercise 4b

What are the categories of the OD structures of exercises 3a, 3b, 2c, 3c, 3d?

Exercise 5: OD groupoid families

Give OD groupoid family symbols of the OD structures of exercises 3a, 3b, 2c, 3c, 3d.