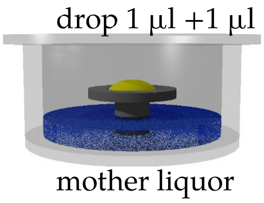
1 Crystal growth



A sample is crystallised by vapour diffusion in a sealed container. Your sample is dissolved in pure EtOH at a concentration c. The mother liquor is a mixture of 7:3 (v/v) $H_2O/EtOH$. Before sealing the container, you mixed 1 µl of the sample with 1 µl of mother liquor in the table.

1. What is the content of the drop immediately after mixing?
2. What is the content of the drop after equilibration?
3. Estimate how long it takes to reach equilibrium
4. What measures are there to reduce the time for equilibration?

Make use of your common sense, rather than a pocket calculator!

2 Symmetry

A mirror seems to swap your hands: left hand becomes right and, and right hand becomes left hand. Why does the mirror not swap up and down?

3 Fractional coordinates

A point inside the "original" unit cell has fractional coordinates between 0 and 1 ($0 \leq x, y, z < 1$). Since each unit cell is the same, one can add or subtract 1 to each of coordinate x, y, or z, without modifying the crystal.

In two dimensions, the atoms of oxalic acid (*cf. lecture* № 2) may have the following coordinates:

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C1  -0.17  0.09  0.00
O3   0.35 -0.10  0.00
O2  -0.19 -0.26  0.00
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1. Sketch these three atoms based on the fractional coordinates!
2. Move all atoms into the "original" unit cell!
3. Why does it make sense to list atoms with negative fractional coordinates, instead of the "normalised" coordinates of part b?
4. Why are some atoms of oxalic acid missing in this list?

4 Bragg's Law

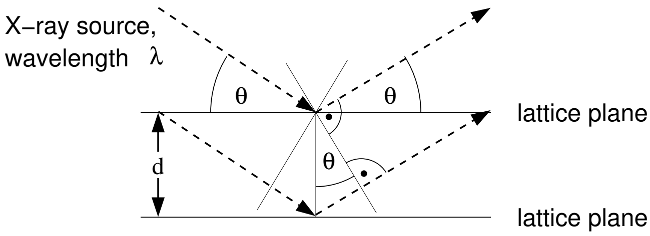
Bragg's law reads

$$\lambda = 2d \sin\theta$$

1. Use Bragg's law to show that the maximum resolution d_{min} of any diffraction experiment is given by

$$d \geq d_{\text{min}} = \lambda/2$$

2. In the next drawing, mark the path difference between the top and the bottom reflected ray!



3. Derive Bragg's law $\lambda = 2d \sin\theta$ from this drawing!

5 Diffraction theory I

Use the Laue equations

$$\vec{a} \cdot \vec{S} = |\vec{a}||\vec{S}| \cos(\vec{a}, \vec{S}) = h$$
$$\vec{b} \cdot \vec{S} = |\vec{b}||\vec{S}| \cos(\vec{b}, \vec{S}) = k$$
$$\vec{c} \cdot \vec{S} = |\vec{c}||\vec{S}| \cos(\vec{c}, \vec{S}) = l$$

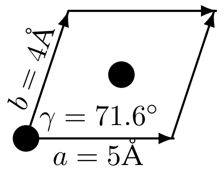
to show that there is always a reflection in the direction of the direct beam S_{in}!

Start with a sketch of the corresponding scattering vector $\vec{S} = \vec{S}_{\text{out}} - \vec{S}_{\text{in}}$!

6 Diffraction theory II

The unit cell in the drawing below contains an atom at the origin $(0, 0, 0)$ and an atom (of the same element type) at the centre of the cell $(0.5, 0.5, 0.5)$ [1]. The crystal is exposed to X-rays so that both atoms emit a spherical wave of amplitude 1.

[1] The Cartesian coordinates for the second atom read (3.12Å, 1.897Å, ???Å)



1. What is the amplitude of the reflections
   a) (1, 0,0)
   b) (0,1,0)
   c) (1,1,0)
2. Which reflections have a different amplitude if the second atoms would have coordinates $(0.5, 0, 0)$?
3. The answer to the previous question is independent of the wavelength λ of the X-rays. Why is this so?