University of Kasdi Merbah - Ouargla-

Faculty of Mathematics and Material Sciences

Chemistry Department

Master 01(Matter Chemistry)

2024-2025

Series of exercises and problems - Radiocrystallography - No. 01

Exercise 1:

1) What is the difference between reflection and diffraction?

2) Why there are two types of rays in the X-ray spectrum emitted by any target material?

Exercise 2:

The energy of an X-ray photon is given in electron volts, in terms of wavelength, by the following relation: $E = \frac{12400}{\lambda}$

1) State the energy range of X-rays used in crystallography.

2) Find the required voltage to produce X-rays by accelerating electrons, to collide with a copper target with an efficiency of 0.3%.

3) Determine a range of atomic numbers (Z) for elements that can be used as anticathode to produce X-rays at a voltage of (500 kV) for a crystallographic structural investigation.

Exercise 3:

1) The tube is equipped with a copper anode. Give the wavelengths and energies of the lines emitted by the anode.

2) Calculate the transmission of 0.4 mm thick beryllium window for the Kα line. We have:

$I = I_0\, e^{-\mu x}$; $\mu = \rho\mu_0$; $l_{bs} = 1/\rho\mu_0 = 5.37\ mm$

3) Repeat questions (1) and (2) for a tungsten anode.

Exercise 4:

The gold and copper alloy crystallizes in the cubic system, where the copper atoms' positions are: $\left(\frac{1}{2},\frac{1}{2},0\right)$,$\left(\frac{1}{2},0,\frac{1}{2}\right)$,$\left(0,\frac{1}{2},\frac{1}{2}\right)$, and the position of gold atom is $(0,0,0)$.

1) Determine the Bravais lattice corresponding to this alloy.

2) Find the number of the first nearest neighbor and its type and calculate the corresponding distance.

3) Deduce the chemical formula of this alloy.

4) If the radius of the gold atom is within the range of 1.36 Å, and the radius of the copper atom is 1.32 Å, calculate the weight density of this alloy.

5) Considering the Lorentz correction for radiation intensity. Calculate the structure factor and the X-ray intensity for the first six peaks, for a powder sample.

The molecular Weight of gold is ***196.97 g/mol,*** *and the* molecular Weight of copper equal to ***63.55 g/mol.***

Exercise 5:

Consider the following space groups (orthorhombic system).

$$P\,ban,\quad C\,mcm \text{ and } I\,bam$$

1) Identify and describe each of the symmetry elements in the previous groups.

2) Find the systematic extinctions for these Space Groups.

Exercise 6:

The lattice parameters for the $Cu_2(OH)_2$ (*copper(II) dihydroxide*) component in its orthorhombic crystal form (space group **$Cmc2_1$**) are typically as follows:

a ≈ 5.02 Å, b ≈ 3.08 Å, c ≈ 9.02 Å.

In the crystal structure of $Cu_2(OH)_2$, the positions of the atoms vary depending on the structure and the space group, in general description of the positions of the atoms in the lattice: : Two sites for the copper ion in the lattice. The positions can be approximately:

Cu: (0, 0, 0), Cu: (1/2, 1/2, 1/4)

The oxygen atoms in hydroxide groups are at specific positions, often bonded to the copper sites. example, the positions for O could be:

O: (0, 0, 1/2), O: (0, 0, 3/4)

The hydrogen atoms in hydroxyl groups are usually bonded to oxygen atoms. they are at a specific distance from the oxygen, usually given by position coordinates, such as:

H: (0, 0, 1/2), H: (0, 0, 3/4)

bonded to the first and the second oxygen respectively.

1) Describe the symmetry space group of this component.

2) Draw the projection of the crystal cell on the planes (100), (010), (001).

3) Find the systematic extinctions for these Space Groups.

4) Considering the Lorentz factor. Calculate the first six peaks for XRD.