

**BOWEN UNIVERSITY, IWO, OSUN STATE**  
**COLLEGE OF AGRICULTURE, ENGINEERING AND SCIENCE**  
**INDUSTRIAL CHEMISTRY PROGRAMME**

**2022/2023 B.SC DEGREE SECOND SEMESTER EXAMINATION**

**Course Code: CHM 423**

**Courses Title: X-Ray Crystallography**

**Date: /02/2023**

**Time Allowed: 2h**

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**INSTRUCTIONS**

- (a) Answer any three questions
- (b) Start to answer each question on a separate sheet
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**USEFUL PHYSICAL CONSTANTS**

Planck's constant, h	= $6.625 \times 10^{-34}$ J.s
Boltzmann's constant, k	= $1.308 \times 10^{-23}$ JK <sup>-1</sup>
Avogadro's number, N <sub>A</sub>	= $6.023 \times 10^{23}$ mol <sup>-1</sup>
1 atomic mass unit, amu	= $1.66 \times 10^{-24}$ g = $1.66 \times 10^{-27}$ kg
Atomic mass of aluminum	= 27 amu

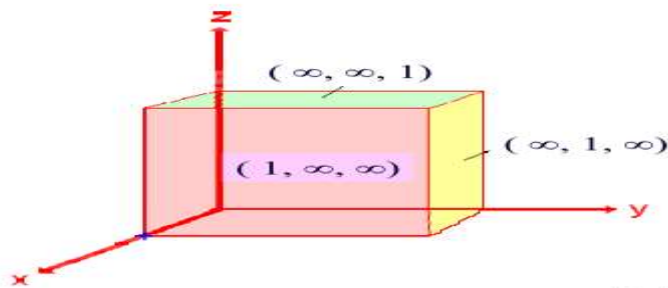
**QUESTION ONE [25 MARKS]**

- a. What is atomic packing factor? **3 marks**
- b. List the packing efficiency of body-centred cubic and face-centred cubic crystal. **2 marks**
- c. A body-centred unit cell has a volume of  $6.32 \times 10^{-23}$  cm<sup>3</sup>. Find the radius of the atom in pm. **5 marks**
- d. Aluminum crystallizes with a face-centred cubic unit cell. Given that the radius of aluminum is 143 pm. Calculate
- i. The unit cell content **3 marks**
  - ii. the mass of the unit cell **3 marks**
  - iii. The length of the unit cell **3 marks**
  - iii. The volume of the unit cell **3 marks**
  - iv. the density of the unit cell **3 marks**

## QUESTION TWO [25 MARKS]

- a. What is a coordination number? **2 marks**
- b. What are the coordination numbers of the following:
- Body-centered cubic packed crystal? **1 mark**
  - Face-centred cubic packed crystal? **1 mark**
- c. What are crystal planes? **3 marks**
- d. What are Miller indices? **3 marks**
- e. State the law of rational intercept. **2 marks**
- f. Determine the Miller indices of the following:
- 3 marks**
  - 3 marks**

- g. Consider the diagram below. Determine the Miller indices of the



- h. List three uses of Miller indices **3 marks**
- i. What is the difference between primitive unit cell and non-primitive unit cell? **3 marks**
- 1 mark**

## QUESTION THREE (25 MARKS)

- a. A first-order reflection from the  $\{111\}$  planes of a cubic crystal was observed at a glancing angle of  $11.2^\circ$  when  $\text{Cu}(K\alpha)$  X-rays of wavelength 154 pm were used. Calculate
- the interplanar distance **4 marks**
  - the length of the side of the unit cell. **5 marks**
- b. i. At room temperature, sodium has a body-centered cubic lattice with a cell of edge length 4.20 Å. Determine the density of sodium. **4 marks**
- ii. At  $-190^\circ\text{C}$ , the density is only 4.5% larger but the cell edge is now 5.35 Å. What type of cubic cell does sodium possess at  $-190^\circ\text{C}$ ? **5 marks**
- iii. Calculate the C-C-bond distance in diamond given points 000 and as well as  $a = 356.7$  pm **5 marks**
- iv. State one difference between  $K_\alpha$  and  $K_\beta$  radiation? **2 marks**

**QUESTION FOUR (25 MARKS)**

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|---|----------------|
| a. Briefly explain how X-rays are generated.  | <b>5 marks</b> |
| b. Prove that the Braggs' equation for a first-order reflection is given by $n\lambda = 2d\sin\theta$ | <b>5 marks</b> |
| c. What do (100), {100} and refer to in x-ray crystallography?  | <b>6 marks</b> |
| d. What do the x and y-axes in an XRD pattern represent?  | <b>3 marks</b> |
| e. What information does the XRD pattern of a crystal provide?  | <b>3 marks</b> |
| f. Why do we observe peaks of different heights in the XRD pattern?                                   | <b>3 marks</b> |

**QUESTION FIVE (25 MARKS)**

Write short notes on the following:

- |   |                |
|---|----------------|
| a. Scattering factor  | <b>6 marks</b> |
| b. Structure factor   | <b>8 marks</b> |
| c. Structure refinement   | <b>5 marks</b> |
| d. The CsCl structure is simple cubic with the Cs atom at the corners of a cube at (0, 0, 0) and the Cl atom at (. . .). What is the structure factor for (2 0 0) reflection? | <b>6 mark</b>  |

