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(University of Choice)

MASINDE MULIRO UNIVERSITY OF SCIENCE AND TECHNOLOGY (MMUST)

MAIN CAMPUS

UNIVERSITY EXAMINATIONS

2022/2023 ACADEMIC YEAR

THIRD YEAR SECOND SEMESTER EXAMINATIONS

FOR THE DEGREE OF BACHELOR OF SCIENCE (CHEMISTRY) AND BACHELOR OF INDUSTRIAL CHEMISTRY

COURSE CODE: SCH 343

COURSE TITLE: CRYSTALLOGRAPHY

DATE: ~~10~~ 20/04/2023 **TH APRIL 2023** **TIME:** 12.00-2.00 PM

INSTRUCTIONS TO CANDIDATES

Total Marks: 70

Answer all the Questions

TIME: 2 Hours

QUESTION ONE (18 Marks)

(a) Define the following terms **(4 marks)**

(i) Lattice

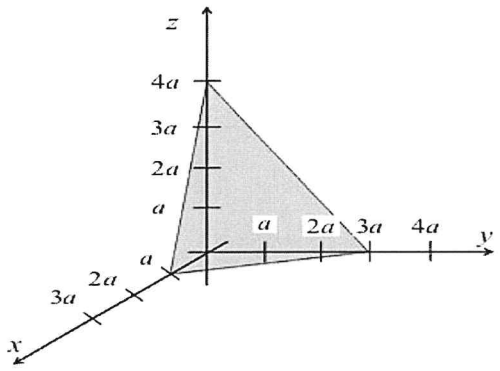
(ii) Unit cell

(iii) Primitive cell

(iv) Bravais lattice

(b) State three differences between crystalline and non-crystalline materials **(3 marks)**

(c) (i) Deduce the Miller indices for the plane shown below **(3 marks)**



(ii) Find the angle between two planes $\mathbf{r}.(2\mathbf{i} - 2\mathbf{j} + \mathbf{k}) = 1$ and $\mathbf{r}.(2\mathbf{i} + \mathbf{k}) = -3$ **(4 marks)**

(iii) If the vector of planes of a crystal are; $\mathbf{a} = 3\mathbf{i} + 2\mathbf{j} + 5\mathbf{k}$ and $\mathbf{b} = \mathbf{i} + 4\mathbf{j} + 6\mathbf{k}$, find $\mathbf{a} \times \mathbf{b}$ **(4 marks)**

QUESTION TWO (17 Marks)

(a) Calculate the smallest observable *d* spacing in a diffraction pattern measured with X-rays from a copper target (λ = 1.54184 Å). State the implication this have for the feasibility of resolving individual atoms in an electron density map **(4 marks)**

(b) State Bragg's Law and sketch the diffraction experiment showing source, collimation (pinholes), sample, detector and the scattering angle. **(4 marks)**

(c) Using a halogen lamp and a pen laser, explain what a collimated beam of electromagnetic radiation is and state why collimation important to Bragg's Law **(4 marks)**

(d) (i) Define packing factor **(2 marks)**

(ii) Determine the packing factor in a body centered crystal (BCC) **(3 marks)**

QUESTION THREE (18 Marks)

(a) Determine the inter-atomic distance between Na and Cl atoms in NaCl crystal of FCC lattice given the density of NaCl = 2.18 g/cm^3 ($N_A = 6.023 \times 10^{23}$ **(5 marks)**

(b) Find the reciprocal lattice vectors for FCC and calculate the primitive volume given the primitive translation vectors to be **(6 marks)**

$$\mathbf{a}^* = \frac{a}{2}(i + j)$$

$$\mathbf{b}^* = \frac{a}{2}(j + k)$$

$$\mathbf{c}^* = \frac{a}{2}(k + i)$$

(c) Find the Miller index for the plane that is parallel to the z axis but which crosses the x and y axes at 3 and -9, respectively. Assume the unit cell length is 3. **(3 marks)**

(d) Miller indices are used as a notation system for atomic planes. State four influences the planes will have on characteristics of materials **(4 marks)**

QUESTION FOUR (17 Marks)

(a) (i) Determine the lattice spacing for (211) reflection of olivine with a = 5.220 Å, b = 10.580 Å, and c = 7.50 Å **(3 marks)**

(ii) Calculate the angle for the above reflection using Cu – α radiation of wavelength 1.6450 Å **(3 marks)**

(b) (i) The d_{321} interplanar spacing in an FCC metal is 0.1545 nm. Determine the lattice constant a **(3 marks)**

(ii) Calculate the atomic radius of the metal **(2 marks)**

(c) Briefly outline steps in construction of Ewald's sphere **(6 marks)**

Periodic Table of the Elements 2006

1 H 1.01												13	14	15	16	17	2 He 4.00
3 Li 6.94	4 Be 9.01											5 B 10.81	6 C 12.01	7 N 14.01	8 O 15.99	9 F 19.00	10 Ne 20.18
11 Na 22.99	12 Mg 24.31	3	4	5	6	7	8	9	10	11	12	13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.87	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.41	31 Ga 69.72	32 Ge 72.64	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.60	53 I 126.90	54 Xe 131.29
55 Cs 132.91	56 Ba 137.33	57 La 138.91	72 Hf 178.49	73 Ta 180.95	74 W 183.84	75 Re 186.21	76 Os 190.23	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.2	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	89 Ac (227)	104 Rf (261)	105 Db (262)	106 Sg (266)	107 Bh (264)	108 Hs (270)	109 Mt (268)	110 Ds (281)	111 Rg (272)							

58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.97	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)