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## AI—308—2017

## FACULTY OF COMPUTER STUDIES

## M.Sc. (Second Year) (Third Semester) EXAMINATION MARCH/APRIL, 2017

## PHYSICAL CHEMISTRY

(Paper CH-534/3A)

(Statistical Thermodynamics)

(Thursday, 27-4-2017)

Time: 2.00 p.m. to 5.00 p.m.

Time— Three Hours

Maximum Marks—75

- N.B. := (i) Attempt All questions.
  - (ii) Use of log table and calculator is allowed.
  - (ii) Attempt MCQ at once only.
- 1. Solve any three:

15

- (a) Explain in brief Lagrange method of undetermined multiplier.
- (b) Define partition function. Explain its significance.
- (c) Derive:

$$S = K_b N \ln \left[ \frac{a_e}{N} \right] + \frac{E}{T}.$$

- (d) Calculate the nuclear partition function.
- (e) Calculate the heat capacity of an element at a temperature equal to its characteristics temperature.
- 2. Solve any three:

15

- (a) Derive the rel. for fluctuation in density and radioactive disintegration.
- (b) Derive the relation for p.f. and thermodynamic function of internal energy, entropy, and Helmoltz work function.

P.T.O.

- (c) Calculate the relative number of distinguishable states in ice and in water at 273 K.
- (d) Explain in brief thermal characteristics of crystaline solid.
- (e) Write a note on mean symmetry and nuclear spin.
- 3. (a) Explain partition function. Derive translational partition function. 8 Or

Derive the derivation of a Maxwell-Boltzmann distribution.

(b) Explain in brief Debye theory its limitations and modification. 7

Or

Using the principle of equipartition of energy, indicate the translational, vibrational and rotational contribution to the heat capacity of the H-molecule.

4. (a) Derive:

$$C_{V} = \left[\frac{nR}{T^{2}}\right] \left[\frac{\partial^{2} \ln a}{\partial (T^{2})}\right]_{V}.$$

 $O_{7}$ 

Derive the relation for a rotational partition function.

Calculate the rotational partition of HCl at 25°C. The rotation constant of HCl is 10.59 cm<sup>-1</sup>.

The value of kT/hc (cm<sup>-1</sup>) at 298 K is 207.20.

(b) Show that the entropy at absolute zero in a canonical ensemble can be expressed as  $S = K \log [g_a]$ .

Or

Find the ratio of Iodine molecules in the ground Ist and IInd excited vibration states at room temperature. The vibrational energy levels are separated by 214.6 cm<sup>-1</sup>.

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5.	(A)	Select the <i>correct</i> alternative :					5
		(i)	The entropywith increasing molar mass.				
			(a)	decreases	(b)	increases	
			(c)	no change	(d)	none of these	
		(ii)	Partition function is aquantity.				
			(a)	Dimensionless	(b)	Dimension	
			(c)	Both (a) and (b)	(d)	None of these	
		(iii)	The entropy of Co at absolute zero is:				
			(a)	Positive	(b)	Negative	
			(c)	Zero	(d)	None of these	
		(iv) Vibration contribution to energy at low temper					e is:
			(a)	Negligible	(b)	Increases	
		aks.	(c)	Decreases	(d)	None of these	
		(v)	Partition function increases withof temperature.				
		000 X	(a)	increases	(b)	decreases	
	5000		(c)	zero	(d)	none of these	
	(B)	Write	se short notes on any two:				2×5=10
		(i)	Combination problem				
		(ii)	Latti	ce model			

(iii)

Mean distribution and mean square deviation.