Birla Institute of Technology and Science, Pilani (Rajasthan)

CHEM C422 : Statistical Thermodynamics

Mid-semester Examination (Closed Book) **Semester I (2016-17)**

Max. Marks: 60 **Duration: 90 minutes** **Date: October 06, 2016**

General Instructions:

1. Enter your name, ID number, course no., course title, tutorial section no. etc. on the front page of answer-sheet and the supplementary answer-sheet(s) clearly and legibly. Incomplete, incorrect or illegible information may result in deduction of up to 5 marks.

2. All the questions are compulsory. You may attempt the questions in any order but the sub-questions of a question must be solved together before attempting the next question(s).

3. Use of non-programmable scientific calculators only is allowed for calculations. Do not use pencil for writing answers.

4. Indicate the "Rough work" clearly. Rough work must be done only on the last page of the main answer-sheet/supplementary answer-sheet(s).

***Useful data*:** π = 3.14159, 1 a.m.u. = 1.67 X 10^{-27} kg

1. Consider a two-dimensional isotropic harmonic oscillator with force constant k. Use Lagrange's equations of motion in cartesian coordinates, derive Hooke's law. Using Lagrange's equations of motion in polar coordinates, check whether the angular momentum is conserved. **[15]**

2. (a) Defining $f\left(\beta,\gamma,\{E_{N,j}\}\right)=\ln\Xi=\ln\sum_{N}\sum_{j}e^{-\beta E_{N,j}}e^{-\gamma N}$, obtain the simplified expression for entropy of an open system. **(b)** Use this to obtain entropy for (I) system of bosons (II) system of fermions. In which case would the entropy be more? Explain mathematically. **[8+4+4+2]**

3. (a) Obtain the expressions for average number of (I) fermions; (II) bosons in k-th quantum state. **(b)** Write the Liouville equation for a system of N molecules of a noble gas in generalized coordinates. **[8+3]**

4. The bond-distance of $^{1}H^{35}Cl$ molecule is 127.45 pm and the value of force constant is 516.3 N m^{-1}. One mole of $^{1}H^{35}Cl$ gas at 400 K was enclosed in a container. **(a)** Calculate thermal de Broglie wavelength and molecular translational partition function. **(b)** Calculate the rotational temperature and molecular rotational partition function. **(c)** Calculate vibrational temperature and molecular vibrational partition function. **(d)** Assuming the molecular electronic and molecular nuclear partition functions to be 1, each, calculate the total molecular partition function and total partition function for one mole of the gas. **[4+4+4+4]**

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