CHEM352: Physical Chemistry I
Homework Set VI - due 17^{th} of Dec, 5.00 pm

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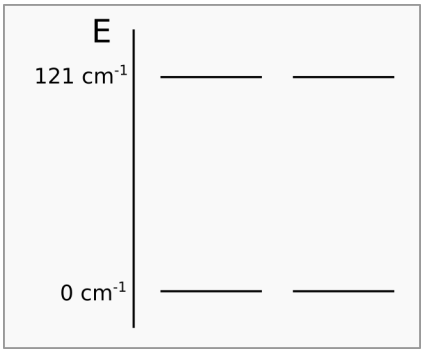
Lecture: Tue, 2.10-3.25 pm & Fri 2.10-3.25 pm, **C111**
Office hours: Thu, 4-6 pm, **HB - 1321B**

Problem 1 — CH31/5pts

Below is simplified electronic energy diagram for radical ·N=O molecule. Determine the probablity of electron to occupy one of the higer energy states at 100, 298 and 3000 K.



Problem 2 — CH32/5pts

A gas absorbed on a surface can sometimes be modelled as a two-dimensional ideal gas which partition fuction is given by:

$$Q(N, A, T) = \frac{1}{N!}\left(\frac{2\pi m k_B T}{h^2}\right)^N A^N \tag{1}$$

where A is the area of the surface. Derive the expression for $< E >$ and compare with the three-dimensional result. Calculate the heat capacity of 2-dimensional gas.

Problem 3 — CH32/5pts

Next, calculate the entropy of 2-dimensional ideal gas. Compare it to the entropy of 3-dimensional ideal gas.

Problem 4 — CH31/5pts

1. Calculate the conribution of each component (translational, rotational and vibrational, neglect electronic) to the partition energy funcion of CO_2 at 500K in volume of 8 nm^3. The vibrations energies are 1388, 667.4 (doubly degenerate) and 2349 cm^{-1}. The rotational constant is 0.39 cm^{-1}.
2. Calculate energy and heat capacity and Gibbs energy of CO_2 at 500K in cavity of 8 nm^3. Show the individual contributions to the gibbs energy.

Problem 5 — CH32/5pts

Detertmine the equilibriun constant for the sodium dissociation at 500K:

$$Na_{2(g)} \rightleftarrows 2Na_{(g)} \tag{2}$$

where B=0.155 cm^{-1}, $\bar{\nu}$ = 159 cm^{-1} and dissociation energy is 70.4 kJ/mol, and ground-state energy-degeneracy is 2.