Using Mathematica to evaluate partition functions

Your skills test on Friday will require that you to be able to construct a partition function given energy levels and then extract thermodynamic information using this partition function. You should begin by defining a set of Mathematica functions that take as input partition functions and give the thermodynamic variables: internal energy, constant volume heat capacity, Helmholtz free energy, pressure, and entropy. (Check out the link: http://en.wikipedia.org/wiki/Statistical_mechanics for assistance.)

Next, construct the translational, rotational, and vibrational partition functions for a diatomic gas. Then:

1) Show that the translational contribution to the molar heat capacity for a diatomic gas is $3R/2$.

2) Show that the rotational contribution to the molar heat capacity for a diatomic gas is $R$.

3) Derive the expression for the heat capacity of a homonuclear diatomic gas in terms of its vibrational temperature, $\Theta_{vib}$.

4) The vibrational temperature for $H_2$ is 6320 K. Plot the vibrational contribution to the molar heat capacity from 10 K to 10000 K. At room temperature, ~300 K, what is the contribution of the vibrational states of $H_2$ to the molar heat capacity?

5) The vibrational temperature for $Cl_2$ is 814 K. Plot the vibrational contribution to the molar heat capacity from 10 K to 2000 K. At room temperature, ~300 K, what is the contribution of the vibrational states of $Cl_2$ to the molar heat capacity?

6) Find the probability that at room temperature a molecule of hydrogen is in an excited vibrational state. Find the probability that at room temperature a molecule of chlorine is in an excited vibrational state.

7) The rotational temperature, $\Theta_{Rot} = h^2/(8 \pi^2 I k_B)$, of $N_2$ is 2.89 K. What is the probability that a nitrogen molecule is in an excited rotational state at 300 K?

8) Derive the partition function for a particle moving in a finite harmonic well containing 5 vibrational states. Assuming this particle has a vibrational temperature of 1000 K, what is the vibrational contribution to the room temperature heat capacity?