Statistical Mechanics Assignment 4

Due: February 6, 11:00 a.m.

Marks: 23

The U.S. National Institute of Standards and Technology (NIST) keeps an extensive database of molecular and thermodynamic data. Pointers to various parts of this web site are available on the course web site. In this assignment, you will look up some data from the NIST web site and do some calculations based on them.

1. Find the vibrational and rotational constants of the electronic ground state of boron monoxide, given in units of cm^{-1} and called, respectively, ω_e and B_e in the NIST Chemistry WebBook. While we haven't discussed this issue in this class, it is important to understand that the vibrational and rotational constants depend on the electronic state of the molecule. The NIST Chemistry WebBook gives vibrational and rotational constants (and other data) for several electronic states. The molecular energy in the lowest rotational and vibrational states for each electronic state (roughly corresponding to the electronic energy) is called T_e in this table and is again given in cm^{-1}. [2 marks]

2. Based on the data in the table, argue that none of the excited electronic states will be relevant to the thermodynamic properties of BO gas at reasonable temperatures. [2 marks]

3. The data you will have found corresponds to a particular isotopic variant of BO. Look up the masses of the relevant isotopes and calculate the mass of this particular isotopic variant. [2 marks]

4. Calculate the translational, rotational and vibrational partition functions for BO gas in a 0.4 L container at 1000 K. [6 marks]

   Hint: You may avoid later problems if you define these partition functions as explicit functions of T using Maple's arrow operator.

5. Calculate the molecular partition function at 1000 K. [1 mark]

6. Calculate the probabilities that a BO molecule occupies each of the four lowest vibrational states at 1000 K. [2 marks]

7. Calculate the probability that a BO molecule occupies the $(v = 1, J = 10)$ vibration-rotation state at 1000 K. [1 mark]

8. Which is the most probable rotational state at 1000 K? [3 marks]

9. Calculate the molar internal energy at 1000 K. [4 marks]