Exercise 08

NAME:	MATRICULATION NUMBER:
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RESULTS:

8.1	OF 5 P
8.2	OF 5 P
8.2	OF 10 P
8.2	OF 5 P
8.2	OF 5 P
TOTAL	OF 30 P

GENERAL INSTRUCTIONS

- SUBMIT YOUR SOLUTION TO LUCA DONATI (R. 35.17) BEFORE **THURSDAY 23. JUNE AT 8.15 AM**.
- FILL OUT THIS COVER SHEET AND SUBMIT IT ALONG WITH YOUR SOLUTION.
- SHOW HOW YOU ARRIVED AT YOUR ANSWER.

8.1 Contribution of the electronic partition function to thermodynamic functions (5 P)

Consider the electronic partition function, determine the following thermodynamic functions :

1. Helmholtz free energy
2. Entropy
3. Internal energy
4. Heat capacity

8.2 Vibrational partition function of N_2 (5 P)

Diatomic nitrogen ($\Theta_{vib} = 3383$) is heated in an electric arc. Spectroscopic measurements yield the following values for the relative populations of excited vibrational states:

- $\frac{N_1}{N_0} = 0.26$
- $\frac{N_2}{N_0} = 0.068$
- $\frac{N_3}{N_0} = 0.018$

Compute the temperature of the arc using the relation:

$$\frac{N_v}{N} = \frac{1}{z}\exp(-v\Theta_{vib}/T)$$

8.3 Vibrational partition function of Cl_2 (10 P)

The ground vibrational frequency of a diatomic molecule of Chlorine is $1.663 \times 10^{13}\ \frac{1}{\mathrm{s}}$.

1. Determine the characteristic temperature Θ_{vib}
2. Verify the relation

$$\exp\left(-\frac{\epsilon_{vib}(v)}{k_B T}\right) = \exp\left(-v\frac{\Theta_{vib}}{k_B T}\right)$$

   for $v = 1, 2, 3$ at temperature $T = 300K$.
3. Plot the population of excited states (relative to the total number of states) as a function of v.

8.4 Occupation of the vibrational states of I_2 (5 P)

From the Raman spectrum of the diatomic Iodine at room temperature, the vibration wave number is $\tilde{\nu_0} = 21460\mathrm{m}^{-1}$.
Determine:

1. The oscillation frequency
2. The characteristic temperature Θ_{vib}
3. The ratio $\frac{\Theta_{vib}}{T}$
4. The partition function z_{vib}.
5. The occupation probability N_v/N of the first 4 vibrational states

8.5 Vibrational contribution to the entropy (5 P)

Plot the contribution to the entropy from a given vibrational mode as function of the quantity

$$x = \frac{hv}{k_B T}$$

for $T = 298K$ and $T = 1000K$.