

1. Hydrogen gas has the following characteristic temperatures:

- Rotational temperature: $\Theta_{\text{rot}} = 87.5 \text{ K}$
- Vibrational temperature: $\Theta_{\text{vib}} = 6215 \text{ K}$

(a) What temperature is required for 50% of the molecules to be rotationally excited?

(b) What temperature is required for 50% of the molecules to be vibrationally excited?

(c) For the temperature found in part (a), what percentage of molecules are vibrationally excited? What does this tell you about the relative accessibility of rotational versus vibrational energy levels?

- (d) If we replaced hydrogen gas with a heavier gas like helium, would the characteristic temperatures increase, decrease, or do something else?

2. Derive the expression for the molar energy \bar{U} of a diatomic ideal gas, excluding the electronic contribution, starting from the molecular partition function:

$$q = q_{\text{trans}} q_{\text{rot}} q_{\text{vib}} = \left(\frac{2\pi m k_{\text{B}} T}{h^2} \right)^{3/2} V \cdot \frac{T}{\sigma \Theta_{\text{rot}}} \cdot \frac{e^{-\Theta_{\text{vib}}/2T}}{1 - e^{-\Theta_{\text{vib}}/T}}$$
$$\bar{U} = \frac{5}{2} RT + R \frac{\Theta_{\text{vib}}}{2} + R \frac{\Theta_{\text{vib}}}{e^{\Theta_{\text{vib}}/T} - 1}$$

Homework Problem 8

1. Derive an expression for J_{\max} , the rotational quantum number that has the highest population at a given temperature T , and verify for NO ($\Theta_{\text{rot}} = 2.39$) that $J_{\max} = 7$ at 300K . Remember quantum numbers must be integers. The probability distribution is given by:

$$P_J = \frac{\Theta_{\text{rot}}}{T} (2J + 1) e^{-\frac{\Theta_{\text{rot}} J(J+1)}{T}}$$