Question

Maxwell-Boltzmann Statistics: The moment of inertia of a H_2 molecule is $4.64 \times 10^{-48}\, kg\, m^2$. (a) Find the relative populations of the $J = 0$, 1, 2, 3, and 4 rotational states at 300 K. (b) Can the populations of the $J = 2$ and $J = 3$ states ever be equal? If so, at what temperature does this occur?

Solution

a) The number of molecules in state J (See example 9.2 in the text)

$$n_J = n_0(2J+1)e^{-J(J+1)\hbar^2/2IkT}$$

At 300 K

$$\frac{\hbar^2}{2IkT} = \frac{(1.055 \times 10^{-34})^2}{2(4.64 \times 10^{-48})(1.381 \times 10^{-23})(300)} = 0.2895$$

For $J = 0$ the population is n_0 and for the remaining values

$J = 1$

$$n_1 = n_0(3)e^{-2(0.2895)} = 1.68\, n_0$$

$J = 2$

$$n_2 = n_0(5)e^{-6(0.2895)} = 0.882\, n_0$$

$J = 3$

$$n_3 = n_0(7)e^{-12(0.2895)} = 0.218\, n_0$$

$J = 4$

$$n_4 = n_0(9)e^{-20(0.2895)} = 0.0277\, n_0$$

Hence the relative populations

$$J_0 : J_1 : J_2 : J_3 : J_4 = 1 : 1.68 : 0.882 : 0.218 : 0.0277$$

b) For $n_2 = n_3$

$$\begin{aligned}
n_0(5)e^{-6\hbar^2/2IkT} &= n_0(7)e^{-12\hbar^2/2IkT} \\
e^{6\hbar^2/2IkT} &= 7/5 \\
\frac{6\hbar^2}{2IkT} &= ln(1.4) \\
T &= \frac{3\hbar^2}{Ik\, ln(1.4)} \\
&= \frac{3(1.055 \times 10^{-34})^2}{(4.64 \times 10^{-48})(1.381 \times 10^{-23})(0.3365)} \\
&= \frac{3.339 \times 10^{-68}}{2.156 \times 10^{-71}} \\
&= 1.549 \times 10^3
\end{aligned}$$

The populations of $J = 2$ and $J = 3$ states are equal at a temperature of $1.55 \times 10^3\, K$.