Problemes T5

5.1 Llei de distribució de Maxwell-Boltzmann, fixats E_e^- i vibracional, el nivell rotacional + poblat d'una diatòmica és $J_{màx} = \sqrt{\frac{kT}{2hB_e}} - 1/2$

$\langle N_s \rangle = \sum p_j N_{sj}$ $\qquad B_e = \frac{h}{8\pi\mu R_e^2}$

$E_{rot} = \frac{J(J+1)\hbar^2}{2\mu R_e^2} = hB_e J(J+1)$

$z_{rot} = \frac{2 I_e kT}{\sigma \hbar^2} = \frac{I_e kT}{\hbar^2}$

↑ 2 homonuclear

$E_{rot} = hB_e J(J+1) - h\alpha_e(v+1/2)J(J+1)$

$E_{rot} = (B_e - \alpha_e(v+1/2))hJ(J+1)$

$\frac{\langle N_s \rangle}{N} = \frac{de^{-E_r/kT}}{z} = \frac{(2J+1)}{z} e^{-E_r/k_b T}$ $\qquad \varepsilon_r = hB_e J(J+1) = hB_e(J^2+J)$

$\langle N_s \rangle = \frac{N}{z}(2J+1) e^{-E_r/k_b T}$

Busquem mínim/màxim $\frac{\partial N}{\partial J} = 0$

$0 = \frac{d\langle N_s \rangle}{dJ} = \frac{N}{z}(2+1) e^{-hB_e(J^2+J)} \cdot (2J+1)\left[-2J\frac{hB_e}{kT} + -\frac{hB}{kT}\right] e^{-hB_v J(J+1)/kT}$

$= \frac{N}{z}\left[2 e^{-hB_e(J^2+J)} + (2J+1)\left(-\frac{hB_x}{kT}(2J+1)\right) e^{-hBJ(J+1)/kT}\right] = 0$

$= 2e^{-hB_e(J^2+J)} - (2J+1)^2 \frac{hB_e}{kT} e^{-hB_e J(J+1)/kT} = 0$

$2 = (2J+1)^2 \frac{hB_e}{kT}$; $2J+1 = \sqrt{\frac{2kT}{hB_e}} \Rightarrow$ $\boxed{J = \sqrt{\frac{kT}{2hB_e}} - 1/2}$

5.2 FP vibracional diatómica osc arm. origen E_0!

$$z_{vibr} = \frac{e^{-h\nu e/2kbT}}{1-e^{-h\nu e/kBT}} \qquad E_0 = \frac{1}{2}h\nu \qquad E_1 = h\nu$$

$$z_{vib} = \sum_{v=0}^{\infty} e^{-E_{vibr,v}/kT} = \sum_{v=0}^{\infty} \left(e^{-h\nu/kbT}\right)^{v} = \frac{1}{1-e^{-h\nu/kT}}$$

b) FP E_0 mínima e^-. ??

5.3. $^1g_{3/2}$ $\frac{\langle N_1\rangle}{\langle N_0\rangle} = 0{,}528$ $\frac{\langle N_2\rangle}{\langle N_0\rangle} = 0{,}279$

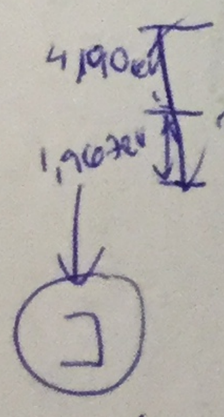
si son d'eq. pq $N_0 > N_1$

$\tilde{\nu}_e = 6{,}39 \cdot 10^2 s^{-1}$ T? $E_0 = \frac{1}{2}h\nu$ $E_1 = 3h\nu$ $\boxed{\Delta E = h\nu}$

$$\ln 0{,}528 = h e^{-h\nu e/kBT}$$

$$T = \frac{h\nu e}{k_B\, 0{,}638} = 480{,}2K$$

5.4. $T = 298{,}15$



$J = 1+1 = 2, 1, 0$

$d(3P) = \cancel{J(J+1)} = (2S+1)(2L+1) = 3\cdot 3 = 9$

$d(1D) = 5$

$d\,^1S = 1$

$$z = 9 \cdot e^{0} \cdot \sum_i g_i e^{-\varepsilon_{ex}/kB}$$