

Chapter 4

Rigid Models and Angular Momentum Eigenstates

Homework Solutions

1. $\vec{A} = 3\vec{i} - \vec{j} + 2\vec{k} \quad \vec{B} = 2\vec{i} + 4\vec{j} - 3\vec{k}$

$$\vec{A} \cdot \vec{B} = A_x B_x + A_y B_y + A_z B_z = (3)(2) + (-1)(4) + (2)(-3) = -4$$

$$\begin{aligned} \vec{A} \times \vec{B} &= \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ A_x & A_y & A_z \\ B_x & B_y & B_z \end{vmatrix} = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ 3 & -1 & 2 \\ 2 & 4 & -3 \end{vmatrix} \\ &= \vec{i} [(-1)(-3) - (2)(4)] - \vec{j} [(3)(-3) - (2)(2)] + \vec{k} [(3)(4) - (-1)(2)] \\ &= -5\vec{i} + 13\vec{j} + 14\vec{k} \end{aligned}$$

2. $\psi = Ae^{-2i\phi} \sin^2 \theta$

(a) $L^2\psi/2I$

$$\begin{aligned} \frac{L^2\psi}{2I} &= -\frac{\hbar^2}{2I} \left[\frac{1}{\sin(\theta)} \frac{\partial}{\partial \theta} \left(\sin(\theta) \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2(\theta)} \frac{\partial^2 \psi}{\partial \phi^2} \right] = \\ &= -\frac{\hbar^2}{2I} [\hat{A}\psi + \hat{B}\psi] \end{aligned}$$

Calculation of $\hat{A}\psi$

$$\sin \theta \frac{\partial \psi}{\partial \theta} = \sin \theta \frac{\partial}{\partial \theta} [Ae^{-2i\phi} \sin^2 \theta] = \sin \theta [Ae^{-2i\phi} 2 \sin \theta \cos \theta] = 2Ae^{-2i\phi} \sin^2 \theta \cos \theta$$

$$\begin{aligned} \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \frac{\partial \psi}{\partial \theta} \right] &= \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} [2Ae^{-2i\phi} \sin^2 \theta \cos \theta] = 2Ae^{-2i\phi} \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} [\sin^2 \theta \cos \theta] \\ &= 2Ae^{-2i\phi} \frac{1}{\sin \theta} [\sin^2 \theta (-\sin \theta) + \cos \theta (2 \sin \theta \cos \theta)] \\ &= 2Ae^{-2i\phi} [-\sin^2 \theta + 2 \cos^2 \theta] = 2Ae^{-2i\phi} [-\sin^2 \theta + 2(1 - \sin^2 \theta)] \\ &= 2Ae^{-2i\phi} [2 - 3 \sin^2 \theta] \end{aligned}$$

Calculation of $B\psi$

$$\begin{aligned}\frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} &= \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} [Ae^{-2i\phi} \sin^2 \theta] = \frac{1}{\sin^2 \theta} [(-2i)^2 Ae^{-2i\phi} \sin^2 \theta] \\ &= -4Ae^{-2i\phi}\end{aligned}$$

Calculation of $L^2\psi/2I$

$$\begin{aligned}\frac{L^2\psi}{2I} &= -\frac{\hbar^2}{2I} [\hat{A}\psi + \hat{B}\psi] = -\frac{\hbar^2}{2I} \{2Ae^{-2i\phi} [2 - 3\sin^2 \theta] - 4Ae^{-2i\phi}\} \\ &= \frac{6\hbar^2}{2I} [Ae^{-2i\phi} \sin^2 \theta] = \frac{6\hbar^2}{2I} \psi\end{aligned}$$

Therefore, the Energy is: $E = \frac{6\hbar^2}{2I} = \frac{l(l+1)\hbar^2}{2I}$

(b) L^2

We've actually already accomplished this. The energy is:

$$E = \frac{L^2}{2I} = \frac{6\hbar^2}{2I} \rightarrow L^2 = 2I(E) = 2I \left(\frac{6\hbar^2}{2I} \right) = 6\hbar^2 = l(l+1)\hbar^2$$

Note: The above result illustrates that ψ is a wavefunction with $l = 2$

(c) L_z

$$\hat{L}_z\psi = \frac{\hbar}{i} \frac{\partial \psi}{\partial \phi} = m\hbar\psi$$

$$\hat{L}_z\psi = \frac{\hbar}{i} \frac{\partial}{\partial \phi} [Ae^{-2i\phi} \sin^2 \theta] = A \sin^2 \theta \frac{\hbar}{i} (-2i) e^{-2i\phi} = -2\hbar (Ae^{-2i\phi} \sin^2 \theta) = -2\hbar\psi$$

Thus we see that, for this wavefunction, $m_z = -2$

3. The energy levels for a 2D Rigid Rotor (see PP) are given by:

$$E_m = \frac{\hbar^2 m^2}{2I} \quad m = 0, \pm 1, \pm 2, \text{etc.}$$

$$\mu = \frac{m_{F_2} \cdot m_{F_2}}{m_{F_2} + m_{F_2}} = \frac{m_{F_2}}{2} = \frac{19 \text{ amu} \cdot \frac{1.66 \times 10^{-27} \text{ kg}}{1 \text{ amu}}}{2} = 1.58 \times 10^{-26} \text{ kg}$$

$$I = \mu r^2 = (1.58 \times 10^{-26} \text{ kg}) (1.42 \times 10^{-10} \text{ m})^2 = 3.18 \times 10^{-46} \text{ kg} \cdot \text{m}^2$$

$$\begin{aligned} \Delta E = E_{fin} - E_{init} &= \frac{\hbar^2 m_{fin}^2}{2I} - \frac{\hbar^2 m_{init}^2}{2I} = \frac{\hbar^2}{2I} [8^2 - 2^2] = \frac{60 (1.05 \times 10^{-34} \text{ J} \cdot \text{s})^2}{2 (3.18 \times 10^{-46} \text{ kg} \cdot \text{m}^2)} \\ &= 1.04 \times 10^{-21} \text{ J} \end{aligned}$$

$$\Delta E = \frac{hc}{\lambda} = hc\tilde{\nu} \rightarrow \tilde{\nu} = \frac{\Delta E}{hc} = \frac{1.04 \times 10^{-21} \text{ J}}{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})(3.00 \times 10^{10} \text{ cm/s})} = 52.3 \text{ cm}^{-1}$$

4. Rotational Raman: Transition $J'' \rightarrow J' = J'' + 2$

$$\Delta E = hc\tilde{B}(J')(J'+1) - hc\tilde{B}J''(J''+1)$$

$$\tilde{\nu} = \frac{\Delta E}{hc} = \tilde{B}(J')(J'+1) - \tilde{B}J''(J''+1)$$

$$\text{First line: } J'' = 0 \rightarrow J' = 2 \quad \tilde{\nu} = \tilde{B}(2)(3) - \tilde{B}(0)(1) = 6\tilde{B} = 50.2 \text{ cm}^{-1} \rightarrow \tilde{B} = 8.37 \text{ cm}^{-1}$$

$$\text{Second line: } J'' = 1 \rightarrow J' = 3 \quad \tilde{\nu} = \tilde{B}(3)(4) - \tilde{B}(1)(2) = 10\tilde{B} = 83.7 \text{ cm}^{-1} \rightarrow \tilde{B} = 8.37 \text{ cm}^{-1}$$

$$\tilde{B} = \frac{h}{8\pi^2 Ic} \rightarrow I = \frac{h}{8\pi^2 \tilde{B}c} = \frac{6.63 \times 10^{-34} \left(\frac{\text{kg} \cdot \text{m}^2}{\text{s}^2} \right) \text{s}}{8(3.14)^2 (8.37 \text{ cm}^{-1})(3.00 \times 10^{10} \text{ cm/s})} = 3.34 \times 10^{-47} \text{ kg} \cdot \text{m}^2$$

$$\mu = \frac{m_H m_{Br}}{m_H + m_{Br}} = \frac{(1.00 \text{ amu})(79.0 \text{ amu})}{1.00 \text{ amu} + 79.0 \text{ amu}} = 0.988 \text{ amu} \cdot \frac{1.66 \times 10^{-27} \text{ kg}}{1 \text{ amu}} = 1.64 \times 10^{-27} \text{ kg}$$

$$\begin{aligned} I = \mu r^2 \rightarrow r &= \sqrt{\frac{I}{\mu}} = \sqrt{\frac{3.34 \times 10^{-47} \text{ kg} \cdot \text{m}^2}{1.64 \times 10^{-27} \text{ kg}}} \\ &= \sqrt{2.04 \times 10^{-20} \text{ m}^2} = 1.43 \times 10^{-10} \text{ m} = 0.143 \text{ nm} = 1.43 \text{ \AA} \end{aligned}$$

5. Any molecule with a dipole moment will have a rotational microwave spectrum.

DO have a rotational microwave spectrum: H_2O , $\text{H-C}\equiv\text{C-Cl}$, cis-1,2-dichloroethylene, NH_3

DO NOT have a rotational microwave spectrum: $\text{H-C}\equiv\text{C-H}$, benzene

6.
$$\tilde{\nu} = \frac{\Delta E}{hc} = \tilde{B}(J')(J'+1) - \tilde{B}J''(J''+1)$$

- (a) First line: $J'' = 0 \rightarrow J' = 1$

$$\tilde{\nu} = \tilde{B}(1)(2) - \tilde{B}(0)(1) = 2\tilde{B} = 3.84 \text{ cm}^{-1} \rightarrow \tilde{B} = 1.92 \text{ cm}^{-1}$$

$$\tilde{B} = \frac{h}{8\pi^2 Ic} \rightarrow I = \frac{h}{8\pi^2 \tilde{B} c} = \frac{6.63 \times 10^{-34} \left(\frac{\text{kg} \cdot \text{m}^2}{\text{s}^2} \right) \text{s}}{8(3.14)^2 (1.92 \text{ cm}^{-1})(3.00 \times 10^{10} \text{ cm/s})} = 1.46 \times 10^{-46} \text{ kg} \cdot \text{m}^2$$

$$\mu = \frac{m_C m_O}{m_C + m_O} = \frac{(12.0 \text{ amu})(16.0 \text{ amu})}{12.0 \text{ amu} + 16.0 \text{ amu}} = 6.86 \text{ amu} \cdot \frac{1.66 \times 10^{-27} \text{ kg}}{1 \text{ amu}} = 1.14 \times 10^{-26} \text{ kg}$$

$$I = \mu r^2 \rightarrow r = \sqrt{\frac{I}{\mu}} = \sqrt{\frac{1.46 \times 10^{-46} \text{ kg} \cdot \text{m}^2}{1.14 \times 10^{-26} \text{ kg}}} \\ = \sqrt{1.28 \times 10^{-20} \text{ m}^2} = 1.13 \times 10^{-10} \text{ m} = 0.113 \text{ nm} = 1.13 \text{ \AA}$$

- (b) 7th. Line: $J'' = 6 \rightarrow J' = 7$

$$\tilde{\nu} = \tilde{B}(7)(8) - \tilde{B}(6)(7) = 14\tilde{B} = 14(1.92 \text{ cm}^{-1}) = 26.9 \text{ cm}^{-1}$$

- (c) 5th. line: $J'' = 4 \rightarrow J' = 5$

2nd. line: $J'' = 1 \rightarrow J' = 2$

$$N_J \propto (2J+1)e^{E_J/kT} = (2J+1)e^{-hc\tilde{B}J(J+1)/kT}$$

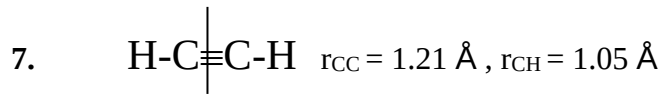
The transition intensity is proportional to N_J where J is the initial state of the absorption.

$$\frac{hc\tilde{B}}{kT} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})(3.00 \times 10^{10} \text{ cm/s})(1.92 \text{ cm}^{-1})}{(1.38 \times 10^{-23} \text{ J/K})(298 \text{ K})} = 9.29 \times 10^{-3}$$

$$\frac{I(4 \rightarrow 5)}{I(1 \rightarrow 2)} = \frac{N_4}{N_1} = \frac{(2 \cdot 4 + 1)e^{-(4)(5)hc\tilde{B}/kT}}{(2 \cdot 1 + 1)e^{-(1)(2)hc\tilde{B}/kT}} = \frac{9}{3}e^{-18hc\tilde{B}/kT} = 3e^{-18(9.29 \times 10^{-3})} = 2.54$$

- (d) The maximum intensity transition is from the value of J with the highest value of N_J
 We can determine this from basic calculus. We will differentiate N_J with respect to J and set the derivative equal to 0 to determine $J_{\max}$

$$\begin{aligned}\frac{dN_J}{dJ} = 0 &= \frac{d}{dJ} \left\{ (2J+1)e^{-(J^2+J)hc\tilde{B}/kT} \right\} = \left\{ (2J+1) \frac{d}{dJ} e^{-(J^2+J)hc\tilde{B}/kT} + e^{-(J^2+J)hc\tilde{B}/kT} \frac{d}{dJ} (2J+1) \right\} \\ 0 &= \left\{ (2J+1)e^{-(J^2+J)hc\tilde{B}/kT} \left[-(2J+1) \frac{hc\tilde{B}}{kT} \right] + e^{-(J^2+J)hc\tilde{B}/kT} \cdot 2 \right\} \\ 0 &= e^{-(J^2+J)hc\tilde{B}/kT} \left\{ -(2J+1)^2 \frac{hc\tilde{B}}{kT} + 2 \right\} \\ (2J_{\max}+1)^2 &= \frac{2}{\frac{hc\tilde{B}}{kT}} = \frac{2}{9.29 \times 10^{-3}} = 215 \\ 2J_{\max}+1 &= \sqrt{215} = 14.7 \rightarrow J_{\max} = 6.9 \approx 7\end{aligned}$$



Therefore, $r_{\text{C}} = 0.50(1.21) = 0.605 \text{ \AA}$
 $r_{\text{H}} = 0.50(1.21) + 1.05 = 1.655 \text{ \AA}$

Calculation of I and B

$$\begin{aligned}I &= \sum_i m_i r_i^2 = 2 \cdot m_{\text{C}} r_{\text{C}}^2 + 2 \cdot m_{\text{H}} r_{\text{H}}^2 = 2(12.0 \text{ amu})(0.605 \text{ \AA})^2 + 2(1.00 \text{ amu})(1.655 \text{ \AA})^2 \\ &= 14.26 \text{ amu} \cdot \text{\AA}^2 \frac{1.66 \times 10^{-27} \text{ kg}}{1 \text{ amu}} \left(\frac{1 \times 10^{-10} \text{ m}}{1 \text{ \AA}} \right)^2 = 2.37 \times 10^{-46} \text{ kg} \cdot \text{m}^2\end{aligned}$$

$$\tilde{B} = \frac{h}{8\pi^2 I c} = \frac{6.63 \times 10^{-34} \left(\frac{\text{kg} \cdot \text{m}^2}{\text{s}^2} \right) \cdot \text{s}}{8(3.14)^2 (2.37 \times 10^{-46} \text{ kg} \cdot \text{m}^2) (3.00 \times 10^{10} \text{ cm/s})} = 1.18 \text{ cm}^{-1}$$

- (a) Line 1: $J''=0 \rightarrow J'=2$:

$$\tilde{\nu} = \tilde{B}(J')(J'+1) - \tilde{B}(J'')(J''+1) = \tilde{B}(2)(3) - \tilde{B}(0)(1) = 6\tilde{B} = 6(1.18 \text{ cm}^{-1}) = 7.08 \text{ cm}^{-1}$$

- Line 2: $J''=1 \rightarrow J'=3$:

$$\tilde{\nu} = \tilde{B}(J')(J'+1) - \tilde{B}(J'')(J''+1) = \tilde{B}(3)(4) - \tilde{B}(1)(2) = 10\tilde{B} = 10(1.18 \text{ cm}^{-1}) = 11.8 \text{ cm}^{-1}$$

- (b) Line 1: $J''=0 \rightarrow J'=3$:

$$\tilde{\nu} = \tilde{B}(J')(J'+1) - \tilde{B}(J'')(J''+1) = \tilde{B}(3)(4) - \tilde{B}(0)(1) = 12\tilde{B} = 12(1.18 \text{ cm}^{-1}) = 14.16 \text{ cm}^{-1}$$

- Line 2: $J''=1 \rightarrow J'=4$:

$$\tilde{\nu} = \tilde{B}(J')(J'+1) - \tilde{B}(J'')(J''+1) = \tilde{B}(4)(5) - \tilde{B}(1)(2) = 18\tilde{B} = 18(1.18 \text{ cm}^{-1}) = 21.24 \text{ cm}^{-1}$$

- (c) $T = 100\text{ }^{\circ}\text{C} = 373\text{ K}$
 Line 20: $J''=19 \rightarrow J'=21$
 Line 5: $J''=4 \rightarrow J'=6$

$$\frac{hc\tilde{B}}{kT} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})(3.00 \times 10^{10} \text{ cm} / \text{s})(1.18 \text{ cm}^{-1})}{(1.38 \times 10^{-23} \text{ J} / \text{K})(373 \text{ K})} = 4.56 \times 10^{-3}$$

$$\begin{aligned} \frac{I(19 \rightarrow 21)}{I(4 \rightarrow 6)} &= \frac{N_{19}}{N_4} = \frac{(2 \cdot 19 + 1)e^{-(19)(20)hc\tilde{B}/kT}}{(2 \cdot 4 + 1)e^{-(4)(5)hc\tilde{B}/kT}} = \frac{39}{9} e^{-360hc\tilde{B}/kT} = 4.33e^{-360(4.56 \times 10^{-3})} \\ &= 4.33(0.194) = 0.84 \end{aligned}$$

8. NO_2 , $T = 150\text{ }^{\circ}\text{C} = 423\text{ K}$, $\sigma = 2$

$$I_a = 3.07 \times 10^{-47} \text{ kg} \cdot \text{m}^2 , I_b = 6.20 \times 10^{-46} \text{ kg} \cdot \text{m}^2 , I_c = 6.50 \times 10^{-46} \text{ kg} \cdot \text{m}^2$$

$$\Theta_a = \frac{h^2}{8\pi^2 I_a k} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{8(3.14)^2 (3.07 \times 10^{-47} \text{ kg} \cdot \text{m}^2)(1.38 \times 10^{-23} \text{ J} / \text{K})} = 13.14 \text{ K}$$

$$\Theta_b = \frac{h^2}{8\pi^2 I_b k} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{8(3.14)^2 (6.20 \times 10^{-46} \text{ kg} \cdot \text{m}^2)(1.38 \times 10^{-23} \text{ J} / \text{K})} = 0.651 \text{ K}$$

$$\Theta_c = \frac{h^2}{8\pi^2 I_c k} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{8(3.14)^2 (6.50 \times 10^{-46} \text{ kg} \cdot \text{m}^2)(1.38 \times 10^{-23} \text{ J} / \text{K})} = 0.621 \text{ K}$$

Preliminary Calculations: Partition Function and Derivative

$$q^{\text{rot}} = \frac{\pi^{1/2}}{\sigma} \left(\frac{T^3}{\Theta_a \Theta_b \Theta_c} \right)^{1/2} = \frac{(3.14)^{1/2}}{2} \left(\frac{(423 \text{ K})^3}{(13.14 \text{ K})(0.651 \text{ K})(0.621 \text{ K})} \right)^{1/2} = 3345$$

$$\begin{aligned} \ln(Q^{\text{rot}}) &= \ln(q^{\text{rot}})^N = nN_A \ln(q^{\text{rot}}) = nN_A \ln \left[\frac{\pi^{1/2}}{2} \left(\frac{T^3}{\Theta_a \Theta_b \Theta_c} \right)^{1/2} \right] \\ &= nN_A \left\{ \ln(T)^{3/2} + \ln \left(\frac{\pi^{1/2}}{2} \right) - \ln(\Theta_a \Theta_b \Theta_c)^{1/2} \right\} \end{aligned}$$

$$\left(\frac{\partial [\ln(Q^{\text{rot}})]}{\partial T} \right)_{V,N} = nN_A \frac{d \ln(T^{3/2})}{dT} = \frac{3nN_A}{2T}$$

$$\left(\frac{\partial [\ln(Q^{\text{rot}})]}{\partial \ln V} \right)_{T,N} = 0 \quad \text{i.e. the rotational partition function is independent of volume.}$$

Internal Energy: U^{rot}

$$U^{\text{rot}} = kT^2 \left(\frac{\partial \ln Q^{\text{rot}}}{\partial T} \right)_{V,n} = kT^2 \left(\frac{3nN_A}{2T} \right) = \frac{3}{2} n(N_A k) T = \frac{3}{2} nRT$$

$$= \frac{3}{2} (2 \text{ mol}) (8.31 \text{ J / mol} \cdot \text{K}) (423 \text{ K}) = 10550 \text{ J} \approx 10.6 \text{ kJ}$$

Note: This result illustrates equipartition of Internal Energy. Each of the three rotations contributes $(1/2)RT$ to U^{rot} .

Enthalpy: H^{rot}

$$H^{\text{rot}} = kT^2 \left(\frac{\partial \ln Q^{\text{rot}}}{\partial T} \right)_{V,N} + kT \left(\frac{\partial \ln Q^{\text{rot}}}{\partial \ln V} \right)_{T,N} = U^{\text{rot}} + 0 = \frac{3}{2} nRT \approx 10.6 \text{ kJ}$$

Constant Pressure Heat Capacity

$$C_p^{\text{rot}} = \left(\frac{\partial H^{\text{rot}}}{\partial T} \right)_{V,n} = \frac{d}{dT} \left(\frac{3}{2} nRT \right) = \frac{3}{2} nR = \frac{3}{2} (2 \text{ mol}) (8.31 \text{ J / mol} \cdot \text{K}) = 24.9 \text{ J / mol} \cdot \text{K}$$

Note: $C_v^{\text{rot}} = \left(\frac{\partial U^{\text{rot}}}{\partial T} \right)_{V,n} = \frac{d}{dT} \left(\frac{3}{2} nRT \right) = \frac{3}{2} nR = 24.9 \text{ J / mol} \cdot \text{K}$

Notice that the rotational contribution to both the constant volume and constant pressure heat capacities are the same. It is only the translational contribution to the two heat capacities which is different.

Entropy: H^{rot}

$$S^{\text{rot}} = k \ln(Q^{\text{rot}}) + \frac{U^{\text{rot}}}{T} = k(nN_A \ln(q^{\text{rot}})) + \frac{U^{\text{rot}}}{T} = nR \ln(q^{\text{rot}}) + \frac{\frac{3}{2} nRT}{T}$$

$$= (2 \text{ mol}) (8.31 \text{ J / mol} \cdot \text{K}) \ln(3345) + \frac{3}{2} (2 \text{ mol}) (8.31 \text{ J / mol} \cdot \text{K})$$

$$= 134.9 \text{ J / K} + 24.9 \text{ J / K} = 159.8 \text{ J / K} \approx 160 \text{ J / K}$$

Helmholtz Energy: A^{rot}

$$A^{\text{rot}} = -kT \ln(Q^{\text{rot}}) = -kT [nN_A \ln(q^{\text{rot}})] = -nRT \ln(q^{\text{rot}})$$

$$= -(2 \text{ mol}) (8.31 \text{ J / mol} \cdot \text{K}) (423 \text{ K}) \ln(3345) = -57050 \text{ J} \approx -57.1 \text{ kJ}$$

Gibbs Energy: G^{rot}

$$G^{\text{rot}} = -kT \ln(Q^{\text{rot}}) + kT \left(\frac{\partial \ln(Q^{\text{rot}})}{\partial V} \right)_{T,n} = -kT \ln(Q^{\text{rot}}) + 0$$

$$= A^{\text{rot}} \approx -57.1 \text{ kJ}$$

9.
$$q^{\text{rot}} = \frac{T}{\sigma \Theta_R} = \frac{T}{\sigma \left(\frac{h^2}{8\pi^2 I k} \right)} = \frac{T \cdot I}{\sigma \left(\frac{h^2}{8\pi^2 k} \right)} = \frac{T \cdot \mu r^2}{\sigma \left(\frac{h^2}{8\pi^2 k} \right)} = C \cdot \mu T$$

C is a constant which cancels out when taking ratios.

(a)
$$\mu_{H_2} = \frac{m_H m_H}{m_H + m_H} = \frac{m_H}{2} = \frac{1.0 \text{ amu}}{2} = 0.5 \text{ amu}$$

$$\mu_D = \frac{m_D m_D}{m_D + m_D} = \frac{m_D}{2} = \frac{2.0 \text{ amu}}{2} = 1.0 \text{ amu}$$

Note: Because we only need the ratio of reduced masses, it is not necessary to convert to SI units.

$$\frac{q^{\text{rot}}(D_2)}{q^{\text{rot}}(H_2)} = \frac{C \cdot \mu_{D_2} \cdot T}{C \cdot \mu_{H_2} \cdot T} = \frac{\mu_{D_2}}{\mu_{H_2}} = \frac{1.0}{0.5} = 2$$

$$q^{\text{rot}}(D_2) = 2 \times q^{\text{rot}}(H_2) = 2(1.70) = 3.40$$

(b) $T_1 = 25^\circ\text{C} = 298 \text{ K}$, $T_2 = 3000^\circ\text{C} = 3273 \text{ K}$

$$\frac{q^{\text{rot}}(T_2)}{q^{\text{rot}}(T_1)} = \frac{C \cdot \mu \cdot T_2}{C \cdot \mu \cdot T_1} = \frac{T_2}{T_1} = \frac{3273 \text{ K}}{298 \text{ K}} = 10.98 \approx 11.0$$

$$q^{\text{rot}}(T_2) = 11.0 \times q^{\text{rot}}(T_1) = (11.0)(1.70) = 18.7$$