

Homework for Chapter 9

Xiping Hu

<https://hxp.plus/>

May 18, 2020

1. HBr 分子的远红外吸收光谱是一些 $\Delta\tilde{\nu}=16.94$ 厘米⁻¹ 等间隔的光谱线。试求 HBr 分子的转动惯量及原子核间的距离。已知 H 和 Br 的原子量分别为 1.008 和 79.92。

$$\begin{cases} \Delta\tilde{\nu} = 2B \\ B = \frac{h}{8\pi^2 Ic} \\ \mu = \frac{m_1 m_2}{m_1 + m_2} \\ I = \mu r^2 \end{cases} \Rightarrow \begin{cases} I = 3.302 \times 10^{-47} \text{ kg} \cdot \text{m}^2 \\ r = 1.42 \text{ \AA} \end{cases}$$

2. HCl 分子有一个近红外光谱带，其相邻的几条谱线的波数是：2925.78、2906.25、2865.09、2843.56、2821.49 厘米⁻¹。H 和 Cl 的原子量分别是 1.008 和 35.46。试求这个谱带的基线波数 $\tilde{\nu}_0$ 和这种分子的转动惯量。

$$\begin{cases} \tilde{\nu}_{R1} = \tilde{\nu}_0 + 2B = 2906.25 \text{ cm}^{-1} \\ \tilde{\nu}_{P1} = \tilde{\nu}_0 - 2B = 2865.09 \text{ cm}^{-1} \\ \tilde{\nu}_{R2} = \tilde{\nu}_0 + 4B = 2925.78 \text{ cm}^{-1} \\ \tilde{\nu}_{P2} = \tilde{\nu}_0 - 4B = 2843.56 \text{ cm}^{-1} \end{cases} \Rightarrow \bar{B} = \frac{1}{2} \left(\frac{\tilde{\nu}_{R1} - \tilde{\nu}_{R2}}{4} + \frac{\tilde{\nu}_{R2} - \tilde{\nu}_{P2}}{8} \right) = 10.285 \text{ cm}^{-1}$$

$$\Rightarrow \begin{cases} I = \frac{h}{8\pi^2 Bc} = 2.72 \times 10^{-47} \text{ kg} \cdot \text{m}^2 \\ \tilde{\nu}_0 = \frac{\tilde{\nu}_{R1} + \tilde{\nu}_{R2} + \tilde{\nu}_{P1} + \tilde{\nu}_{P2}}{4} = 2885.17 \text{ cm}^{-1} \end{cases}$$

3. Cl 原子的两同位素 Cl^{35} 和 Cl^{37} 分别与 H 原子化合成两种分子 HCl^{35} 和 HCl^{37} ，试求这两种分子的振动光谱中相应光谱带基线的频率 ν_0 之比。

$$\tilde{\nu} = \frac{1}{2\pi c} \sqrt{\frac{k}{m}} \Rightarrow \frac{\tilde{\nu}_{01}}{\tilde{\nu}_{02}} = \sqrt{\frac{m_2}{m_1}} = 1.002$$

5. 怎样解释分子的组合散射有下列两个特点：

(1) 波长短的伴线比波长长的伴线的强度弱；

(2) 随散射体温度的升高，波长短的伴线强度明显增强而波长长的伴线的强度几乎不变。

According to statistics regulations, molecules tend to stay on low energy levels, thus the amount of molecules on high energy levels is far more smaller than the amount of molecules on low energy levels. So that the majority of molecules will emit light with long wavelength, while few molecules emit light with short wavelength. This causes the irradiance of light with short wavelength lower than those with long wavelength.

But when the temperature becomes higher, according to Boltzmann Statistics, more molecules will exist in high energy levels, thus the irradiance of light with short wavelength will become higher.