

Quantum Chemistry

Exercises 4

1. In the far infrared spectrum of H^{79}Br , there is a series of lines separated by 16.72 cm^{-1} . Calculate the moment of inertia and internuclear separation in H^{79}Br .
2. The $I=0 \rightarrow I=1$ transition for carbon monoxide ($^{12}\text{C}^{16}\text{O}$) occurs at $1.153 \cdot 10^5 \text{ MHz}$. Calculate the bond length in carbon monoxide.
3. In Cartesian coordinates the z-component of the angular momentum operator is given by:

$$\hat{L}_z = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

Use the following equations that relate Cartesian and spherical coordinates

$$\begin{aligned} x &= r \sin\theta \cos\varphi & r &= \sqrt{x^2 + y^2 + z^2} \\ y &= r \sin\theta \sin\varphi & \varphi &= \tan^{-1} \left(\frac{y}{x} \right) \\ z &= r \cos\theta & \theta &= \cos^{-1} \left(\frac{z}{\sqrt{x^2 + y^2 + z^2}} \right) \end{aligned}$$

to show that in spherical polar coordinates,

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \varphi}$$