3.9: Rotation of Linear Molecules

The rotational motion of a linear polyatomic molecule can be treated as an extension of the diatomic molecule case. One obtains the $Y_{J,M}(\theta,\phi)$ as rotational wavefunctions and, within the approximation in which the centrifugal potential is approximated at the equilibrium geometry of the molecule (R_e), the energy levels are:

$$E_J^0 = \hbar^2 \frac{J(J+1)}{2I}.$$

Here the total moment of inertia I of the molecule takes the place of μR_e^2 in the diatomic molecule case

$$I = \sum_a m_a (R_a - R_{CofM})^2;$$

m_a is the mass of atom a whose distance from the center of mass of the molecule is $(R_a - R_{CofM})$. The rotational level with quantum number J is (2J+1)-fold degenerate again because there are (2J+1) M- values.