SOLUTION MANUAL FOR HW # 6

8.7)

$$\tilde{\nu}(n) = 2170.21(n + 1/2)cm^{-1} - 13.461(n + 1/2)^2\, cm^{-1}$$

In Morse Potential;

$$E_n = h\nu_0(n + 1/2) - x_e(n + 1/2)^2 \quad \& \quad x_e = \frac{(h\nu_0)^2}{4D_e}$$

$$\Rightarrow x_e(cm^{-1}) = \frac{(\tilde{\nu}_0)^2}{4D_e}$$

$$\Rightarrow 13.461cm^{-1} = \frac{(2170.21cm^{-1})^2}{4D_e} \Rightarrow D_e = \frac{(2170.21cm^{-1})^2}{4(13.461cm^{-1})} = 87417.43cm^{-1}$$

$$\Rightarrow D_e = \tilde{\nu}(0) + D_0 \Rightarrow D_0 = D_e - \tilde{\nu}(0) = (87417.43 - 1081.74)cm^{-1} = 86389.68cm^{-1}$$

$$D_e = 1.74 * 10^{-18}\, J \quad \& \quad D_0 = 1.72 * 10^{-18}\, J$$

8.11) Acetone

8.13)

CO_2: Asymmetric and Doubly degenerate bending modes are IR active (Dipole moment changing) (2349 cm^{-1} and 667 cm^{-1} respectively)

H_2O: Both modes IR active (Dipole moment changing) (Symmetric stretch, 3657 cm^{-1}, Asymmetric stretch 3756 cm^{-1} and Bending 1595 cm^{-1})

8.20)

$$J_{\max} = \frac{1}{2}\left[\sqrt{\frac{4kTI}{\hbar^2}} - 1\right] \Rightarrow T = (2J_{\max} + 1)^2\left(\frac{\hbar^2}{4kI}\right)$$

$$\mu = \frac{m_H m_{Cl}}{m_H + m_{Cl}} = 1.61 * 10^{-27} kg \quad \& \quad r = 1.27 * 10^{-10} m \Rightarrow I = \mu r^2 = 2.60 * 10^{-47} kgm^2$$

1^{st} *Spectrum*:

$$\Rightarrow J_{\max} = 2 \Rightarrow T = 192K$$

2^{nd} *spectrum*

$$\Rightarrow J_{\max} = 3 \Rightarrow T = 375K$$