Harmonic oscillator transition dipole

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Solution: First, we obtain an analytical expression for the transition dipole moment based on the harmonic oscillator model.

$$\left(\frac{\partial \mu_0}{\partial Q}\right)\langle \chi_0|Q|\chi_1\rangle = \left(\frac{\alpha}{\pi}\right)^{1/2}\left(\frac{\partial \mu_0}{\partial Q}\right)\int_{-\infty}^{\infty} e^{-\alpha Q^2/2}\, Q\sqrt{2\alpha}Qe^{-\frac{\alpha Q^2}{2}}dQ$$

$$= \left(\frac{2}{\pi}\right)^{1/2}\alpha\left(\frac{\partial \mu_0}{\partial Q}\right)\int_{-\infty}^{\infty} e^{-\alpha Q^2}\, Q^2 dQ = \left(\frac{\partial \mu_0}{\partial Q}\right)\left(\frac{1}{2\alpha}\right)^{1/2}$$

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Next we calculate α.

$$\alpha = \frac{\mu\omega}{\hbar} = \frac{4\pi^2\mu c\widetilde{\nu_0}}{h}$$

$$\alpha = \frac{4\pi^2(0.95)(1.66\ x\ 10^{-27})(2.99\ x\ 10^{10})(3900)}{6.626\ x\ 10^{-34}}$$

$$\alpha = 1.153\ x\ 10^{22}\ m^{-2}$$

$$\alpha = 115.3\ \text{Å}^{-2}$$

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Combining these results we find that the transition dipole moment is:

$$M_{01} = \left(\frac{\partial \mu_0}{\partial Q}\right)\left(\frac{1}{2\alpha}\right)^{1/2}$$

$$M_{01} = \left(9.5\ \frac{D}{\text{Å}}\right)\left(\frac{1}{2(115.3\ \text{Å}^{-2})}\right)^{1/2}$$

$$M_{01} = 0.625\ D$$