Spectroscopy Light

$$\frac{dN_1}{dt} = B_{1\leftarrow 0}\,\rho(\nu)\,N_o \;-\; B_{1\rightarrow 0}\,\rho(\nu)\,N_1 \;-\; A_{1\rightarrow 0}\,N_1 \qquad \hat{\vec{\mu}} = \hat{\vec{\mu}}_{el} + \hat{\vec{\mu}}_{nuclei} = -\sum_{i=1}^{n} e\,\hat{\vec{r}}_i + \sum_{j=1}^{m} q_j\,\hat{\vec{r}}_j$$

$$\vec{\mu} = -e\vec{r} \qquad \vec{\mu} = -e\int \Psi^* \vec{r}\,\Psi\,d\tau \qquad \vec{\mu}_{tr} = \langle\vec{\mu}\rangle = \int \Psi_j^*\,\hat{\vec{\mu}}\,\Psi_i\,d\tau = \vec{\mu}_{tr,el}\int \chi_{\upsilon'}(R)^*\chi_{\upsilon''}(R)\,dR$$

$$\tilde{B} = \frac{\hbar}{4\pi Ic} = \frac{\hbar}{4\pi\mu r^2 c} \qquad \tilde{F}_J = \frac{E_J}{hc} = \tilde{B}\,J(J+1) \qquad E_J = \tilde{B}\,hc\,J(J+1)$$

$$\tilde{F}_J = \tilde{B}_e\,J(J+1) - \tilde{D}_e\,[J(J+1)]^2 \qquad \tilde{D}_e = \frac{4\tilde{B}^3}{\tilde{\nu}_o^2} \qquad I = \Sigma\, m_i r_i^2 = \mu r^2$$

$$\tilde{B} = \frac{\hbar}{4\pi I_\perp c} \qquad \tilde{A} = \frac{\hbar}{4\pi I_\parallel c} \qquad \tilde{F}_{JK} = \tilde{B}J(J+1) + (\tilde{A} - \tilde{B})K^2$$

$$E_\upsilon = h\nu_e\,(\upsilon + \tfrac{1}{2}) = \hbar\omega_e\,(\upsilon + \tfrac{1}{2}) \qquad \tilde{G}_\upsilon = \tilde{\nu}_e\,(\upsilon + {}^1\!/_2) \qquad \tilde{\nu}_e = \frac{\nu_e}{c} \;\text{ in cm}^{-1}$$

$$\Delta\tilde{G} = \tilde{\nu}_e \qquad \omega_e = 2\pi\nu_e = \sqrt{\frac{k}{\mu}} \qquad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$E_\upsilon = h\nu_e\,(\upsilon + \tfrac{1}{2}) - \chi_e\,h\nu_e\,(\upsilon + \tfrac{1}{2})^2 + \gamma_e\,h\nu_e\,(\upsilon + \tfrac{1}{2})^3 + \ldots.$$

$$V = D_e\,(1 - e^{-a(R-Re)})^2 \qquad a = \omega_e\left(\frac{\mu}{2D_e}\right)^{1/2} \qquad \chi_e = \frac{a^2\hbar}{2\mu\omega_e} = \frac{\hbar\omega_e}{4D_e} = \frac{\tilde{\nu}_e}{4\tilde{D}_e}$$

$$E_\upsilon = h\nu_e\,(\upsilon + \tfrac{1}{2}) - \chi_e\,h\nu_e\,(\upsilon + \tfrac{1}{2})^2 \qquad h\nu_o = hc\tilde{\nu}_e - 2hc\tilde{\nu}_e\chi_e$$

$$\Delta E = h\nu_e - h\chi_e\nu_e\,2(\upsilon + 1) \qquad \Delta\tilde{G}_\upsilon = \tilde{\nu}_e - \chi_e\tilde{\nu}_e\,2(\upsilon + 1)$$

$$D_e = D_o + \tfrac{1}{2}\,h\nu_e - \tfrac{1}{4}\,\chi_e\,h\nu_e \qquad \tilde{D}_e = \tilde{D}_o + \tfrac{1}{2}\,\tilde{\nu}_e - \tfrac{1}{4}\,\tilde{\nu}_e\chi_e \qquad \tilde{D}_e = \tilde{\nu}_e^2/4\chi_e\tilde{\nu}_e$$

$$ZPE = \tilde{G}_o = \tfrac{1}{2}\,\tilde{\nu}_e - \tfrac{1}{4}\,\tilde{\nu}_e\,\chi_e \qquad \tilde{\nu}_m = \tilde{\nu}_o + (2\tilde{B}_e - 2\tilde{\alpha}_e)\,m - \tilde{\alpha}_e\,m^2$$

$$\Delta E_{\upsilon',J'\leftarrow\upsilon'',J''} = E_{\upsilon',J'} - E_{\upsilon'',J''} = h\nu_o\,(\upsilon' - \upsilon'') + \tilde{B}'\,hc\,J'(J'+1) - \tilde{B}''\,hc\,J''(J''+1)$$

$$\tilde{B}_\upsilon = \tilde{B}_e - \tilde{\alpha}_e\,(\upsilon + \tfrac{1}{2}) \qquad k = 4\pi^2c^2\tilde{\nu}_o^2\mu \qquad \Delta E_{\upsilon''+1,J''+1\leftarrow\upsilon'',J''} = h\nu_o + 2\tilde{B}hc\,(J''+1)$$

$$\tilde{B}_e = \frac{\hbar}{4\pi\mu R_e^2 c} \qquad \Delta\tilde{\nu}_\upsilon = (\tilde{\nu}_e^{ex} - 2\chi_e^{ex}\,\tilde{\nu}_e^{ex}) - 2\chi_e^{ex}\,\tilde{\nu}_e^{ex}\,\upsilon = \Delta\tilde{\nu}_o - 2\chi_e^{ex}\,\tilde{\nu}_e^{ex}\,\upsilon$$

$$\tilde{D}_o = \tilde{\nu}_o + \sum_{i=1}^{\infty}\Delta\tilde{\nu}_i = \tilde{\nu}_o + \tfrac{1}{2}\,\Delta\tilde{\nu}_1\,\upsilon_{cl} \qquad \upsilon_{cl} = \frac{\Delta\tilde{\nu}_o}{2\chi_e^{ex}\,\tilde{\nu}_e^{ex}}$$

$$\tilde{\nu}_{\infty o} = \tilde{D}_o + \Delta\tilde{E}_{atomic} = \tilde{\nu}_{oo} + \tilde{D}_o^{ex} = \tilde{\nu}_{oo} + \sum_{i=0}^{\infty}\Delta\tilde{\nu}_i = \tilde{\nu}_o + \tfrac{1}{2}\,\Delta\tilde{\nu}_o\,\upsilon_{cl} \qquad \rho \equiv \frac{I_\perp}{I_\parallel}$$

$$\vec{\mu}_{ind} = \alpha\vec{E} \qquad \begin{pmatrix}\mu_x\\ \mu_y\\ \mu_z\end{pmatrix}_{ind} = \begin{pmatrix}\alpha_{xx} & \alpha_{xy} & \alpha_{xz}\\ \alpha_{yx} & \alpha_{yy} & \alpha_{yz}\\ \alpha_{zx} & \alpha_{zy} & \alpha_{zz}\end{pmatrix}\begin{pmatrix}E_x\\ E_y\\ E_z\end{pmatrix} \qquad \vec{\mu}_{ind} = \underset{\approx}{\alpha}\,\vec{E}$$

1 H = 2625.5 kJ/mol = 627.52 kcal/mol = 27.2116 eV = 219,474.6 cm^{-1}

a_o = 0.529Å = 52.9 pm 1 cal = 4.184 J 1ev = 96.485 kJ/mol = 8065.5 cm^{-1}

1 cm^{-1} = 11.962 J/mol kT/hc = 207.224 cm^{-1} at 298.2K