Chapter 1

$$s = \sigma.\rho.N \qquad (1.1.a)$$

$$s = \sigma.n.\Phi \qquad (1.1.b)$$

$$p = \frac{h\nu}{c} \qquad p = mv \qquad (1.2)$$

$$E = h\nu \qquad E_k = \frac{mv^2}{2} \qquad (1.3)$$

$$\varepsilon_1 + E_1 = \varepsilon_2 + E_2 \qquad \left[h(\nu_1 - \nu_2) << h\nu_1\right] \qquad (1.3)$$

$$\varepsilon_1 + E_1 = E_2^* \qquad (1.4)$$

$$h\nu_1 + E_1^* = 2h\nu_1 + E_2 \qquad (1.5)$$

$$\varepsilon_1 + E_1^* = \varepsilon_2 + E_2 \qquad (\varepsilon_2 > \varepsilon_1) \qquad (1.6a)$$

$$\varepsilon_1 + E_1 = \varepsilon_2 + E_2^* \qquad (\varepsilon_2 < \varepsilon_1) \qquad (1.6b)$$

$$\varepsilon_{1a} + \varepsilon_{1b} + E_1 = 2\varepsilon_{1b} + E_2^* \qquad (\varepsilon_{1a} > \varepsilon_{1b}) \qquad (1.7)$$

$$E_1^* = E_2 + \varepsilon_2 \qquad (1.8)$$

$$\varepsilon_{1a} + E_1 = \varepsilon_{2b} + E_2^* \qquad (1.9)$$

$$h\nu_{1a} = I + \frac{m_e v_e^2}{2} \qquad I = E_2^* - E_1 \qquad (1.10)$$

$$U = \frac{1}{4\pi\varepsilon}\sum_i \frac{Q_i}{|\mathbf{R} - \mathbf{r}_i|} \qquad (1.11)$$

$$\mathbf{p} = \sum_i Q_i \mathbf{r}_i \qquad (1.12)$$

$$\mathbf{F} = Q\mathbf{E} \qquad (1.13)$$

$$\mathbf{p} = \mathbf{p}_o + \alpha\mathbf{E} + \frac{1}{2}\beta\mathbf{E}^2 + \ldots \qquad (1.14)$$

$$\mathbf{T} = \mathbf{p} \times \mathbf{E} \qquad (1.15)$$

$$\mathbf{P} = \frac{\sum_i \mathbf{p}_i}{V} \qquad (1.16)$$

$$\mathbf{P} = \varepsilon_o \chi_e \mathbf{E} \qquad (1.17)$$

$$\mathbf{D} = \varepsilon\mathbf{E} \qquad (1.18)$$

$$\mathbf{D} = \varepsilon_o\mathbf{E} + \mathbf{P} = \varepsilon_o(1 + \chi_e) \qquad (1.19)$$

$$\varepsilon_r \equiv \frac{\varepsilon}{\varepsilon_o} = 1 + \chi_e \qquad (1.20)$$

$$P_M \equiv \frac{\varepsilon_r - 1}{\varepsilon_r + 2}\frac{M}{\rho} \qquad (1.21)$$

$$P_M \equiv \frac{\varepsilon_r - 1}{\varepsilon_r + 2}\frac{M}{\rho} = \frac{N_A}{3\varepsilon_o}\left(\overline{\alpha} + \frac{\mathbf{p}^2}{3kT}\right) \quad (1.22)$$

$$\mathbf{F} = Q\mathbf{v} \times \mathbf{B} \quad (1.23)$$

$$\mathbf{T} = \mathbf{m} \times \mathbf{B} \quad (1.24)$$

$$\frac{e}{m_e}\mathbf{s} = -\mathbf{m}_S \quad (1.24)$$

$$\mu_B \hat{\mathbf{s}} = -\frac{\hbar}{2}\hat{\mathbf{m}}_s \quad (1.25)$$

$$\mu_B = \frac{e\hbar}{2m_e} \quad (1.26)$$

$$\frac{e}{m_e}\mathbf{l} = -2\mathbf{m} \quad (1.27)$$

$$\mu_B \hat{\mathbf{l}} = -\hbar\hat{\mathbf{m}} \quad (1.28)$$

$$g\mu_B \hat{\mathbf{L}} = -\hbar\hat{\mathbf{M}} \quad (1.29)$$

$$g_N \mu_N \hat{\mathbf{I}} = \hbar\hat{\mathbf{M}}_I \quad (1.30)$$

$$\mu_N = \frac{e\hbar}{2m_p} \quad (1.31)$$

$$\Delta m = \frac{e^2 r^2}{4m_e}B \quad (1.32)$$

$$\omega = g\frac{\mu_B}{h}B = \gamma_e B \quad (1.33)$$

$$\omega = g_N\frac{\mu_B}{h}B = \gamma_N B \quad (1.34)$$

$$M = \int \psi_i^* \Delta\mathbf{m}\psi_j d\tau \quad (1.35)$$

$$\mathbf{M} = \sum_i \frac{\mathbf{m}_i}{V} \quad (1.36)$$

$$\mathbf{M} = \mu_o \chi_m \mathbf{H} \quad (1.37)$$

$$\mathbf{B} = \mu\mathbf{H} \quad (1.38)$$

$$\mu_r = 1 + \chi_m \quad (1.39)$$

$$\chi_m = \frac{A}{T} + B \quad (1.40)$$

$$\Delta E \equiv E_i - E_j = h\nu \equiv \hbar\omega \quad (1.41)$$

$$a_{i\leftarrow j} = \frac{1}{\hbar^2}\left|\int_0^{t_p} K_{ij}(t)\,exp(i\omega_{ij}t)dt\right|^2 \qquad (1.42)$$

$$K_{ij} = \int \psi_i^* \hat{K} \psi_j d\tau \qquad (1.43)$$

$$V = \Delta\mathbf{pE} \qquad (1.44)$$

$$K_{ij} = \mathbf{E}\int \psi_i^* \Delta\mathbf{p} \psi_j d\tau \qquad (1.45)$$

$$P = \int \psi_i^* \Delta\mathbf{p} \psi_j d\tau \qquad (1.46)$$

$$\frac{N_i}{N_j} = exp\left(-\frac{E_i - E_j}{kT}\right) = exp\left(-\frac{h\nu}{kT}\right) \qquad (1.47)$$

$$r + a + t = 1 \qquad (1.48)$$

$$\delta E.\delta t \geq \frac{h}{2\pi} \qquad (1.49)$$

$$\delta\nu \geq \frac{1}{2\pi\tau} \qquad (1.50)$$

$$\Delta\nu = \nu - \nu_0 = \nu_o \frac{v}{c} \qquad (1.51)$$

$$T \equiv \frac{I}{I_o} \qquad (1.52)$$

$$A \equiv \lg\left(\frac{I_o}{I}\right) = -\lg(T) \qquad (1.53)$$

$$R \equiv \lg\left(\frac{I_o}{I_r}\right) = -\lg(r) \qquad (1.54)$$

$$\tilde{\nu} \equiv \frac{\nu}{c} \qquad (1.55)$$

Chapter 2

$$\hat{H}\psi = E\psi \qquad (2.1)$$

$$\psi(r,\varphi,\theta) = R(r)Y(\varphi,\theta) \qquad (2.2)$$

$$\hat{H} = \hat{T} + \hat{V} \qquad (2.3)$$

$$V = -\frac{1}{4\pi\varepsilon_o}\frac{e^2}{r} \qquad (2.3)$$

$$\hat{T} = -\frac{\hbar^2}{2m_e}\left(\hat{T}_r + \hat{T}_{\varphi,\theta}\right) - \frac{\hbar^2}{2m_p}\hat{T}_p \tag{2.4}$$

$$Y(\varphi,\theta)\left[-\frac{\hbar^2}{2m_e}\hat{T}_r + \hat{V}\right]R(r) - \frac{\hbar^2}{2m_e}R(r)\hat{T}_{\varphi,\theta}\left[Y(\varphi,\theta)\right] = ER(r)Y(\varphi,\theta) \tag{2.5}$$

$$\frac{1}{R(r)}\left[-\frac{\hbar^2}{2m_e}\hat{T}_r + \hat{V}\right]R(r) = \frac{\hbar^2}{2m_e}\frac{1}{Y(\varphi,\theta)}\hat{T}_{\varphi,\theta}\left[Y(\varphi,\theta)\right] - E \tag{2.6}$$

$$E_n = -\frac{e^4 m_e}{32\pi\varepsilon_o \hbar^2 n^2} = -hc\frac{R_H}{n^2} \tag{2.7}$$

$$\psi(n,l,m) = N_{n,l,m}\frac{1}{r}R_n^l\left(\frac{2r}{na_o}\right)Y_l^m(\varphi,\theta) \tag{2.8}$$

$$a_o = \frac{4\pi\varepsilon_o \hbar^2}{m_e e^2} = 52.9\,\text{pm} \tag{2.9}$$

$$\int \psi^* \psi \, d\tau = 1 \tag{2.10}$$

$$\hat{\mathbf{l}}^2 Y_l^m = l(l+1)\hbar^2 Y_l^m \tag{2.11}$$

$$l = \sqrt{l(l+1)}\hbar = l^*\hbar \tag{2.12}$$

$$\hat{l}_z Y_l^m = m\hbar Y_l^m \tag{2.13}$$

$$l_z = m\hbar \tag{2.14}$$

$$m = -\mu_B l^* \tag{2.15}$$

$$m_z = -\mu_B m \tag{2.16}$$

$$\hat{\mathbf{s}}^2\varphi(\sigma) = s(s+1)\hbar\varphi(\sigma) \tag{2.17}$$

$$s = \sqrt{s(s+1)}\hbar = s^*\hbar \tag{2.18}$$

$$\hat{s}_z\varphi(\sigma) = m_s\hbar\varphi(\sigma) \tag{2.19}$$

$$s_z = m_s\hbar \tag{2.20}$$

$$m_s = -2\mu_B s^* \tag{2.21}$$

$$m_{s,z} = -2\mu_B m_s \tag{2.22}$$

$$\mathbf{j} = \mathbf{l} + \mathbf{s} \tag{2.23}$$

$$j = \sqrt{j(j+1)}\hbar = j^*\hbar \qquad (j = l + s) \tag{2.24}$$

$$j_z = m_j\hbar \; (-j \le m_j \le +j) \tag{2.25}$$

$$\hat{\mathbf{I}}^2\psi = I(I+1)\hbar^2\psi \tag{2.26}$$

$$I = \sqrt{I(I+1)}\hbar = I^*\hbar \qquad \text{for hydrogen } I = \frac{1}{2} \tag{2.27}$$

$$I_z = M_I\hbar \qquad (-I \le M_I \le +I) \tag{2.28}$$

$$M_I = g_p\mu_N I^* \tag{2.29}$$

$$M_{I,z} = g_p \mu_N \mathrm{M}_I \tag{2.30}$$

$$\Delta E = E_i - E_j = h\nu \tag{2.31}$$

$$\mathbf{P} = \int \psi_i^* \Delta\mathbf{p} \psi_j \mathrm{d}\tau \neq 0 \tag{2.32}$$

$$\Delta\mathbf{p} = -\mathrm{e}\Delta\mathbf{r} \tag{2.33}$$

$$\Delta \mathrm{p_x} = -\mathrm{e}\Delta \mathrm{r} \sin\theta \cos\varphi \tag{2.34}$$

$$\Delta \mathrm{p_y} = -\mathrm{e}\Delta \mathrm{r} \sin\theta \sin\varphi \tag{2.35}$$

$$\Delta \mathrm{p_z} = -\mathrm{e}\Delta \mathrm{r} \cos\theta \tag{2.36}$$

$$d\tau = r^2 \sin\theta d\varphi d\theta dr \tag{2.37}$$

$$\mathrm{P_x} = -\mathrm{e}\int_0^\infty \int_0^\pi \int_0^{2\pi} \psi_i^*(\mathrm{r},\varphi,\theta)\psi_j(\mathrm{r},\varphi,\theta)\mathrm{r}^2 \Delta \mathrm{r}\, sin^2\theta\, cos\,\varphi \mathrm{d}\varphi \mathrm{d}\theta \mathrm{dr} \tag{2.38}$$

$$\mathrm{P_y} = -\mathrm{e}\int_0^\infty \int_0^\pi \int_0^{2\pi} \psi_i^*(\mathrm{r},\varphi,\theta)\psi_j(\mathrm{r},\varphi,\theta)\mathrm{r}^2 \Delta \mathrm{r}\, sin^2\theta\, sin\,\varphi \mathrm{d}\varphi \mathrm{d}\theta \mathrm{dr} \tag{2.39}$$

$$\mathrm{P_x} = -\mathrm{e}\int_0^\infty \int_0^\pi \int_0^{2\pi} \psi_i^*(\mathrm{r},\varphi,\theta)\psi_j(\mathrm{r},\varphi,\theta)\mathrm{r}^2 \Delta \mathrm{r}\, sin\,\theta\, cos\,\theta \mathrm{d}\varphi \mathrm{d}\theta \mathrm{dr} \tag{2.40}$$

$$\tilde{\nu} = \frac{\Delta \mathrm{E}}{\mathrm{hc}} = \mathrm{R_H}\left(\frac{1}{\mathrm{n}_j^2} - \frac{1}{\mathrm{n}_i^2}\right) \qquad \mathrm{n_i} > \mathrm{n_j} \tag{2.41}$$

$$\tilde{\nu}_{\mathrm{lim}it} = T_j = \frac{\mathrm{R}_H}{\mathrm{n}_j^2} \tag{2.42}$$

$$\mathrm{E}_n = -\frac{\mathrm{z}^2 \mathrm{hc} R_\mathrm{H}}{n^2} = -\mathrm{hc}\frac{R_\mathrm{z}}{n^2} \tag{2.43}$$

$$\tilde{\nu} = \mathrm{R_z}\left[\frac{1}{(\mathrm{n_j} - \mathrm{a_j})^2} - \frac{1}{(\mathrm{n_i} - \mathrm{a_i})^2}\right] \tag{2.44}$$

$$\hat{\mathrm{H}} = -\frac{\hbar^2}{2\mathrm{m_e}}\sum_i \nabla^2 - \sum_i \frac{\mathrm{ze}^2}{\mathrm{r_i}} + \sum_i \sum_{j>i} \frac{\mathrm{e}^2}{\mathrm{r_{ij}}} \tag{2.45}$$

$$E_{1s} < E_{2s} < E_{2p} < E_{3s} < E_{3p} < E_{4s} < E_{3d} < E_{4p} < E_{5s} \ldots \tag{2.46}$$

$$\mathbf{L} = \sum_i \mathbf{l}_i \tag{2.47}$$

$$L = \sqrt{\mathrm{L}(\mathrm{L}+1)}\hbar = \mathrm{L}^*\hbar \tag{2.48}$$

$$\mathbf{S} = \sum_i \mathbf{s}_i \qquad 2.49)$$

$$S = \sqrt{\mathrm{S}(\mathrm{S}+1)}\hbar = \mathrm{S}^*\hbar \tag{2.50}$$

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}} \tag{2.51}$$

$$J = \sqrt{\mathrm{J}(\mathrm{J}+1)}\hbar = \mathrm{J}^*\hbar \qquad \mathrm{J} = \mathrm{L}+\mathrm{S}, \mathrm{L}+\mathrm{S}-1, \ldots, |\mathrm{L}-\mathrm{S}| \tag{2.52}$$

$$J_z = \mathrm{M}_J\hbar \qquad -\mathrm{J} \le \mathrm{M}_J \le +\mathrm{J} \qquad \mathrm{M}_J = \mathrm{M}_L + \mathrm{M}_S \tag{2.53}$$

$$\begin{aligned} \iota &= 2\mathrm{S}+1 \qquad (\mathrm{L} \ge \mathrm{S}, \text{usually}) \\ \iota &= 2\mathrm{L}+1 \qquad (\mathrm{L} < \mathrm{S}, \text{very rarely}) \end{aligned} \tag{2.54}$$

$$\hat{\mathbf{J}} = \sum_i \hat{\mathbf{j}}_i \qquad \textit{for two electrons}: \quad \mathrm{J} = \mathrm{j}_1 + \mathrm{j}_2, \mathrm{j}_1 + \mathrm{j}_2 - 1, \ldots, |\mathrm{j}_1 - \mathrm{j}_2| \tag{2.55}$$

$$\mathrm{E} = \mathrm{E}_o + \frac{1}{2}\mathrm{A}(\mathrm{J}^*)^2 + \mathrm{g}\mu_\mathrm{B}\mathrm{M}_\mathrm{J}\mathrm{B} \tag{2.56}$$

$$\mathrm{g} = 1 + \frac{(\mathrm{J}^*)^2 + (\mathrm{S}^*)^2 - (\mathrm{L}^*)^2}{2(\mathrm{J}^*)^2} \tag{2.57}$$

$$\mathrm{E} = \mathrm{E}_o + \mathrm{AM}_\mathrm{L}\mathrm{M}_\mathrm{S} + \mathrm{g}(\mathrm{M}_\mathrm{L} + 2\mathrm{M}_\mathrm{S})\mathrm{B} \tag{2.58}$$

$$\mathrm{E} = \mathrm{E}_o - \mathrm{g}_\mathrm{N}\mu_\mathrm{N} M_\mathrm{I}\mathrm{B} \tag{2.59}$$

$$\mathrm{E} = \mathrm{E}_o + \frac{1}{2}\mathrm{E}^2\left[\mathrm{a} + 2\mathrm{b}\left(\mathrm{M}_\mathrm{J}^2 - \frac{1}{3}(\mathrm{J}^*)^2\right)\right] \tag{2.60}$$

$$\mathrm{A} - \mathrm{e}^- = \mathrm{A}^+ \tag{2.61}$$

$$\begin{aligned} \mathrm{A} + \mathrm{e}^- &= \mathrm{A}^- \\ \mathrm{A}^- + \mathrm{e}^- &= \mathrm{A}^{2-} \end{aligned} \tag{2.62}$$

$$I(O^-) = -A(O) \tag{2.63}$$

$$\mathrm{A} + \mathrm{e}^- = \mathrm{A}^+ + 2\mathrm{e}^- \tag{2.64}$$

$$\mathrm{M} + \mathrm{e}^- = \mathrm{M}^+ + 2\mathrm{e}^- \tag{2.65}$$

$$\mathrm{ABC} + \mathrm{e}^- = \mathrm{AB}^- + \mathrm{C} \tag{2.66}$$

$$A + h\nu = A^{+} + e^{-} \tag{2.67}$$

$$A^{*} + B = A + B^{+} + e^{-} \tag{2.68}$$

$$A^{*} + BC = AC^{+} + B + e^{-} \tag{2.69}$$

$$A^{*} + B = A^{+} + B + e^{-} \tag{2.70}$$

$$A^{*} + B = A^{+} + B^{-} \tag{2.71}$$

$$A^{*} + B = AB^{+} + e^{-} \tag{2.72}$$

$$X^{+} + M = X + M^{+} \tag{2.73}$$

$$X^{+} + M = XM^{+} \tag{2.74}$$

$$XH^{+} + M = X + MH^{+} \tag{2.75}$$

$$\mathbf{F} = Q\mathbf{E} \tag{2.76}$$

$$\mathbf{F} = Q\mathbf{v} \times \mathbf{B} \tag{2.77}$$

Chapter 3

$$E \times X = X \times E = X \tag{3.1}$$

$$X \times Y = E \tag{3.2}$$

$$Y = X^{-1} \quad \text{and} \quad X = Y^{-1} \tag{3.3}$$

$$(A \times B) \times C = A \times (B \times C) \tag{3.4}$$

$$Y = Z \times X \times Z^{-1} \quad \text{i.e.} \quad X = Z \times Y \times Z^{-1} \tag{3.5}$$

$$\begin{bmatrix} x_2 \\ y_2 \\ z_2 \end{bmatrix} = \begin{bmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} \tag{3.6}$$

$$\begin{bmatrix} x_2 \\ y_2 \\ z_2 \end{bmatrix} = \begin{bmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} \tag{3.7}$$

$$\chi_j = \pm 1 + 2\cos\left(2\pi\frac{p}{n}\right) \qquad p = 1,2,\ldots,n-1 \tag{3.8}$$

$$\hat{H} = -\frac{\hbar^2}{2m_e}\sum_{i=1}^{n}\nabla^2 + \sum_{i=1}^{n}\sum_{j>i}^{n}\frac{e^2}{r_{ij}} - \sum_{i=1}^{n}\sum_{\alpha=1}^{N}\frac{Z_\alpha e^2}{r_{i\alpha}} + \sum_{\alpha=1}^{N}\sum_{\beta>\alpha}^{N}\frac{Z_\alpha Z_\beta e^2}{r_{\alpha\beta}} \tag{3.9}$$

$$S_{12} = \int \psi_1^* \psi_2 d\tau \tag{3.10}$$

$$X = \frac{1}{2}(I + A) \tag{3.11}$$

species	molecular orbital	
Σ_g^+	$\sigma_g = \frac{1}{\sqrt{2(1+S)}}(1s_A + 1s_B)$	(3.12)
Σ_u^+	$\sigma_u^* = \frac{1}{\sqrt{2(1-S)}}(1s_A - 1s_B)$	(3.13)

$$\psi_1 = \frac{1}{2}\left[\chi(2s) + \chi(2p_x) + \chi(2p_y) + \chi(2p_z)\right] \tag{3.14}$$

$$\psi 2 = \frac{1}{2}\left[\chi(2s) + \chi(2p_x) - \chi(2p_y) - \chi(2p_z)\right] \tag{3.15}$$

$$\psi 3 = \frac{1}{2}\left[\chi(2s) - \chi(2p_x) + \chi(2p_y) - \chi(2p_z)\right] \tag{3.16}$$

$$\psi_4 = \frac{1}{2}\left[\chi(2s) - \chi(2p_x) - \chi(2p_y) + \chi(2p_z)\right] \tag{3.17}$$

$$S_{ij} = 0 \qquad i \neq j \tag{3.18}$$

$$S_{ij} = 1 \qquad i = j \tag{3.19}$$

$$H_{ij} = \int \psi_i^* \hat{H} \psi_j d\tau \tag{3.20}$$

$H_{ij} = \alpha$ if i and j belongs to the same atom (Coulomb integral) (3.21)

$H_{ij} = \beta$ if i and j belong to neighbour atoms (resonance integral) (3.22)

$H_{ij} = 0$ in all other cases (3.23)

$$|\mathbf{H} - E\mathbf{S}| = 0 \qquad (3.24)$$

$$\begin{vmatrix} \alpha - E & \beta \\ \beta & \alpha - E \end{vmatrix} = 0 \qquad (3.25)$$

$$\alpha_X = \alpha + h_X\beta \qquad (3.26)$$

$$\beta_{XY} = k_{XY}\beta \qquad (3.27)$$

$$T = E_r = \frac{1}{2}I\omega^2 = \frac{1}{2}\frac{L^2}{I} \qquad (3.28)$$

$$L = \sqrt{J(J+1)}\hbar = J^*\hbar \qquad J = 0,1,2,3,... \qquad (3.29)$$

$$L_z = M_J\hbar \qquad -J \le M_J \le J \qquad (3.30)$$

$$E_r = \frac{\hbar^2}{2I}J(J+1) = B'J(J+1) \qquad (3.31)$$

$$B' = \frac{\hbar^2}{2I} \qquad (3.32)$$

$$I = \sum_{i=1}^{N} m_i r_i^2 \qquad (3.33)$$

$$I = \mu r_o^2 \qquad (3.34)$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \qquad (3.35)$$

$$\Delta J = \pm 1 \quad \text{and} \quad M_J = \pm 1 \qquad (3.36)$$

$$\tilde{\nu} = \frac{E_{r,i} - E_{r,j}}{hc} = B[(J+1)(J+2) - J(J+1)] = 2B(J+1) \qquad (3.37)$$

$$B = \frac{B'}{hc} = \frac{h}{8\pi^2 cI} \qquad (3.38)$$

$$N_J = N_0(2J+1)\exp\left(-\frac{E_{r,J}}{kT}\right) = N_0(2J+1)\exp\left[-\frac{B'J(J+1))}{kT}\right] \qquad (3.39)$$

$$\Delta\mathbf{p} = \Delta\alpha * \mathbf{E} \qquad (3.40)$$

$\Delta J = \pm 2$ for identical atoms (3.41)

$\Delta J = \pm 1, \pm 2$ for different atoms (3.42)

$$E_r = hc\left[BJ(J+1) + (A - B)K^2\right] \quad (3.43)$$

$$E_r = hc\left[BJ(J+1) + (C - B)K^2\right] \quad (3.44)$$

$$E_r = hc\left[BJ(J+1) + (A - B)K^2\right] \quad (3.43)$$

$$E_r = hc\left[BJ(J+1) + (C - B)K^2\right] \quad (3.44)$$

$\Delta J = \pm 1$ $\Delta K = 0$ (IR) (3.45)

$\Delta J = \pm 1, \pm 2$ $\Delta K = 0$ (RA) (3.46)

$\Delta J = \pm 1$ (IR) (3.47)

$\Delta J = \pm 2$ (RA) (3.48)

$$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{d^2}{dq^2} + \frac{1}{2}kq^2 \quad (3.49)$$

$$E_v = h\nu\left(v + \frac{1}{2}\right) \qquad v =,1,2,... \quad (3.50)$$

$\Delta v = \pm 1$ (+: absorption, -: emission) (3.51)

$$E_v = h\nu\left[\left(v + \frac{1}{2}\right) - x\left(v + \frac{1}{2}\right)^2\right] \quad (3.52)$$

$$2V = 4\pi^2 c^2 \sum_{i=1}^{3N-6} \tilde{\nu}_i^2 Q_i^2 \qquad 2T = \sum_{i=1}^{3N-6} \dot{Q}_i^2 \quad (3.53)$$

$$2V = \mathbf{q}'\mathbf{f}\mathbf{q} \qquad 2T = \dot{\mathbf{q}}'\mathbf{g}^{-1}\dot{\mathbf{q}} \quad (3.54)$$

$$2V = \mathbf{S}'\mathbf{F}\mathbf{S} \qquad 2T = \dot{\mathbf{S}}'\mathbf{G}^{-1}\dot{\mathbf{S}} \quad (3.55)$$

$$\left|\mathbf{GF} - \lambda\mathbf{E}\right| = 0 \quad (3.56)$$

$$\lambda_i = 4\pi^2 c^2 \tilde{\nu}^2 \qquad i = 1,2,...,3N-6 \quad (3.57)$$

$$\mathbf{Q} = \mathbf{L}^{-1}\mathbf{S} \quad (3.58)$$

$$F_{ij} = \left(\frac{\partial^2 E}{\partial S_i \partial S_j}\right)_0 \quad \text{or} \quad f_{ij} = \left(\frac{\partial^2 E}{\partial q_i \partial q_j}\right)_0 \tag{3.59}$$

$$\rho = \frac{I_{\perp}}{I_{||}} \tag{3.60}$$

$$\chi_j = \pm 1 + 2\cos\left(2\pi \frac{p}{n}\right) \qquad p = 1,2,...,n-1 \tag{3.61}$$

$$m_i = \frac{1}{h}\sum_j n_j \chi_j(R)\chi_{ij} - r_i \tag{3.62}$$

$$\tilde{\nu} = \frac{E}{hc} = \frac{kT}{hc} = \frac{h}{2m_n c\lambda^2} \tag{3.63}$$

$$A = \alpha \ell c \tag{3.63}$$

$$A = \int_{band} \alpha(\nu) d\nu \tag{3.64}$$

$$f = A\frac{4m_e c\varepsilon_o}{N_A e^2} ln(10) \approx 1.44 \times 10^{-19} \times A \qquad dm^3\ cm^{-1}s^{-1}mol^{-1} \tag{3.65}$$

$$f = \frac{4\pi m_e \nu}{3he^2} P^2 \tag{3.66}$$

$$-CH_3 < -C_2H_5 < -CH(CH_3)_2 < -C(CH_3)_3 < -S^- < O^- \tag{3.67}$$

$$-F > -NO_2 > -OH > -Cl > -NH_2 - Br > -I > -C = O > -COOH > -CN > -SH > -R_3N^+ \tag{3.68}$$

$$-F < -Cl < -Br < -OH < -OCH_3 < -NH_2 < -O^- \tag{3.69}$$

$$-NO_2 > -CHO > -COCH_3 > -COOH > COO^- \approx -CN > -SO_2NH_2 \tag{3.70}$$

$$h\nu = \frac{1}{2}m_e v^2 + I \tag{3.71}$$

$$h\nu = \frac{1}{2}m_e v^2 + I + \Delta E_v + \Delta E_r \tag{3.72}$$

$$n = \frac{c}{v} \tag{3.73}$$

$$v = \nu\lambda \tag{3.74}$$

$$n = \sqrt{\varepsilon_r \mu_r} \approx \sqrt{\varepsilon_r} \tag{3.75}$$

$$E = E_o\, exp\left[i2\pi\nu\left(t - \frac{nz}{c}\right)\right] \tag{3.76}$$

$$E = E_o \, exp\left(-2\pi \frac{n_k z}{c}\right) exp\left[i 2\pi\nu\left(t - \frac{nz}{c}\right)\right] \tag{3.77}$$

$$n = n - in_k \tag{3.78}$$

$$n_k = \frac{c \, ln 10}{4\pi\tilde{\nu}}\alpha \tag{3.79}$$

$$\Delta p_o = \frac{a}{\nu_o^2 - \nu^2} \tag{3.80}$$

$$R_M \equiv \frac{n^2 - 1}{n^2 + 2}\frac{M}{\rho} \tag{3.81}$$

$$\frac{n^2 - 1}{n^2 + 2} = \frac{\rho_N}{3}\sum_i \frac{C_i A_i}{\nu_{o,i}^2 - \nu^2} \tag{3.82}$$

$$\Delta\vartheta = 2\pi\ell \frac{n_L - n_R}{\lambda} \tag{3.83}$$

$$[\alpha] = \frac{\Delta\vartheta}{\ell c} \tag{3.84}$$

$$[M] = 10^{-3} M[\alpha] \tag{3.85}$$

$$\Delta\alpha = \alpha_R - \alpha_L \tag{3.86}$$

$$zvB = \frac{mv^2}{r} \tag{3.87}$$

$$zU = \frac{mv^2}{2} \tag{3.88}$$

$$m/z = \frac{B^2 r^2}{2U} \tag{3.89}$$

$$m/z = \frac{5.7V}{4\pi^2\nu^2} \tag{3.90}$$

$$m/z = \frac{2U}{s^2}t^2 \tag{3.91}$$

$$m^* \approx \frac{m_2^2}{m_1} \tag{3.92}$$

$$\Delta E = +\mu_B B - (-\mu_B B) = 2\mu_B B \tag{3.93}$$

$$h\nu = 2\mu_B B \tag{3.94}$$

$$\Delta m_s = \pm 1 \tag{3.95}$$

$$B = \frac{h}{2\mu_B}\nu \tag{3.96}$$

$$B - aM_I = \frac{h}{2\mu_B}\nu \tag{3.97}$$

$$B' = (1-\sigma)B \tag{3.98}$$

$$M_{I,z} = g_a M \mu_N \qquad M = -I, -I+1, ..., I-1, I \tag{3.99}$$

$$E = -\mathbf{M_I B} = -g_a \mu_N M B \tag{3.100}$$

$$\Delta E = \mp g_a \mu_N B \tag{3.101}$$

$$\nu_0 = \frac{\gamma_a}{2\pi} B \tag{3.102}$$

$$\nu = \frac{\gamma_a}{2\pi} B_l = (1-\sigma)\frac{\gamma_a}{2\pi} B = (1-\sigma)\nu_r \tag{3.103}$$

$$\nu = \frac{\gamma_a}{2\pi} B_\ell = (1-\sigma)\frac{\gamma_a}{2\pi} B = (1-\sigma)\nu_o \tag{3.104}$$

$$\tau = 10 - \delta \tag{3.105}$$

$$E = E_o - g_a \mu_B B \sum_i (1-\sigma_i) M_i - \frac{h}{2}\sum_i \sum_j J_{ij} M_i M_j \tag{3.106}$$

$$\Delta M_A = \pm 1 \qquad \Delta M_{B_i} = \pm \qquad i = 1, 2, ..., n \tag{3.107}$$

$$\Delta \sum_i M_i = \pm 1 \tag{3.108}$$

$$\nu_i = \frac{g_a \mu_N B (1-\sigma_i)}{h} + \sum_{j \neq i} J_{ij} M_j = \nu_i^0 + \sum_{j \neq i} J_{ij} M_j \tag{3.109}$$

$$I = 1 \pm \frac{2qJ}{q^2 + J^2} \tag{3.110}$$

$$I_{NOE} = I\left(1 + \frac{P_{32} - P_{41}}{P_{32} + P_{41} + 2P_o}\frac{\gamma_H}{\gamma_C}\right) = I(1+\eta) \tag{3.111}$$

$$\frac{dn}{dt} = 2P(n_e - n) \qquad n = N_+ - N_- \tag{3.112}$$

$$n_e - n = (n_e - n)_o \, exp\left(-\frac{t}{T_1}\right) \qquad T_1 = \frac{1}{2P} \tag{3.113}$$

$$\vartheta = \frac{\gamma B_i t_r}{2\pi} \tag{3.114}$$

$$\frac{1}{T_2^*} = \frac{1}{T_2} + \frac{\gamma_a}{2\pi}\left(B - B_\ell\right) \tag{3.115}$$

$$\Delta\nu_{1/2} = \frac{1}{\pi T_2^*} \qquad T_2^* \le T_2 \le T_1 \tag{3.116}$$

$$\mathbf{I}_o = h\mathbf{k}_o \tag{3.120}$$

$$\mathbf{I} = h\mathbf{k} \tag{3.121}$$

$$|\mathbf{k}| = \tilde{\nu} = \frac{1}{\lambda} \tag{3.122}$$

$$s = 2|\mathbf{k}_o|\sin\frac{\vartheta}{2} \tag{3.123}$$

$$\psi_j = A\frac{\exp(i\mathbf{k_o R})}{R} f_j(s)\exp(i\mathbf{sr_j}) \tag{3.124}$$

$$\Psi = \sum_{j=1}^{N} \psi_j \tag{3.125}$$

$$I(s) = K\sum_{j=1}^{N}\sum_{k=1}^{N} f_j(s) f_k(s)\frac{\mathit{sin}(\mathbf{sr}_{jk})}{\mathbf{sr}_{jk}} \tag{3.126}$$

$$I_m(s) = K\sum_{j=1}^{N}\sum_{k=1}^{N} f_j(s) f_k(s)\frac{\mathit{sin}(\mathbf{sr}_{jk})}{\mathbf{sr}_{jk}} \qquad j \ne k \tag{3.127}$$

$$f_j^{\varphi}(s) = \int \rho_j(\mathbf{r}')\,\mathit{exp}(-isr')dr' \tag{3.128}$$

$$f_j^{e}(s) = \frac{C}{s^2}\left[Z_j - f_j^{\varphi}(s)\right] \tag{3.129}$$

$$M(s) = \frac{I_m(s)}{I_g(s)} \tag{3.130}$$

$$r_g = \int_0^\infty r\frac{p(r)}{r}dr \tag{3.131}$$

$$r_a = \frac{\int_0^\infty r\frac{p(r)}{r}dr}{\int_0^\infty \frac{p(r)}{r}dr} \tag{3.132}$$

Chapter 4

$$E_{ia} = E - \sum_{i=1}^{N} E_i \tag{4.1}$$

$$E_{ia} = \sum_{i=1}^{N} \sum_{j=i+1}^{N} E_{ij} + \sum_{i=1}^{N} \sum_{j=i+1}^{N} \sum_{k=j+1}^{N} E_{ijk} + \ldots + E_{i,j,k,\ldots,N} \tag{4.2}$$

$$E_{ia} = \sum_{i=1}^{N} \sum_{j=i+1}^{N} E_{ij} \tag{4.3}$$

$$\hat{H}_{ij} = \hat{H}_i + \hat{H}_j + \hat{V} = \hat{H}^0 + \hat{V} \tag{4.4}$$

$$E_{ij} = \int \varphi_j^* \varphi_i^* \hat{V} \varphi_i \varphi_j \, d\tau \tag{4.5}$$

$$E_{ij} = E_{ij}^1 + E_{ij}^2 \tag{4.6}$$

$$Q_i^{lm} = \frac{4\pi}{2l+1} \left[\sum_{\alpha=1}^{N_j} Z_\alpha r_{i\alpha}^l Y_m^l (\vartheta_{i\alpha}, \varphi_{i\alpha}) - \int \rho_j(r_j) r_j Y_m^l (\vartheta_j, \varphi_j) dr_j \right] \tag{4.7}$$

$$E_{ij}^2 = -\frac{C_4^{ij}}{R^4} - \frac{C_6^{ij}}{R^6} - \frac{C_8^{ij}}{R^8} - \frac{C_{10}^{ij}}{R^{10}} \tag{4.8}$$

$$-\frac{\hbar^2}{2m_e} \frac{d^2\psi}{dx^2} = E\psi \tag{4.9}$$

$$\psi_k(x) = \exp(ikx) \tag{4.10}$$

$$E_k = \frac{k^2 h^2}{2m_e} \tag{4.11}$$

$$I = hk = \frac{\kappa}{N} \frac{h}{d} = \frac{h}{\lambda} \tag{4.12}$$

$$N = N_F \frac{2}{1 + exp\left(\frac{E - E_F}{kT} \right)} \tag{4.13}$$

$$2d \sin\alpha = n\lambda \quad n = 0, \pm 1, \pm 2, \ldots \tag{4.14}$$

$$E = E_o F(s) \tag{4.15}$$

$$F(s) = \sum_{j=1}^{N} f_j \exp(isr_j) = \sum_{j=1}^{N} f_j \exp\left[i\left(\frac{h}{d_1} x_j + \frac{k}{d_2} y_j + \frac{l}{d_3} z_j \right) \right] \tag{4.16}$$

$$\Delta x = d \sin \vartheta \tag{4.17}$$

$$\Delta\varphi = 2\pi \frac{\Delta x}{\lambda} = \frac{2\pi d}{\lambda} \sin \vartheta \tag{4.18}$$

$$\Delta\varphi = 4\pi \frac{\Delta x}{\lambda} = \frac{4\pi d}{\lambda} \sin \vartheta = 2n\pi \qquad n = 1,2,3,... \tag{4.19}$$

$$\Delta\varphi_{ij} = \frac{4\pi(d_i \pm d_{ij})}{\lambda} \sin \vartheta = 2n\pi \qquad i = 1,2,3 \qquad j = 1,2,..., N \tag{4.20}$$