

EQUATIONS

The conversion of the manuscript from .doc to .pdf files has led to a bad resolution of the Equations, caused by a problem with our software. Therefore, we are attaching this separate file to make easier the revision process.

$$\phi = \frac{k_r}{k_{nr} + k_r} \quad (1)$$

$$\tau = \frac{1}{k_{nr} + k_r} \quad (2)$$

$$\Psi_{S_1} = {}^1\Omega \times \psi_{S_1} = {}^1\Omega \times \frac{1}{\sqrt{2}} \left[\psi_{d_{(Ir)}\pi(N^{\wedge}C)}^{(1)} \cdot \psi_{\pi_{(L^{\wedge}X)}^*}^{(2)} + \psi_{d_{(Ir)}\pi(N^{\wedge}C)}^{(2)} \cdot \psi_{\pi_{(L^{\wedge}X)}^*}^{(1)} \right] \quad (3)$$

$$\Psi_{T_1} = {}^3\Omega \times \psi_{T_1} = {}^3\Omega \times \frac{1}{\sqrt{2}} \left[\psi_{d_{(Ir)}\pi(N^{\wedge}C)}^{(1)} \cdot \psi_{\pi_{(L^{\wedge}X)}^*}^{(2)} - \psi_{d_{(Ir)}\pi(N^{\wedge}C)}^{(2)} \cdot \psi_{\pi_{(L^{\wedge}X)}^*}^{(1)} \right] \quad (4)$$

$$\Delta E_{S_1-T_1} = 2K_{S_1-T_1} = 2 \iint \psi_{d_{(Ir)}\pi(N^{\wedge}C)}^{(1)} \psi_{\pi_{(L^{\wedge}X)}^*}^{(1)} \frac{e^2}{r_{1,2}} \psi_{d_{(Ir)}\pi(N^{\wedge}C)}^{(2)} \psi_{\pi_{(L^{\wedge}X)}^*}^{(2)} d_{v1} d_{v2} \quad (5)$$

$$k_r = \frac{64\pi^4 n^3}{3\hbar} |\vec{M}_{T1}|^2 \langle \bar{\nu}^{-3} \rangle^{-1} \quad (6)$$

$$H_{SO} = \vec{B}_1 \vec{s}_1 + \vec{B}_2 \vec{s}_2 \quad (7a)$$

$$H_{SO} = \frac{1}{2}(\vec{B}_1 + \vec{B}_2)(\vec{s}_1 + \vec{s}_2) + \frac{1}{2}(\vec{B}_1 - \vec{B}_2)(\vec{s}_1 - \vec{s}_2) \quad (7b)$$

$$\vec{B}_i = \frac{e^2 \hbar^2}{2m^2 c^2} \sum \frac{Z_{eff}}{r^3} \times \vec{l}_i = \zeta \times \vec{l}_i \quad (8)$$

$$\Psi_{T_1}=\sqrt{1-\beta_{a-b}^2}|a\rangle+\beta_{a-b}|b\rangle \tag{9}$$

$$\beta_{a-b}=\frac{\langle \psi_a|H_{SO}|\psi_b\rangle}{(\Delta E_{a-b})} \tag{10}$$

$$\beta_{^3_{MLCT}-^1_{MLCT}}=\frac{\langle ^3\psi_{MLCT}|H_{SO}|^1\psi_{MLCT}\rangle}{\left(\Delta E_{^3_{MLCT}-^1_{MLCT}}\right)} \tag{11a}$$

$$\beta_{^3_{MLCT}-^3_{LC}}=\frac{\langle ^3\psi_{MLCT}|H_{SO}|^3\psi_{LC}\rangle}{\left(\Delta E_{^3_{MLCT}-^3_{LC}}\right)} \tag{11b}$$

$$M_{T_1}=\left\langle \psi_a|M|\psi_{S_0}\right\rangle \times \beta_{a-b} \tag{12}$$

$$M_{T_1}=\left\langle \psi_{^1_{MLCT}}|M|\psi_{S_0}\right\rangle \times \beta_{^3_{MLCT}-^1_{MLCT}} \tag{13}$$

$$\ln k_{nr}=\ln \frac{\sqrt{2\pi}}{\hbar} \frac{V_k^2}{(1000\;cm^{-1})}-\frac{1}{2}\ln \left[\frac{\hbar\omega_M E_{em}}{(1000\;cm^{-1})^2}\right]-S_M-\frac{\gamma_0 E_{em}}{\hbar\omega_M}+\frac{(\gamma_0+1)^2}{\hbar\omega_M}\left(\frac{\tilde{v}_{1/2}}{16\ln 2}\right)^2 \tag{14a}$$

$$\gamma_0=\ln\left(\frac{E_{em}}{S_M\hbar\omega_M}\right)-1 \tag{14b}$$

$$\tag{15a}$$

$$X=\int\limits_{380}^{780}I(\lambda)\bar{x}(\lambda)d\lambda \tag{15b}$$

$$Y=\int\limits_{380}^{780}I(\lambda)\bar{y}(\lambda)d\lambda \tag{15c}$$

$$Z=\int\limits_{380}^{780}I(\lambda)\bar{z}(\lambda)d\lambda \tag{16a}$$

$$x=\frac{X}{X+Y+Z} \tag{16b}$$

$$y = \frac{Y}{X + Y + Z}$$