Quantum Dynamics of Photochemical Model Reactions via Conical Intersections: Erratum

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Quantendynamik Photochemischer Modellreaktionen entlang konischer Durchschneidungen: Erratum

INAUGURAL – DISSERTATION

to obtain the academic degree
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p.34, eq. (2.47)

$$\sum_i \hat{H}_{ji}(R)|\Psi_{iN}\rangle = \sum_i [\hat{T}_N + E_i(R) + \hat{V}_N(R)\delta_{ji} + \sum_A \frac{-1}{2M_A}\left[2T_{ji}^{(1)} \cdot \nabla_A\right] + \sum_A \frac{-1}{2M_A} T_{ji}^{(2)}]|\Psi_{iN}(R)\rangle.$$

should be replaced with

$$\sum_i \hat{H}_{ji}(R)|\Psi_{iN}\rangle = \sum_i [(\hat{T}_N + E_i(R) + \hat{V}_N(R))\delta_{ji} + \sum_A \frac{-1}{2M_A}\left[2T_{ji}^{(1)} \cdot \nabla_A\right] + \sum_A \frac{-1}{2M_A} T_{ji}^{(2)}]|\Psi_{iN}(R)\rangle.$$

p.34, eq. (2.51)

$$T_{ji}^{(1)} = -T_{ji}^{(1)^*}.$$

should be replaced with

$$T_{ji}^{(1)} = -T_{ij}^{(1)^*}.$$

p.34, eq. (2.52)

$$[\hat{T}_N + \hat{V}_N(R)\delta_{ji} - E_j]\,|\,\Psi(R)_{jN}\rangle = \sum_i \Lambda_{ji}|\,\Psi(R)_{iN}\rangle,$$

should be replaced with

$$[\hat{T}_N + \hat{V}_N(R)\delta_{ji} + E_j(R) - E_{tot}]|\,\Psi(R)_{jN}\rangle = \sum_i \Lambda_{ji}|\,\Psi(R)_{iN}\rangle,$$

p. 35, eq. (2.53)

$$\Lambda_{ji} = -\langle\Psi_j \mid T_N \mid \Psi_i\rangle + \sum_A \frac{-1}{2M_A}\langle\Psi_j \mid \nabla_A \mid \Psi_i\rangle\nabla_A.$$

should be replaced with

$$\Lambda_{ji} = -\left[\langle\Psi_j \mid T_N \mid \Psi_i\rangle + \sum_A \frac{-1}{M_A}\langle\Psi_j \mid \nabla_A \mid \Psi_i\rangle\nabla_A\right].$$

p. 36, eq. (2.56)

$$\alpha_{ij}(R) = \int \langle \Psi_i^{ad} \mid \frac{\partial}{\partial R} \mid \Psi_j^{ad} \rangle dR.$$

should be replaced with

$$\alpha_{ij}(R) = \alpha_{ij}(R_0) + \int_{R_0}^{R} \langle \Psi_i^{ad} \mid \frac{\partial}{\partial R'} \mid \Psi_j^{ad} \rangle dR'.$$

p. 38, eq. (2.63)

$$|\Psi_i^{MCSCF}\rangle = \sum_k C_{ik} |\Psi_k\rangle,$$

should be replaced with

$$|\Psi_i^{MCSCF}\rangle = \sum_k C_{ik} |\Psi_k^{ad}\rangle,$$

p. 39, eq. (2.64)

$$\langle \Psi_j^{ad} \mid \frac{\partial}{\partial R} \mid \Psi_i^{ad} \rangle = \langle \sum_l C_{jl} \Psi_l^{ad} \mid \frac{\partial}{\partial R} \mid \sum_k C_{ik} \Psi_k^{ad} \rangle$$

should be replaced with

$$\langle \Psi_j^{MCSCF} \mid \frac{\partial}{\partial R} \mid \Psi_i^{MCSCF} \rangle = \langle \sum_l C_{jl} \Psi_l^{ad} \mid \frac{\partial}{\partial R} \mid \sum_k C_{ik} \Psi_k^{ad} \rangle$$

p. 39, eq. (2.67)

$$\langle \Psi_i^{d} \mid \frac{\partial}{\partial R} \mid \Psi_j^{d} \rangle_R \simeq \frac{1}{2\Delta R} \langle \Psi_i^{d}(R + \Delta R) \mid \Psi_j^{d}(R - \Delta R) \rangle,$$

should be replaced with

$$\langle \Psi_i^{ad} \mid \frac{\partial}{\partial R} \mid \Psi_j^{ad} \rangle_R \simeq \frac{1}{2\Delta R} \langle \Psi_i^{ad}(R + \Delta R) \mid \Psi_j^{ad}(R - \Delta R) \rangle,$$

p. 49, eq. (2.113)

$$A = \int_0^{t_p} \Omega(t) dt = \frac{\vec{\mu}_{ij}}{\hbar} \int_0^{t_p} |\vec{E}_i^0| s(t) dt = (2N + 1) \cdot \pi \quad with \quad N = 0, 1, \ldots$$

should be replaced with

$$A = \int_0^{t_p} \Omega(t)dt = \frac{\vec{\mu}_{ij}}{\hbar} \int_0^{t_p} \vec{E}_i^0 s(t)dt = (2N+1) \cdot \pi \quad with \quad N = 0, 1, \ldots$$

p. 65, Figure (3.7)

W_{11} and W_{22}

should be replaced with

W_{00} and W_{11}

, respectively

p. 70, Figure (3.12)

W_{00} and W_{11}

should be replaced with

V_0 and V_1

, respectively

p. 74, Figure (3.15)

($\phi = 0^\circ$ and $\lambda = 16.2$ eV/$\mathring{A}$)

should be replaced with

($\lambda = 16.2$ eV/$\mathring{A}$)

p. 80, Figure (4.3)

center of mass of the HF fragment

should be replaced with

F atom in the HF fragment

p. 81, eq. (4.5)

$$\vec{b}_F(q) = F(q) - b(q),$$

should be replaced with

$$\vec{b}_F(q) = \vec{F}(q) - \vec{b}(q),$$

p. 81, eq. (4.6)

$$\vec{b}_H(q) = H(q) - b(q),$$

should be replaced with

$$\vec{b}_H(q) = \vec{H}(q) - \vec{b}(q),$$

p. 81, eq. (4.7)

$$\vec{R}_{HF}(q) = F(q) - H(q),$$

should be replaced with

$$\vec{R}_{HF}(q) = \vec{F}(q) - \vec{H}(q),$$

p. 81, eq. (4.8)

$$\vec{R}(q) = F(q) - a(q),$$

should be replaced with

$$\vec{R}(q) = \vec{F}(q) - \vec{a}(q),$$

p. 82, line above eq. (4.10)

$$H_d(R) \text{ and } F_d(R)$$

should be replaced with

$$\vec{H}_d(R) \text{ and } \vec{F}_d(R)$$

p. 82, eq. (4.10)

$$H_d(q) = H(q) + u\vec{R}(q)\ (|R| - |R_0|)\,,$$

should be replaced with

$$\vec{H}_d(q) = \vec{H}(q) + u\vec{R}(q)\ (|R| - |R_0|)\,,$$

p. 82, eq. (4.11)

$$F_d(q) = F(q) + u\vec{R}(q)\ (|R| - |R_0|)\,,$$

should be replaced with

$$\vec{F}_d(q) = \vec{F}(q) + u\vec{R}(q)\ (|R| - |R_0|)\,,$$

p. 91, eq. (4.16)

$$\hat{H}^{ad}_{ij} = -\frac{\hbar^2}{2m_r}\left(\frac{\partial^2}{\partial R^2} + T_{ij}{}^{R(2)} + 2T_{ij}{}^{R(1)}\frac{\partial}{\partial R}\right) - \frac{\hbar^2}{2I_r}\left(\frac{\partial^2}{\partial \phi^2} + T_{ij}{}^{\phi(2)} + 2T_{ij}{}^{\phi(1)}\frac{\partial}{\partial \phi}\right) + V_i.$$

should be replaced with

$$\hat{H}^{ad}_{ij} = -\frac{\hbar^2}{2m_r}\left(\frac{\partial^2}{\partial R^2}\delta_{ij} + T_{ij}{}^{R(2)} + 2T_{ij}{}^{R(1)}\frac{\partial}{\partial R}\right) - \frac{\hbar^2}{2I_r}\left(\frac{\partial^2}{\partial \phi^2}\delta_{ij} + T_{ij}{}^{\phi(2)} + 2T_{ij}{}^{\phi(1)}\frac{\partial}{\partial \phi}\right) + V_i\delta_{ij}.$$

p. 121, line 2 from bottom

$$\mathrm{S}_0$$

should be replaced with

$$\mathrm{S}_1$$