ERRATA: Electronic Relaxation in Benzaldehyde Evaluated via TD-DFT and Localized Diabatization: Intersystem Crossings, Conical Intersections, and Phosphorescence

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Eqn. (3) should read

$$\hat{H}_{SO_y} \;=\; -\frac{\alpha_0^2}{2}\sum_{pq}\tilde{L_{y}}_{pq}\cdot\frac{\hbar}{2i}\left(a_p^\dagger a_{\bar{q}} - a_{\bar{p}}^\dagger a_q\right)$$

Eqn. (9) should read:

$$\langle\Phi_{singlet}|\hat{H}_{SO}|\Phi_{triplet}^{m_s=0}\rangle \;=\; -\frac{\alpha_0^2\hbar}{2}\left(\sum_{i,a,b}\tilde{L}_{zab}s_i^a t_i^b - \sum_{i,j,a}\tilde{L}_{zji}s_i^a t_j^a\right)$$

Eqn. (10) should read:

$$\begin{aligned}\langle\Phi_{singlet}|\hat{H}_{SO}|\Phi_{triplet}^{m_s=\pm1}\rangle \;=\; &-\frac{\alpha_0^2\hbar}{2\sqrt{2}}\left(\sum_{i,a,b}\tilde{L}_{xab}s_i^a t_i^b - \sum_{i,j,a}\tilde{L}_{xji}s_i^a t_j^a\right)\\ &\pm\frac{\alpha_0^2\hbar}{2\sqrt{2}i}\left(\sum_{i,a,b}\tilde{L}_{yab}s_i^a t_i^b - \sum_{i,j,a}\tilde{L}_{yji}s_i^a t_j^a\right)\end{aligned}$$

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