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111Equation Chapter 1 Section 1Correction to “Ruthenium Dye Excitations and Relaxations in Natural Sunlight”

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An error in computing the optical rate coefficients for dye RuP was discovered in Table S4 of the Supporting Information (SI) Section S8 Model S λ for this article, published in *J. Phys. Chem. A*, 125, 4365-4372 (2021), DOI: 10.1021/acs.jpca.1c02386. The optical rate coefficients include absorption, stimulated emission, and ground state bleach associated with the ground state and the singlet and triplet excited states, as well as for the excited state absorption between the excited states and implicit higher energy excited states. The optical rate coefficients for continuous solar irradiance were computed using Equation 3 of the main text in which the product of the individual signal components and the solar spectrum are integrated and multiplied by the fundamental optical rate coefficient. We determined the incorrect signal components were used for RuP in the published SI Table S4. The corrected Table S4 column for RuP is presented with the reported values from the original paper in the corrected SI.

New simulations have been performed using the corrected values, and the results used to update Figures 5 and 6, and Figure S9 in the corrected SI. The published conclusions are unchanged. The populations of RuP excited states, Figure 5, are only marginally smaller, which should be expected with minor changes to the optical rate coefficients. There is not a significant change in the results for the number of radiative and non-radiative interactions per dye per second (the optical transitions and non-radiative transitions increased respectively by approximately 2% and 10%, Figure 6A). The occurrence of ESA and ESE events, Figure 6C, both decreased from the original simulation results by 20% and

33%. The most notable difference is exhibited in Figure 6B, the fraction of population moving from the lowest energy singlet state (i.e., intersystem crossing or ultrafast non-radiative relaxation) and non-radiative relaxation from the triplet state have decreased from ~ 0.45 to ~ 0.4 and increased from ~ 0.35 to ~ 0.4 respectively.

Associated Content

Supporting information

The Supporting Information is available free of charge.

Table of corrected rate coefficients for RuP. Corrected excited state populations figure.

Corrected figure 5 and figure S9 data (XSLX).

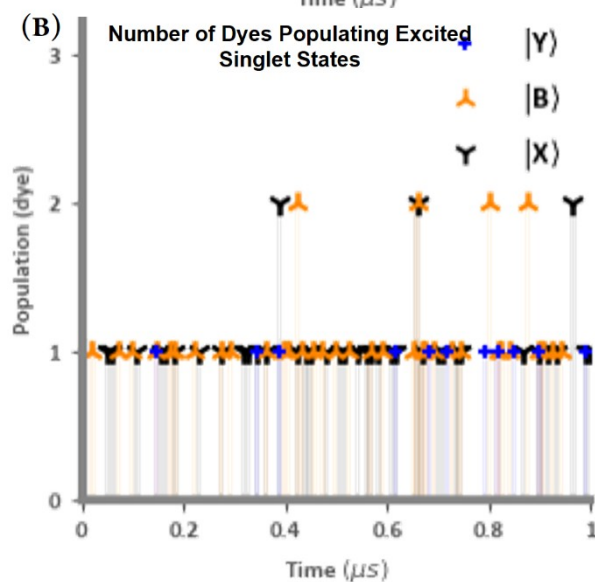
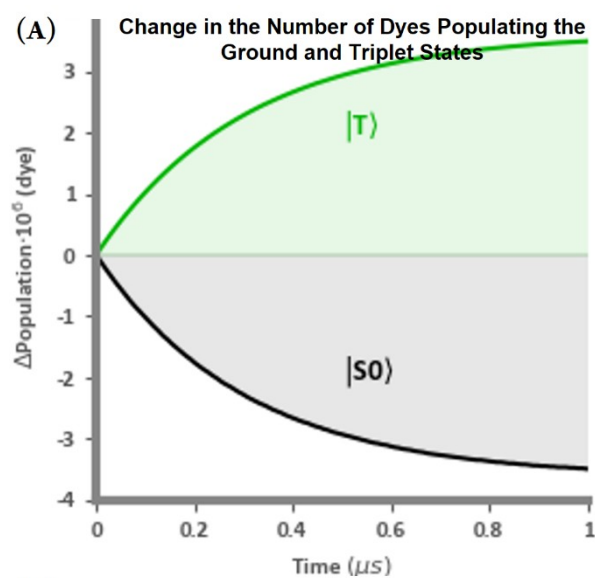


Figure 5. (A) Time-dependent ground state $|S_0\rangle$ and excited triplet $|T\rangle$ state populations and (B) excited singlet state populations ($|Y\rangle$, $|B\rangle$, and $|X\rangle$) of the dye RuP from continuous illumination of a $1500 \mu\text{m}^2$ region under 1-sun conditions. Steady-state in the simulations is reached in approximately $1 \mu\text{s}$. The full data for $10 \mu\text{s}$ are shown in the corrected SI Figure S9 and the original published SI Section S10, Figures S10-S14.

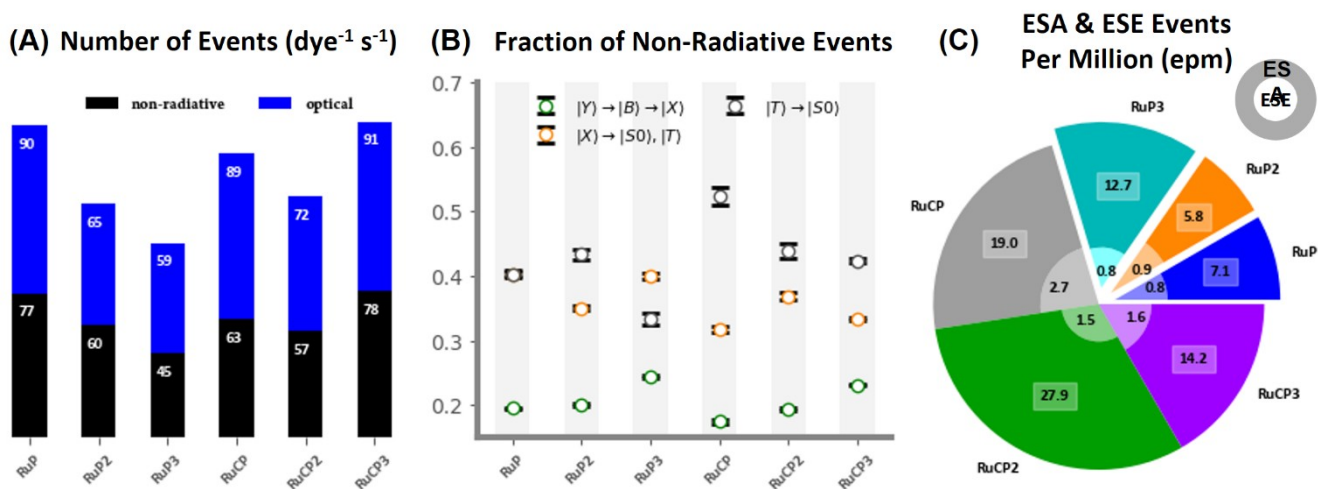


Figure 6. (A) Frequency of non-radiative (black) and optical (blue) events per dye, (B) fraction of non-radiative relaxation events within the excited singlet manifold (green), from the lowest energy singlet state (orange), and from the triplet manifold (gray) to total non-radiative events, and (C) and excited state absorption (ESA) and excited state emission (ESE) events per million (epm) total events for the set of dyes 6-Ru.