Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for:

One Order of Magnitude Increase of Triplet State Lifetime Observed in Deprotonated Form Selenium Substituted Uracil

Peipei Jin[1], Xueli Wang[1]*, Haifeng Pan[1], and Jinquan Chen[1,2]*

1. State Key Laboratory of Precision Spectroscopy, East China Normal University, Shanghai 200062, China

2. Collaborative Innovation Center of Extreme Optics, Shanxi University, Taiyuan, Shanxi 030006, China

*Corresponding author E-mail: xlwang@lps.ecnu.edu.cn; jqchen@lps.ecnu.edu.cn

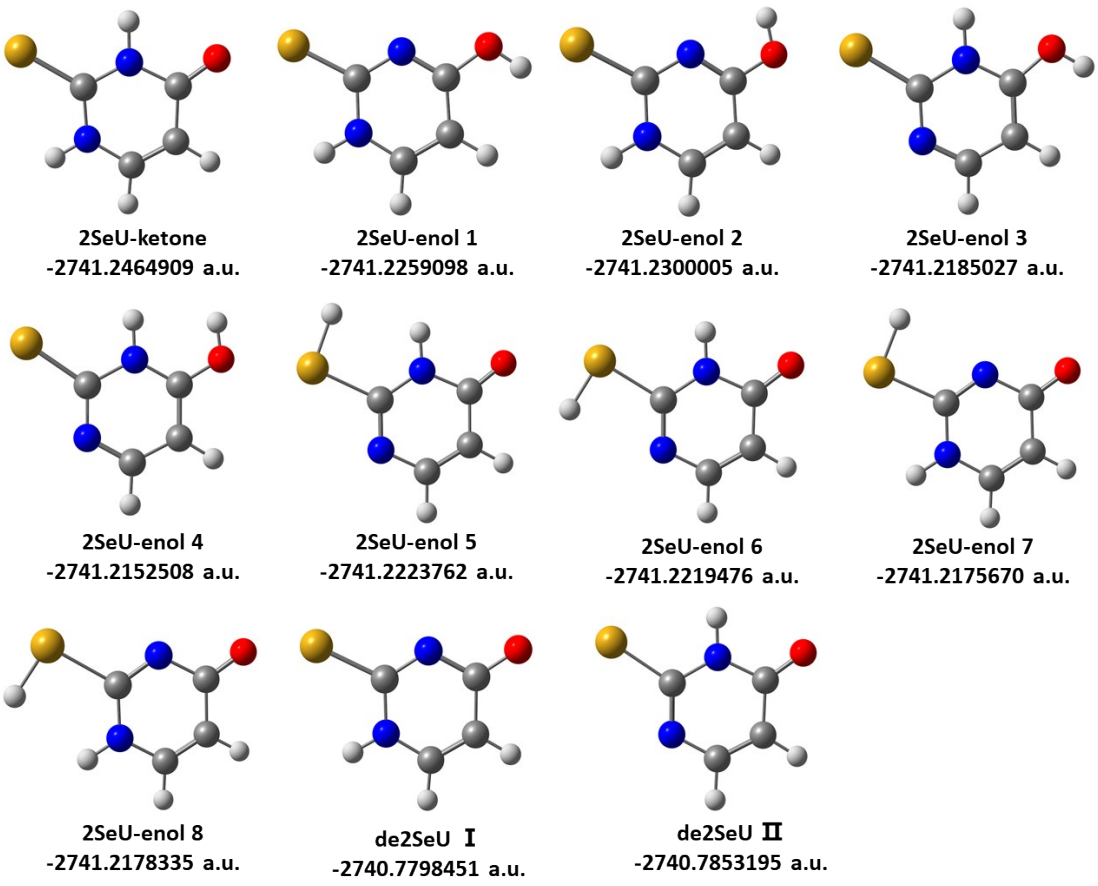

Figure S1. The ground state geometry and energies of 2SeU (ketone isomer), 2SeU (alcohol isomers), de2SeU I and de2SeU II optimized at B3LYP/ IEF-PCM /6-311++G(d,p) level.

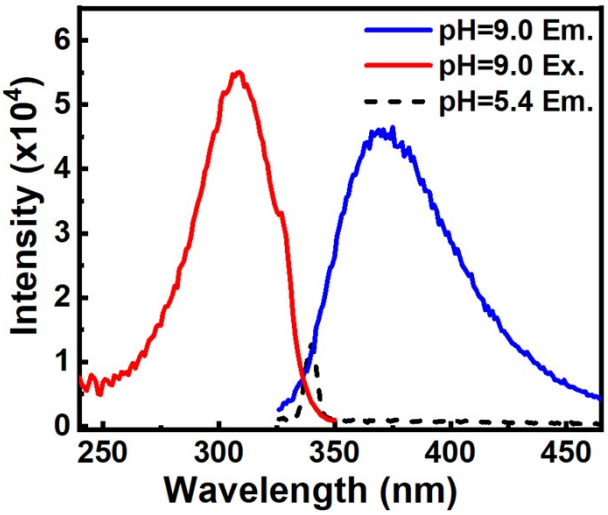

Figure S2. Steady state excitation spectra (red line, ex. 370 nm) and emission spectra (blue line, ex. 285 nm) of 2-selenouracil in PBS at pH=9.0. Steady state emission spectra of 2SeU in pH 5.4 PBS excited by 305 nm (dash line).

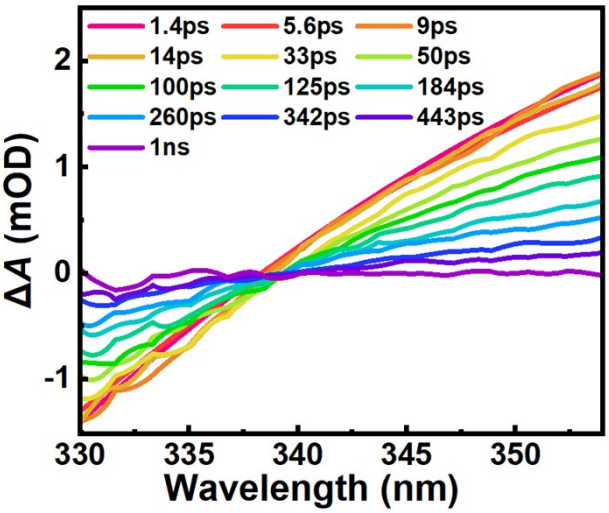

Figure S3. TAS of 2SeU under 305 nm excitation.

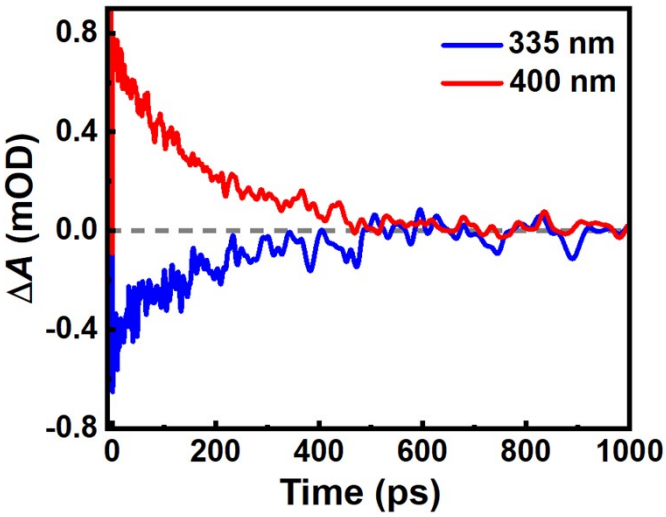

Figure S4. Kinetics decay traces for 2SeU monitored at 335 nm and 400 nm.

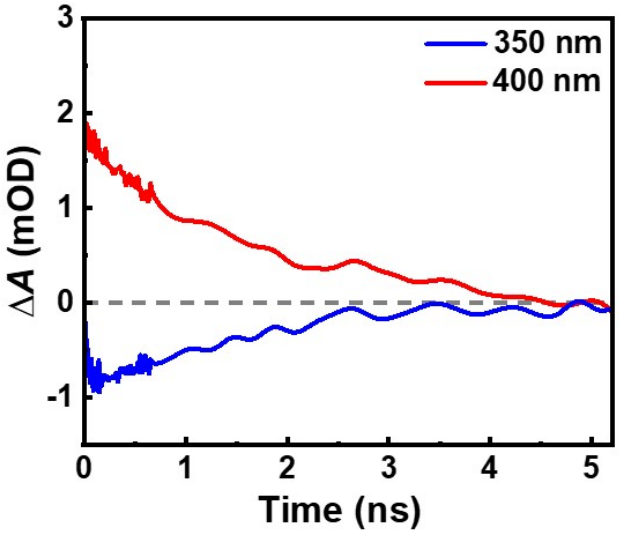

Figure S5. Kinetics decay traces for de2SeU II monitored at 350 nm and 400 nm.

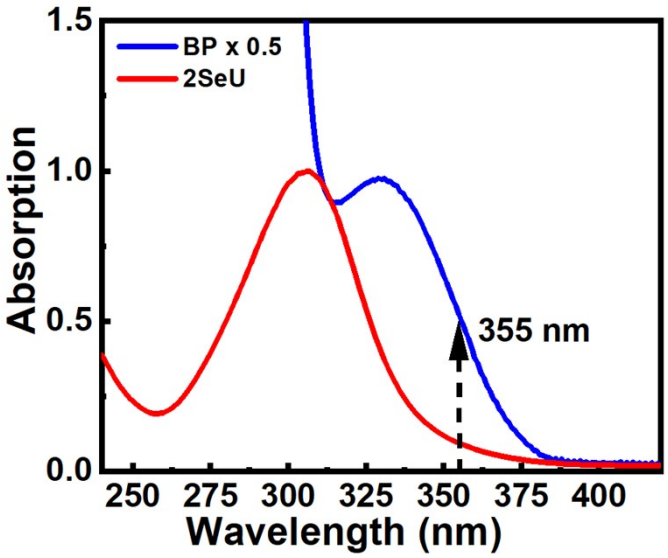

Figure S6. Steady state spectra of (blue) benzophenone (BP) and (red) 2SeU in 1:1 ACN/pH 5.4 PBS.

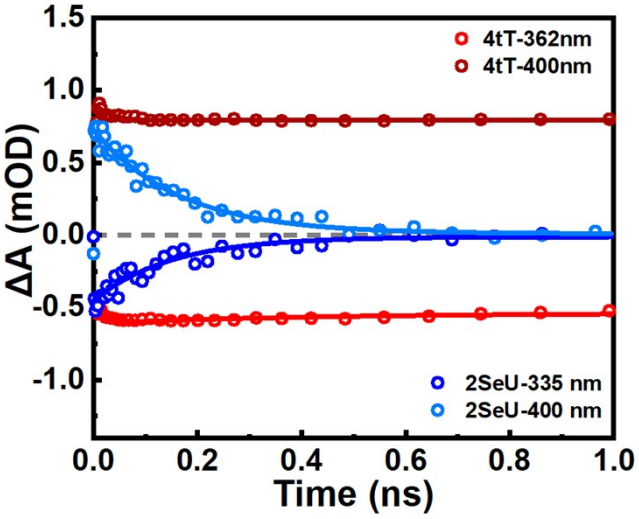

Figure S7. Kinetics decay traces for 4tT monitored at 362 nm and 400 nm and kinetics decay traces for 2SeU monitored at 335 nm and 400 nm excited by 305 nm.

The triplet quantum yield of 2SeU was measured using 4-thiothymine (4tT, Φ_T=85% ± 15%[1]) as the reference sample. The transient absorption kinetics of the 4tT and 2SeU were measured under exactly the same experimental conditions, and the 2SeU triplet quantum yield was calculated according to the following formula.

$$\phi_T(2SeU) = \frac{\Delta A_{2SeU}(\lambda_2)\phi_T(4tT)\varepsilon^*_{4tT}(\lambda_1)}{\Delta A_{4tT}(\lambda_1)\varepsilon^*_{2SeU}(\lambda_2)}$$

In the specific experimental operation, it is necessary to keep the tested sample and the reference sample under exactly the same experimental conditions, including the same steady state absorption value, pump power in the transient absorption experiment, and so on.

References

1. C. Reichardt, C. Crespo-Hernández, E., *J. Phys. Chem. Lett.,* 2010, **1**, 2239-2243.