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

Supporting information

for

Comparison of charge transfer dynamics in polypyridyl ruthenium sensitizers for solar cells and water splitting systems

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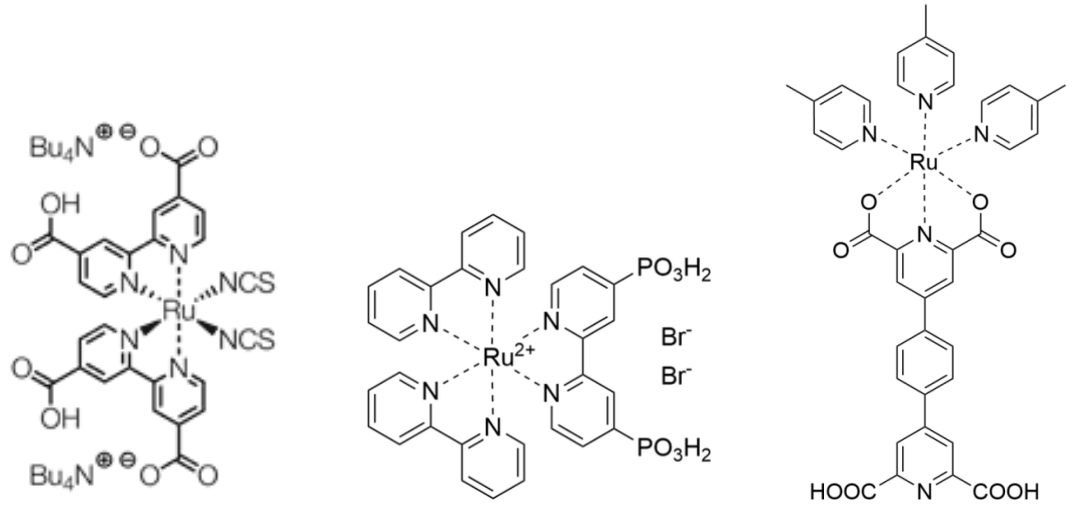
A: B: C:



Scheme S1. The chemical structures of N719 dye (A), RuP dye (B) and RuOEC (C).

Table S1. Averaged photovoltaic parameters of the studied solar cells (fresh and 1 day after preparation): open circuit voltage (V_{OC}), fill factor (FF), photocurrent density (J_{SC}), efficiency (Eff) with standard errors of the mean.

Cell	$\overline{V_{OC}}$ [mV]	$\overline{FF}$	$\overline{J_{SC}}$ [mA/m^2]	$\overline{Eff}$ [%]
N719	81.80 +/- 0.38	0.684 +/- 0.011	5.18 +/- 0.44	2.89 +/- 0.21
N719 (1day)	83.60 +/- 0.69	0.7300 +/- 0.0084	3.39 +/- 0.43	1.99 +/- 0.23
N719_noTBP	58.60 +/- 0.82	0.5720+/- 0.0059	6.35 +/- 0.46	2.13 +/- 0.19
N719_noTBP (1day)	61.7 +/- 2.2	0.5100 +/- 0.0058	6.0 +/- 0.4	1.87 +/- 0.12
RuP	65.83 +/- 0.41	0.6750 +/- 0.0042	1.282 +/- 0.093	0.572 +/- 0.038
RuP (1day)	65.00 +/- 0.45	0.638 +/- 0.014	0.972 +/- 0.091	0.404 +/- 0.045
RuP_noTBP	56.67 +/- 0.84	0.600 +/- 0.031	3.22 +/- 0.15	1.100 +/- 0.091
RuP_noTBP (1day)	55.7 +/- 3.4	0.534 +/- 0.026	1.64 +/- 0.59	0.48 +/- 0.18
RuOEC_noTBP	33.5 +/- 1.5	0.535 +/- 0.005	1.105 +/- 0.005	0.195 +/- 0.005

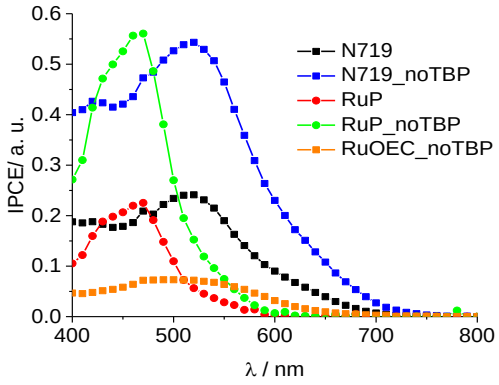


Figure S1. IPCE spectra of selected cells sensitized with N719, RuP or RuOEC containing iodide electrolyte with or without TBP addition.

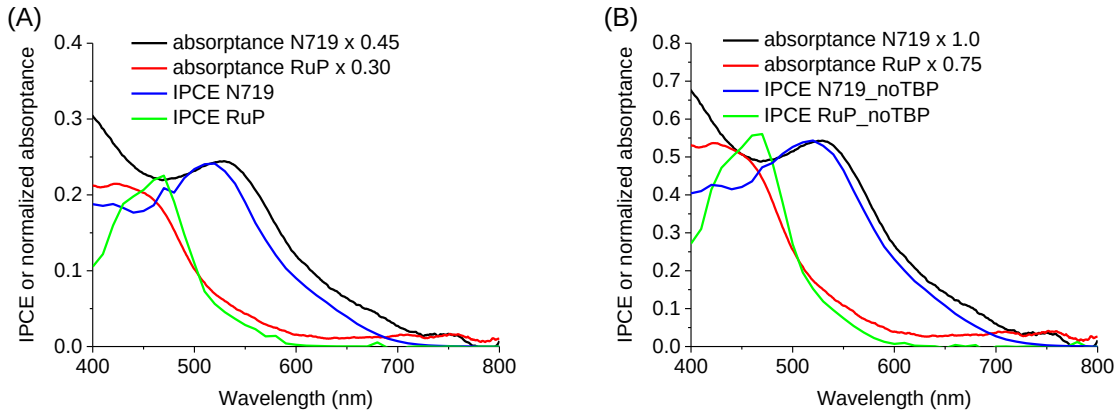
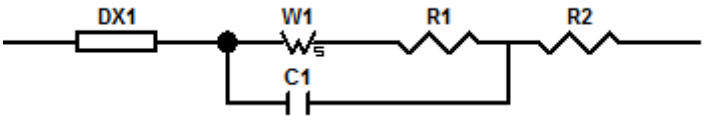


Figure S2. Normalized absorptance ($1\text{-}10^{-A}$, where A is absorbance) spectra to the IPCE spectra of selected cells sensitized with N719 or RuP containing iodide electrolyte with or without TBP addition.

(A)



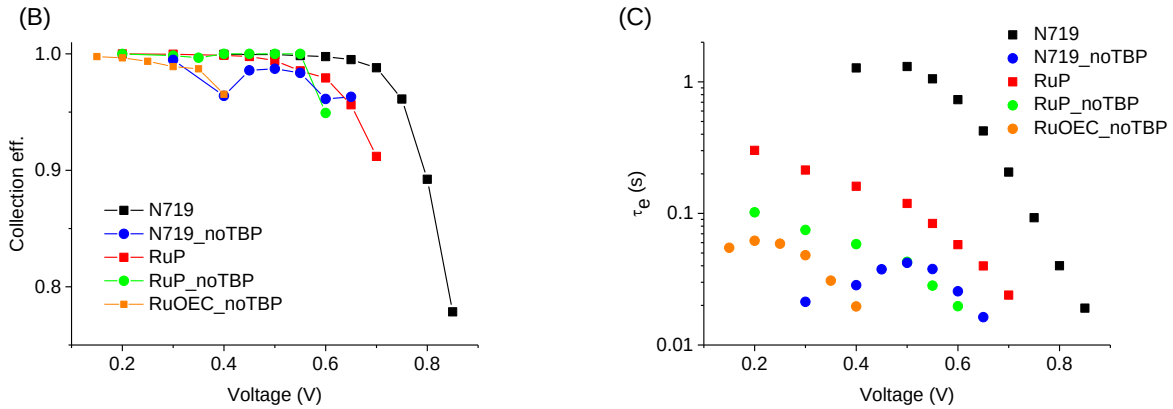


Figure S3. (A) Equivalent circuits for DSSCs, DX1 is transmission line element [*Phys. Chem. Chem. Phys.* **2011**, *13* (20), 9083]. Averaged values of: electron collection efficiency (B) and electron lifetime (C) of cells sensitized by N719 or RuP in different cell configurations using iodide electrolyte with or whithout TBP addition.

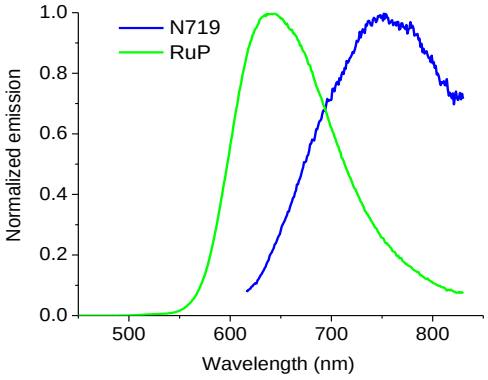


Figure S4. Emission spectra for N719 and RuP cells with iodide electrolyte containing TBP. Excitation wavelength was set at 421 nm.

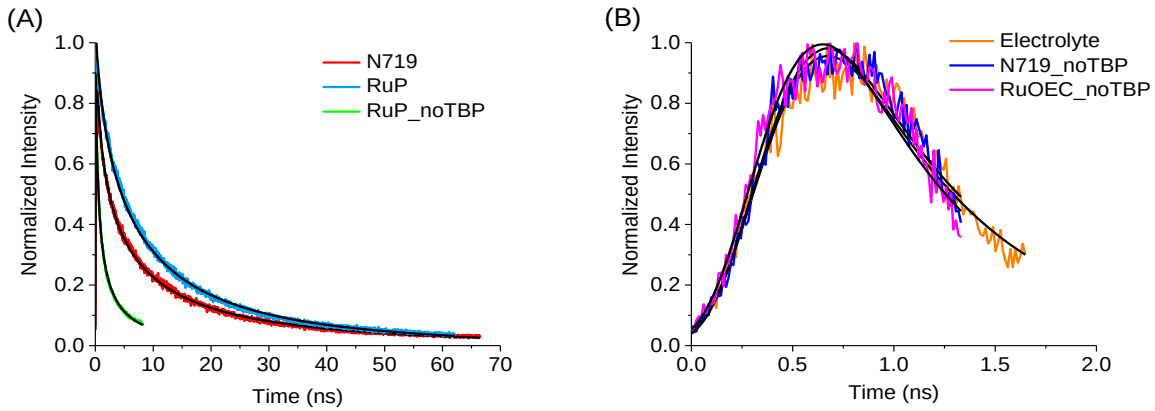


Figure S5. Representative emission decay traces for the indicated cells exhibits electron injection time longer (A) and faster (B) than electrolyte. In the figure (B) emission decay trace for iodide electrolyte without TBP is also shown. The black solid lines represent the best fits.

Table S2. Calculated ideality factor (m) and trap distribution parameter (α) for obtained cells sensitized by N719 + CDCA in different configurations. The parameters α and m were obtained from the fit (Figure 3) of the following functions: $C\mu = C_0 \exp(\alpha\, Ve/kT)$ and $R_{ct} = R_0 \exp(-Ve/m\, kT)$.

Sample / configuration	m	α
N719	1.98 +/- 0.18	0.21 +/- 0.01
N719_noTBP	2.60 +/- 0.11	0.23 +/- 0.03
RuP	2.32 +/- 0.02	0.23 +/- 0.01
RuP_noTBP	2.65 +/- 0.05	0.22 +/- 0.01
RuOEC_noTBP	2.28 +/- 0.10	0.24 +/- 0.01

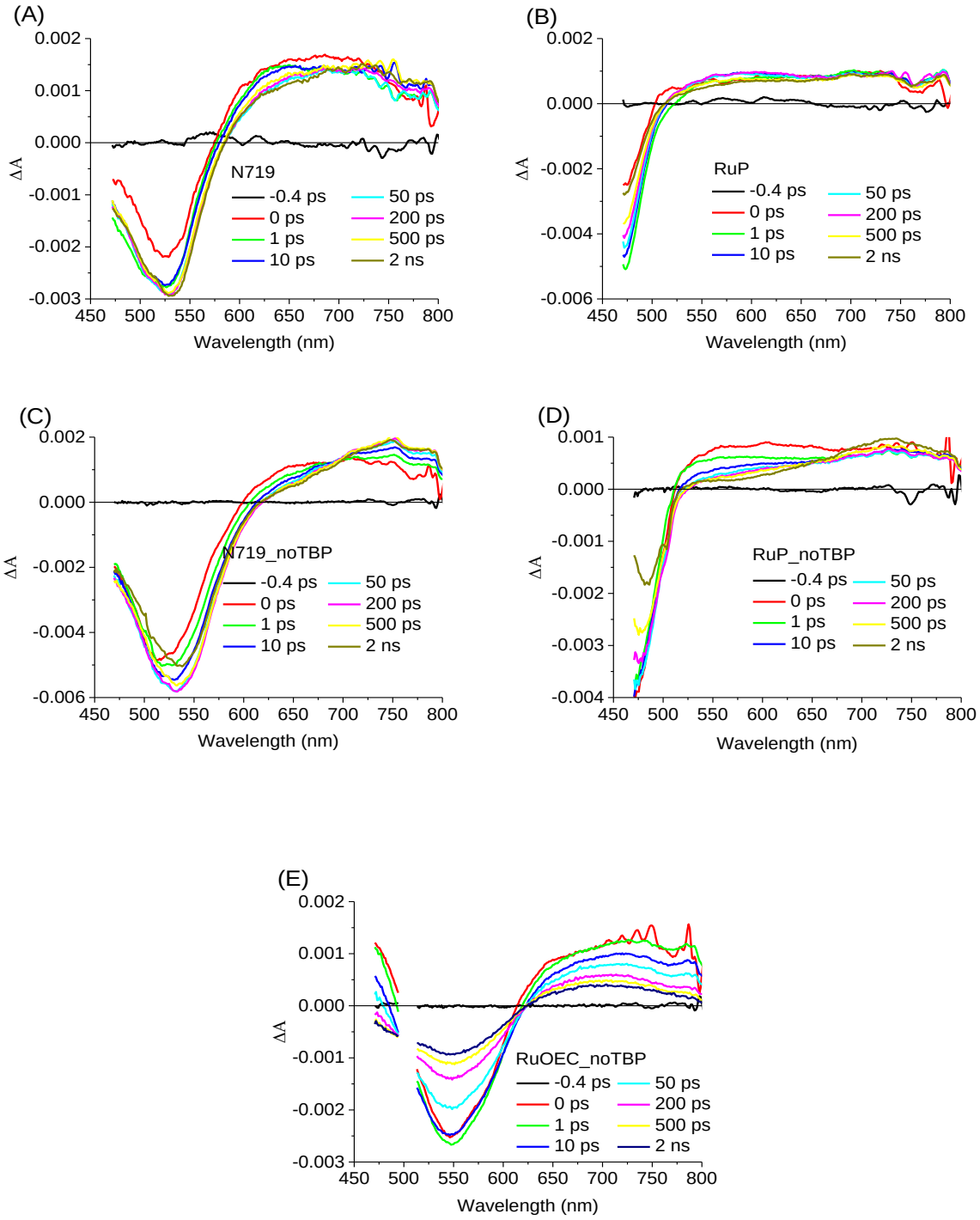


Figure S6. Exemplary transient spectra in the VIS range for selected delay time between pump and probe pulses for the cells sensitized with N719 (left: A, C), RuP (right: B, D) and RuOEC (E) in configurations with electrolyte containing or not TBP additive.

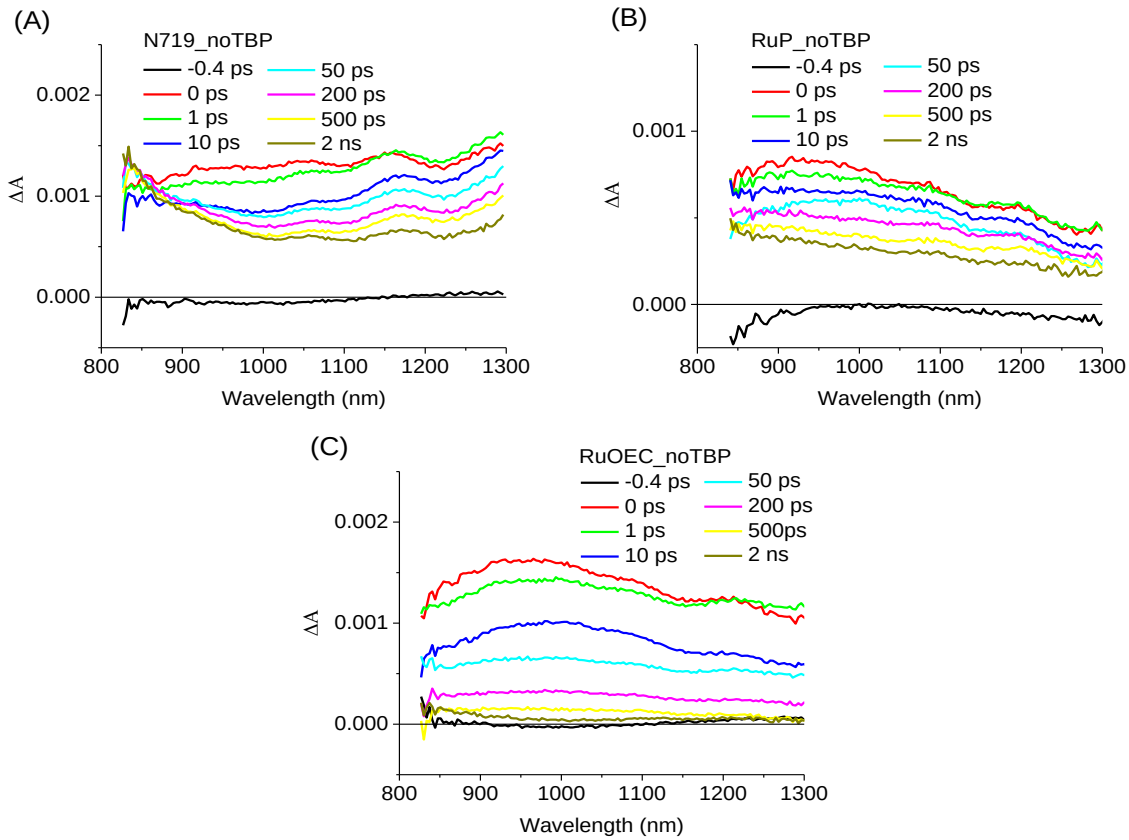


Figure S7. Exemplary transient absorption spectra in the NIR range for selected delay time between pump and probe pulses for the cells sensitized with N719 (A), RuP (B) and RuOEC (C) in configurations with electrolyte not containing TBP additive.

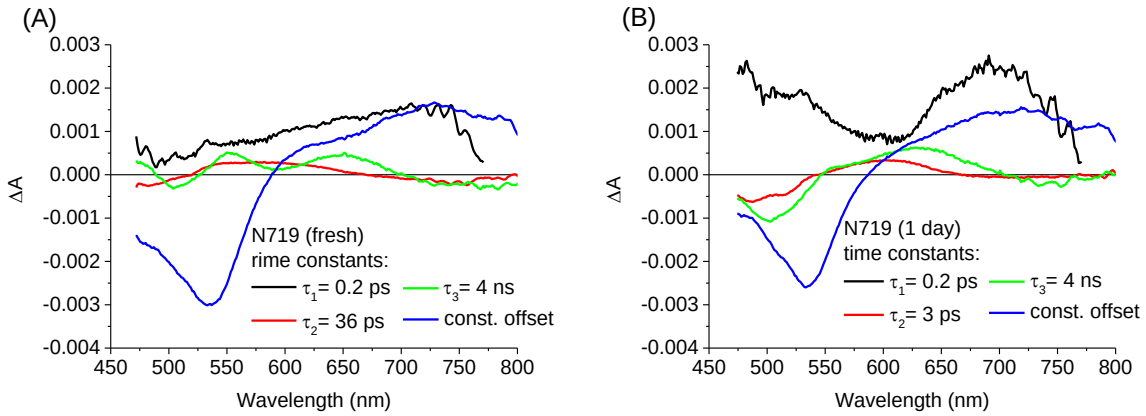


Figure S8. Cell aging effect in transient absorption spectra: wavelength dependent amplitudes of the indicated time constants obtained from global analysis for the fresh cells sensitized with N719 (A) and one day after prepration (B).