Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Complementary Supporting Information's

Light harvesting zinc naphthalocyanine-perylenediimide supramolecular dyads: Long-lived charge-separated states in nonpolar media

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Fig. S15 (Upper) Differential absorption spectra obtained upon nanosecond flash photolysis (430 nm) of ZnNc (0.06 mM) in the presence of PDIpy (0.07 mM) in deaerated benzonitrile with several time delays between 2 and 30 μs at room temperature. (Lower) Decay profile of the ^{3}ZnNc* at 600 nm and the rise profile of the ZnNc$^{\bullet+}$ at 980 nm.

Fig. S16 (Upper) Differential absorption spectra obtained upon nanosecond flash photolysis (430 nm) of ZnNc (0.06 mM) in the presence of PDIpy (0.12 mM) in deaerated benzonitrile with several time delays between 2 and 18 μs at room temperature. (Lower) Decay profile of the ^{3}ZnNc* at 600 nm and the rise profile of ZnNc$^{\bullet+}$ at 980 nm.

Fig. S17 (Left) Decay profiles of the triplet ZnPc at 600 nm with increasing concentrations of PDIpy in deaerated benzonitrile; λ_{ex} = 430 nm. (Right): Pseudo-first-order plot.

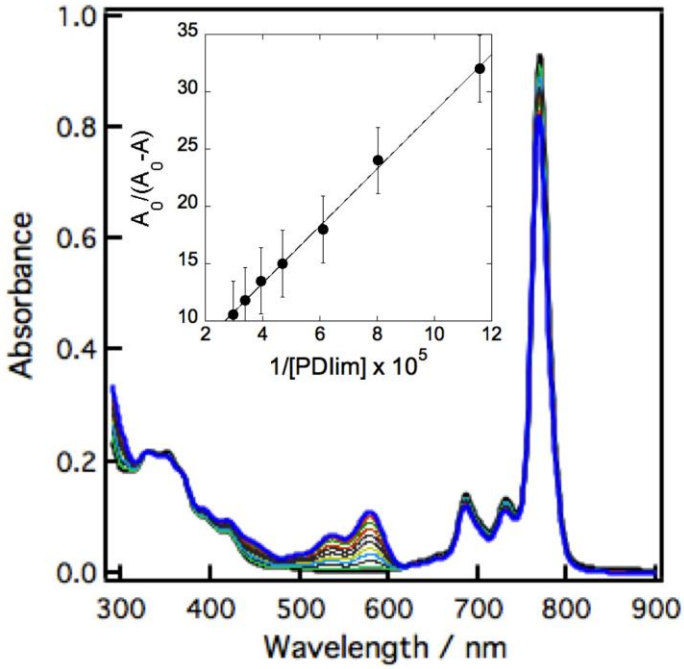


Fig. S1 UV-visible spectral changes observed during the complexation of ZnNc with PDIim to form **2** in toluene. Inset: Benesi-Hildebrand analysis of the absorbance data.

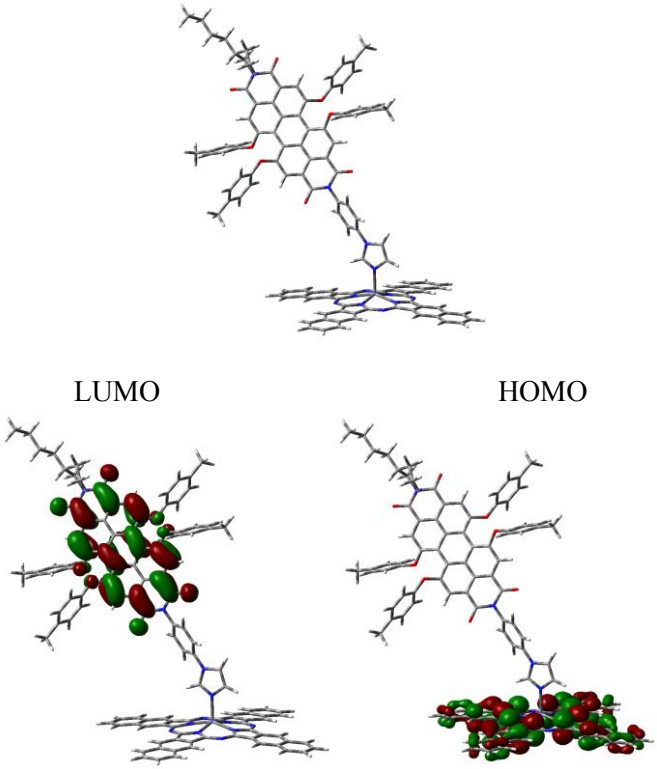


Fig. S2 Optimized structure and *ab initio* B3LYP/6-311G calculated frontier HOMO and LUMO for the self-assembled dyad **2**.

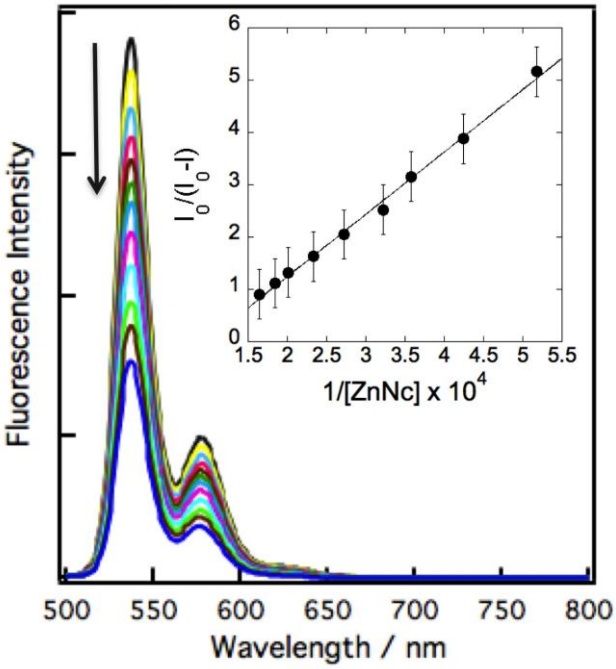


Fig. S3 Fluorescence spectra of PDIpy (1.46 μM) in the presence of increasing amounts of ZnNc (0-100 μM) in toluene (λ_{ex} = 480 nm). Inset: Benesi-Hildebrand analysis of the fluorescence data.

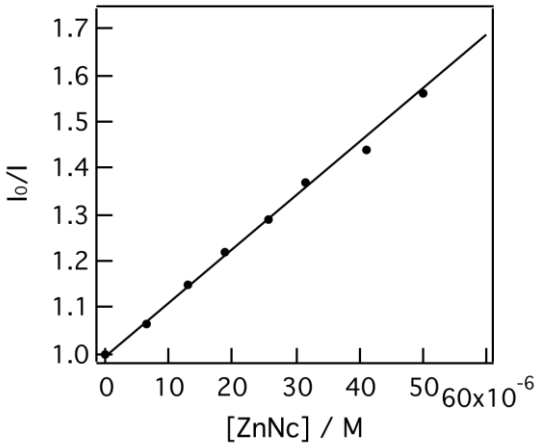


Fig. S4 Stern-Volmer plot for the fluorescence quenching of PDIpy by ZnNc in benzonitrile; λ_{ex} = 480 nm.

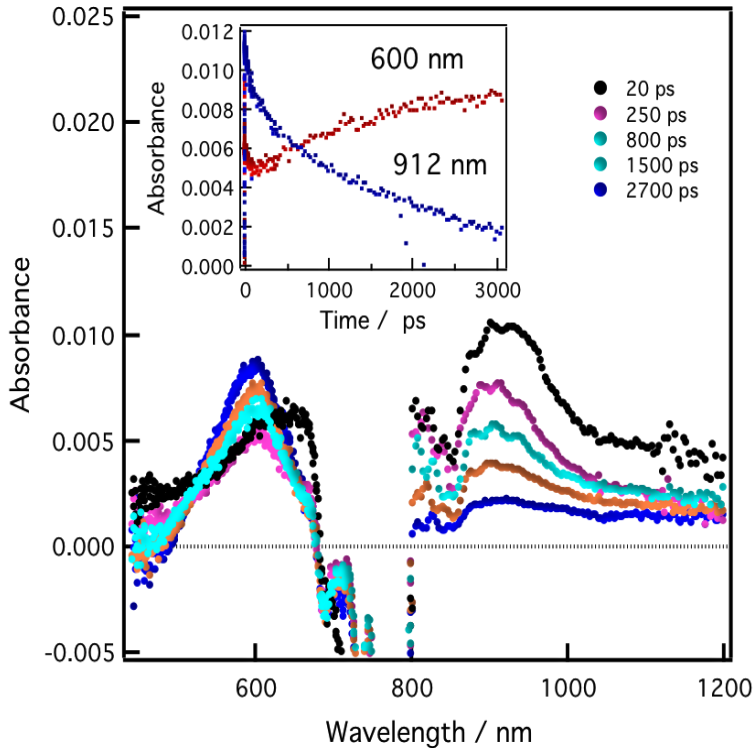


Fig. S5 Differential absorption spectra obtained upon femtosecond flash photolysis (390 nm) of ZnNc in deaerated toluene with several time delays between 20 and 2700 ps at room temperature. Inset: Decay profile of the ^{1}ZnNc* and rise profile of the ^{3}ZnNc* at 912 and 600 nm, respectively.

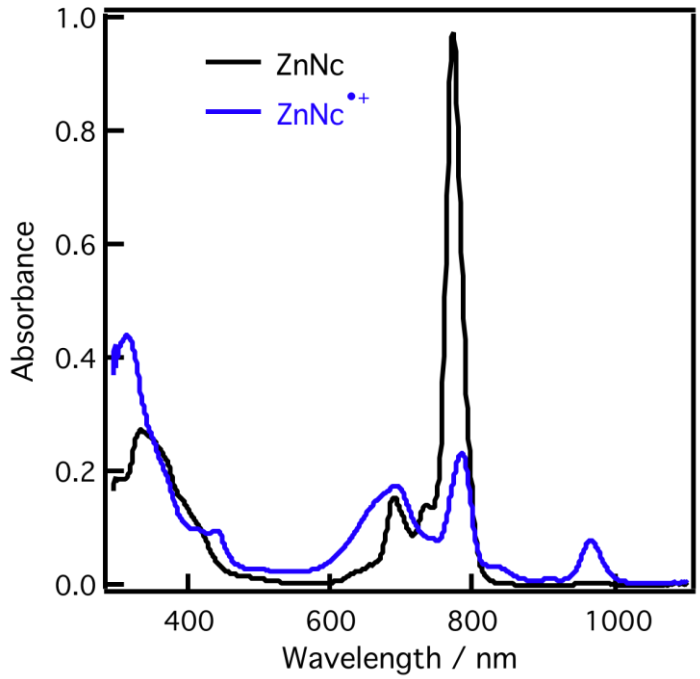


Fig. S6 Absorption spectra of ZnNc radical cation ($ZnNc^{\bullet+}$) obtained by treating ZnNc with tris(4-bromophenyl)aminium hexachloroantimonate in benzonitrile.

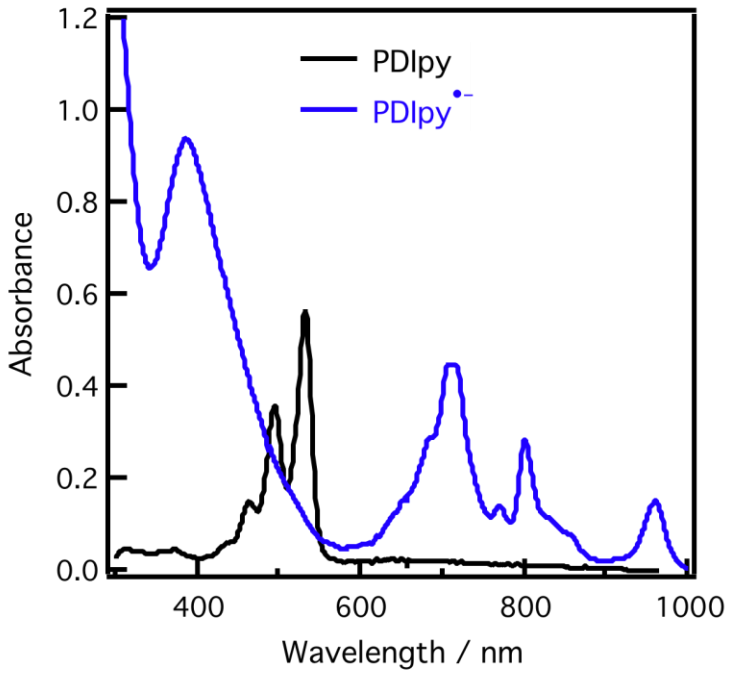


Fig. S7 Absorption spectra of PDIpy radical anion ($PDIpy^{\bullet-}$) obtained by treating PDIpy with tetrakis(dimethylamino)ethylene (TDAE) in benzonitrile.

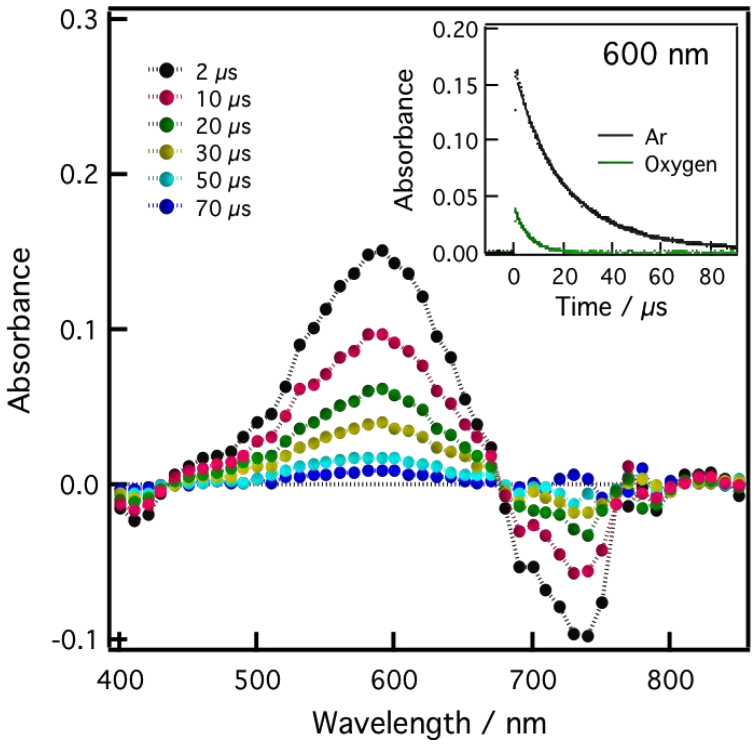


Fig. S8 Differential absorption spectra obtained upon nanosecond flash photolysis (430 nm) of ZnNc (0.05 mM) in the presence of PDIpy (0.05 mM) in deaerated toluene with several time delays between 2 and 70 μs at room temperature. Inset: Decay profiles of the ^{3}ZnNc* at 600 nm in the argon- and oxygen-saturated solutions.

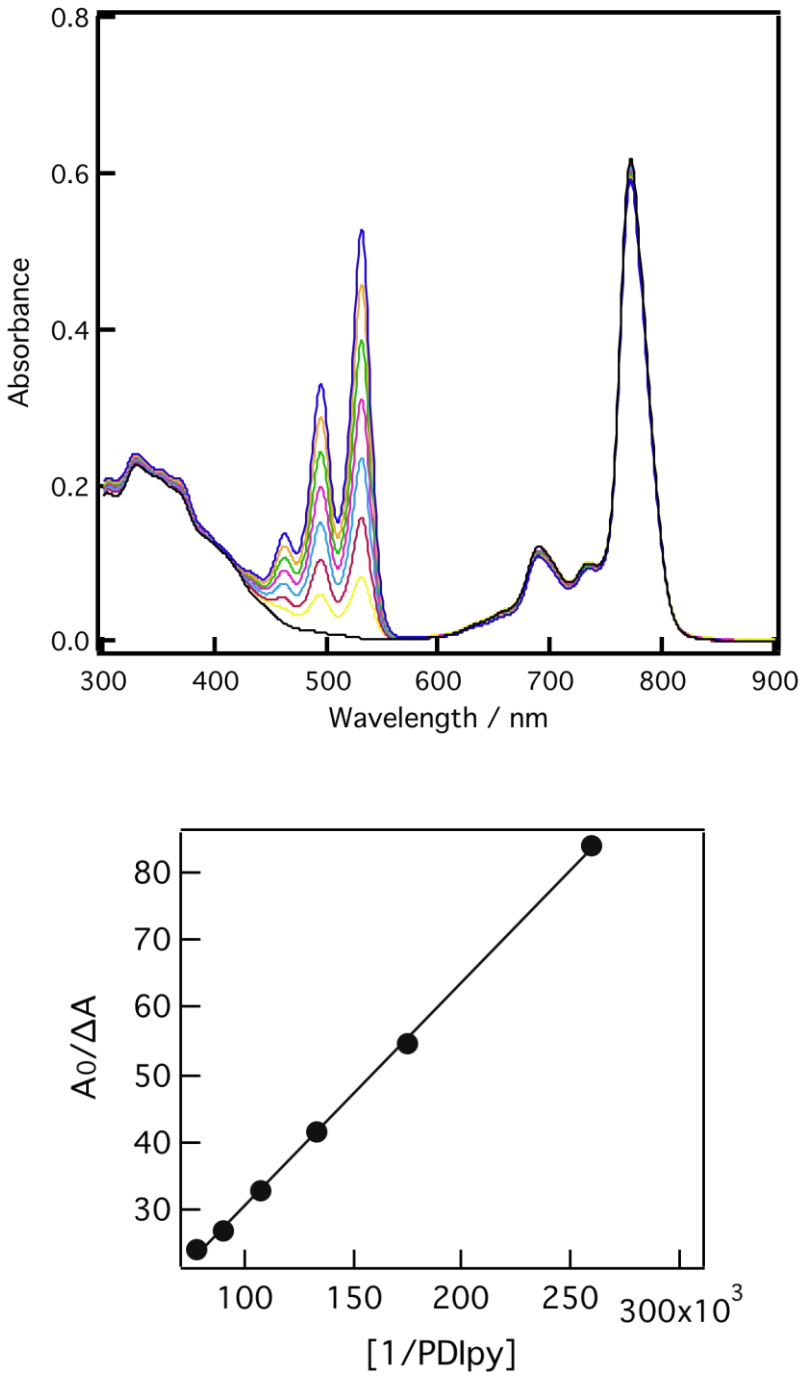


Fig. S9 (Upper) UV-visible spectral changes observed during the complexation of ZnNc with PDIpy in benzonitrile. (Lower) Benesi-Hildebrand analysis of the absorbance data.

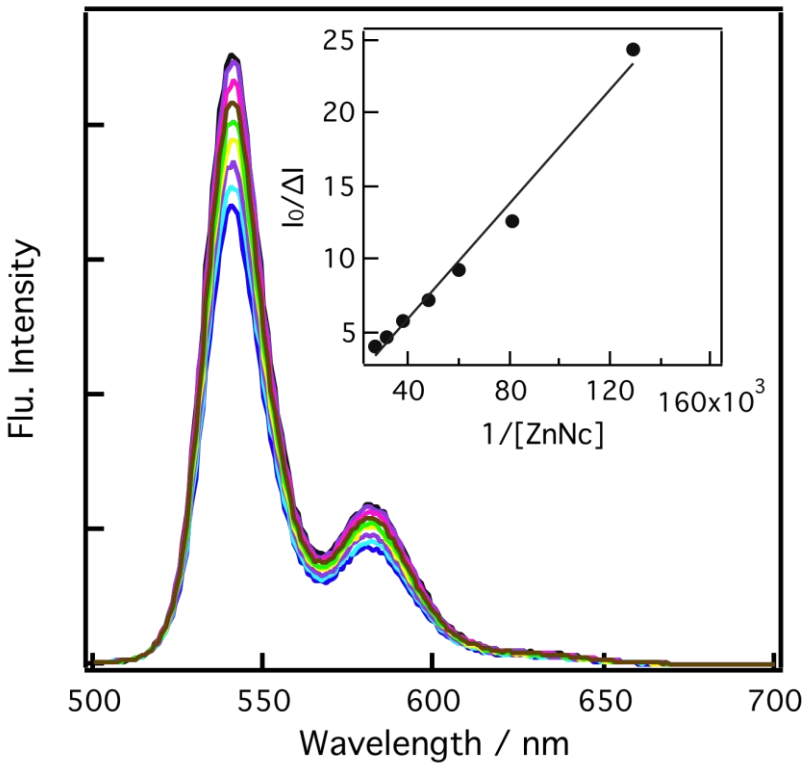


Fig. S10 Fluorescence spectra of PDIpy in the presence of various amounts of ZnNc in benzonitrile (λ_{ex} = 490 nm). Inset: Benesi-Hildebrand analysis of the fluorescence data.

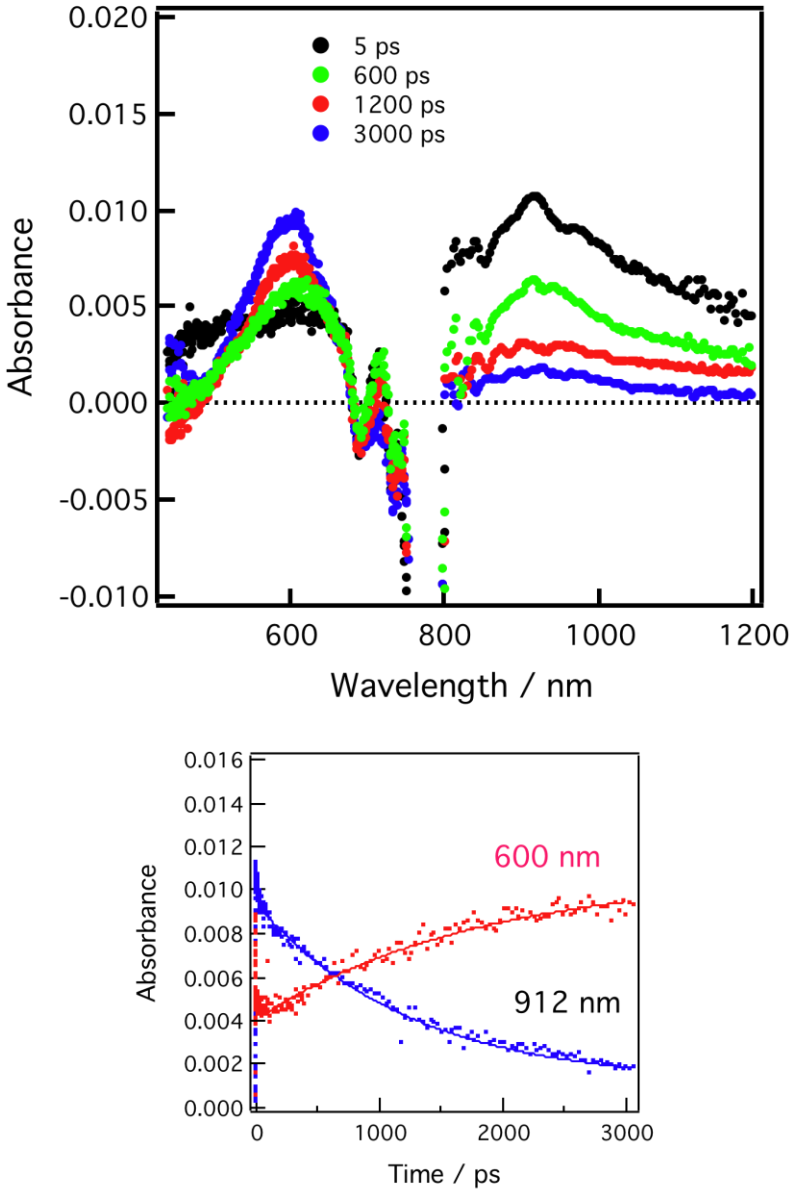
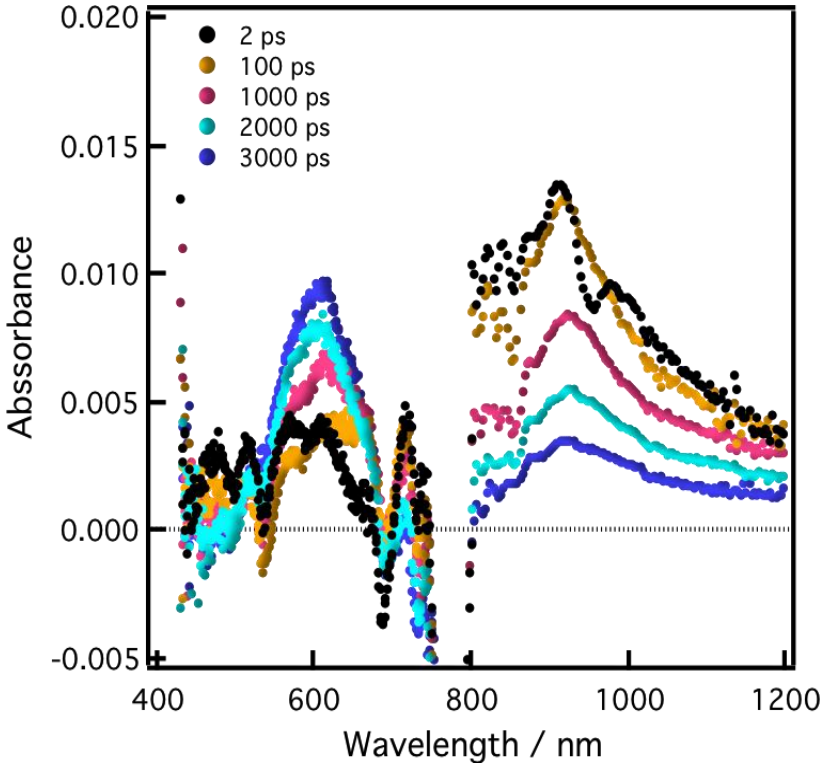


Fig. S11 (Upper) Differential absorption spectra obtained upon femtosecond flash photolysis (390 nm) of ZnNc in deaerated benzonitrile with several time delays between 5 and 3000 ps at room temperature. (Lower) Decay profile of the ^{1}ZnNc* at 912 nm and rise profile of ^{3}ZnNc* at 600 nm.



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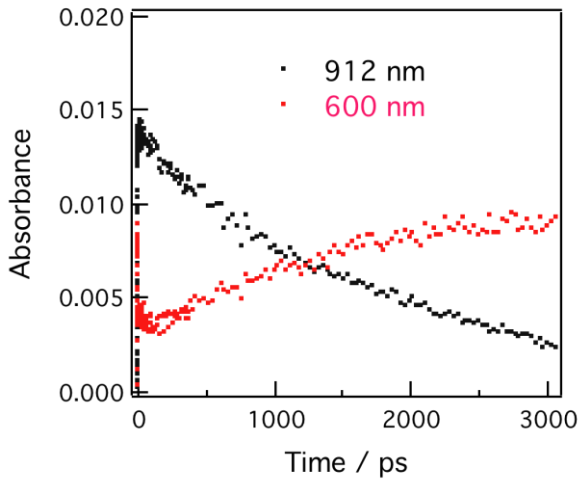

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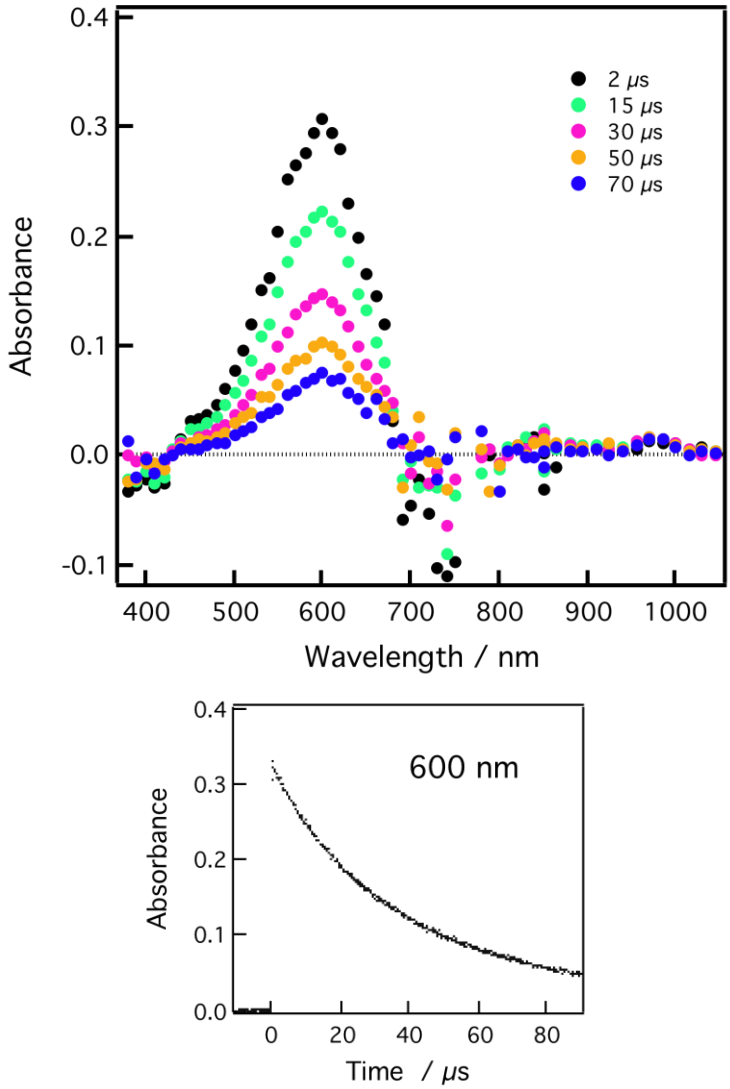
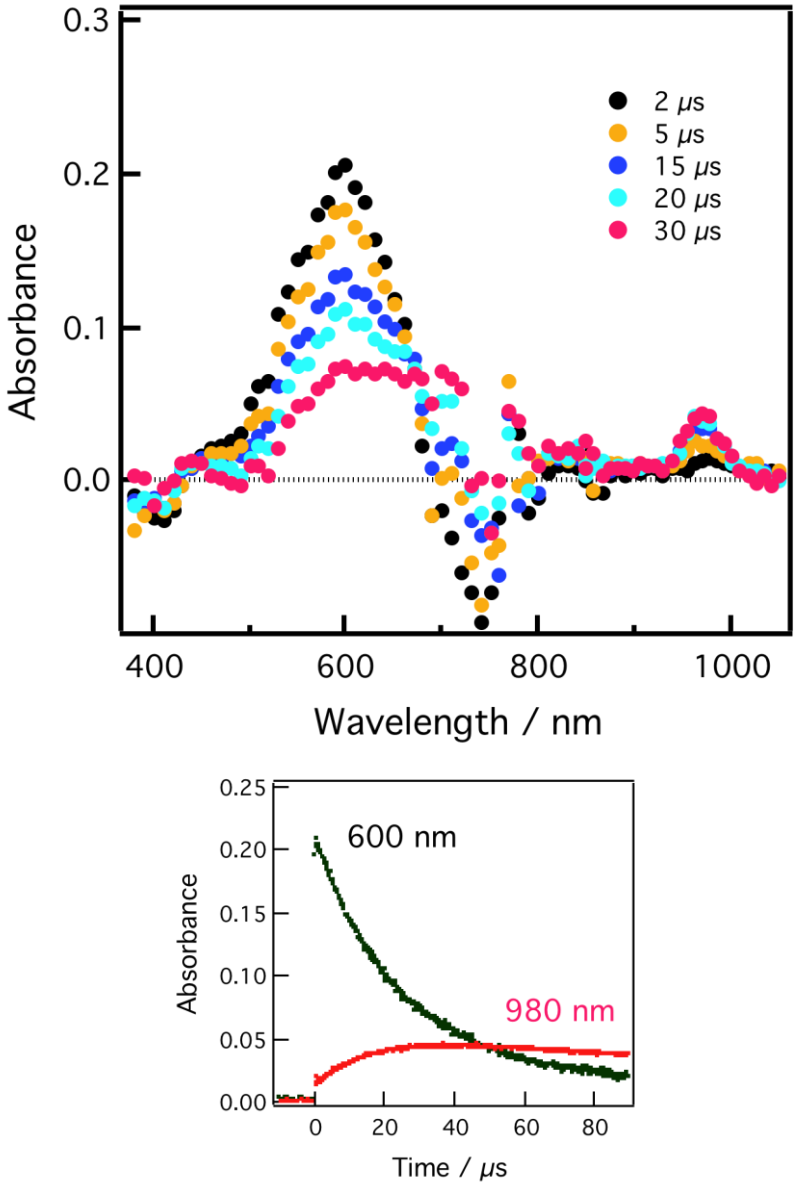


Fig. S14 (Upper) Differential absorption spectra obtained upon nanosecond flash photolysis (430 nm) of ZnNc in deaerated benzonitrile with several time delays between 2 and 70 μs at room temperature. (Lower) Decay profile of the ^{3}ZnNc* at 600 nm.



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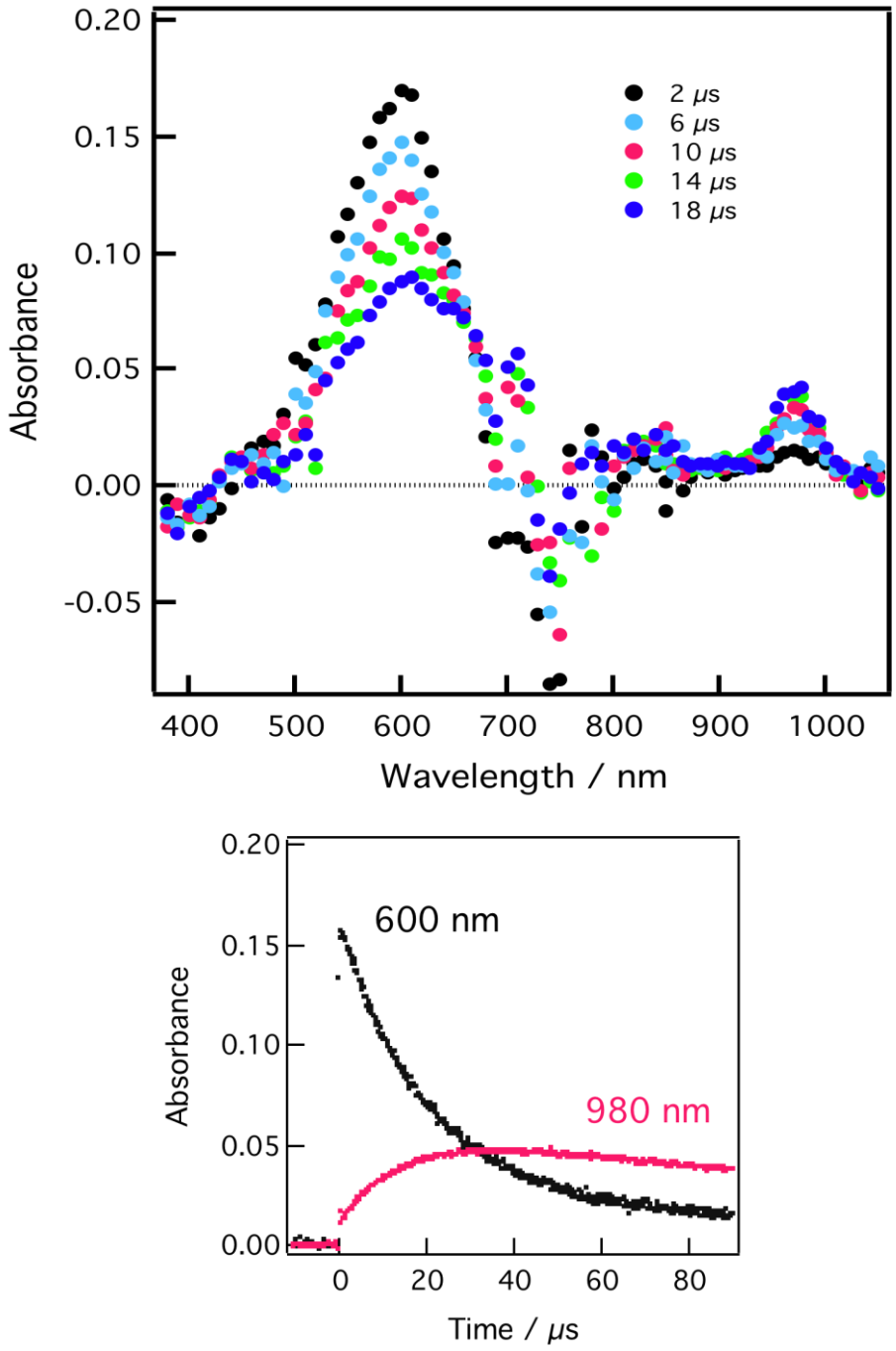

Fig. S16 (Upper) Differential absorption spectra obtained upon nanosecond flash photolysis (430 nm) of ZnNc (0.06 mM) in the presence of PDIpy (0.12 mM) in deaerated benzonitrile with several time delays between 2 and 18 μs at room temperature. (Lower) Decay profile of the ^{3}ZnNc* at 600 nm and the rise profile of $ZnNc^{\bullet+}$ at 980 nm.

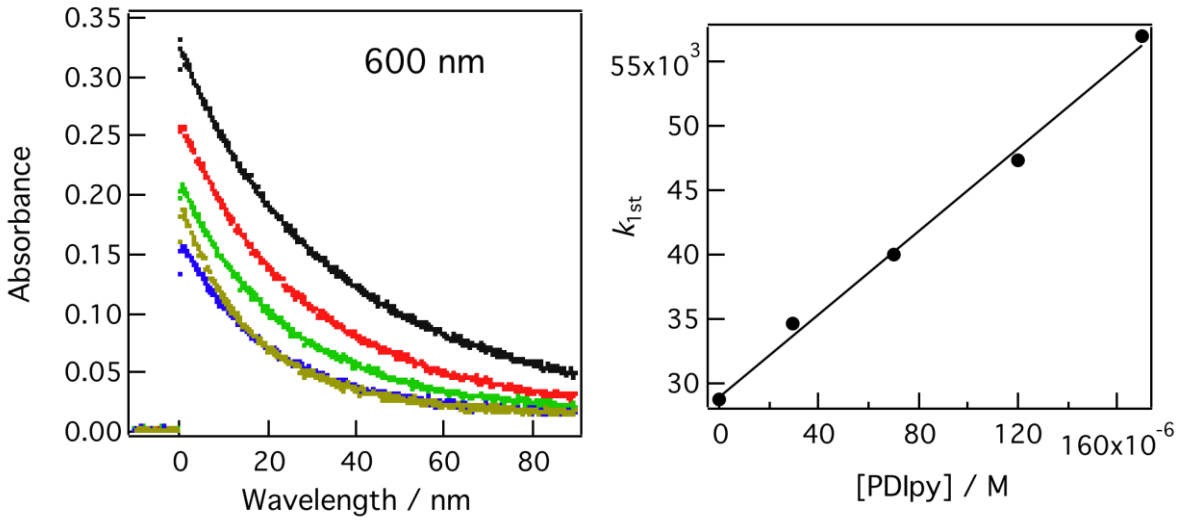

Fig. S17 (Left) Decay profiles of the triplet ZnPc at 600 nm with increasing concentrations of PDIpy in deaerated benzonitrile; λ_{ex} = 430 nm. (Right): Pseudo-first-order plot.