Supporting information

Unveiling Excited State Energy Transfer and Charge Transfer in a Host/Guest Coordination Cage

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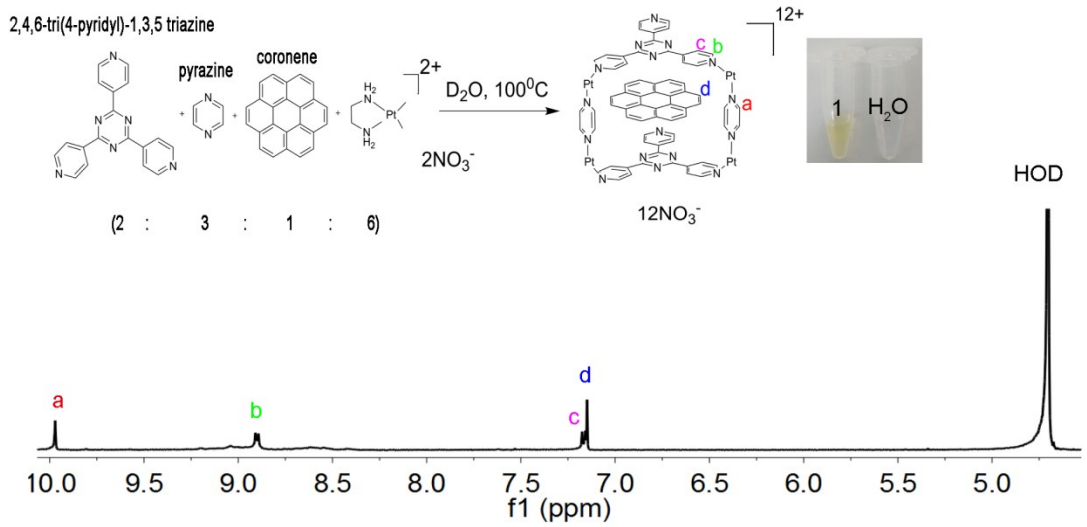

Figure S1. ^{1}H NMR spectra of **1** in D_2O.

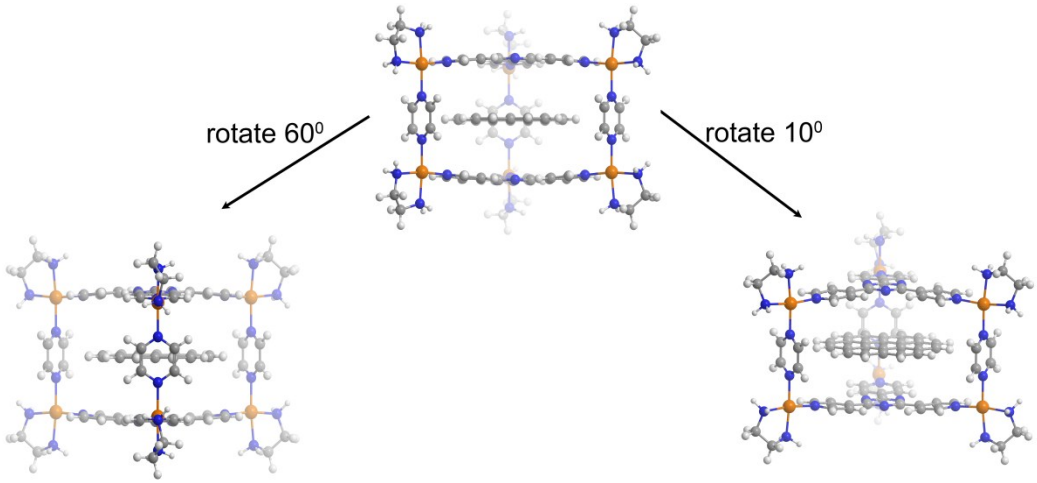

Figure S2. Views of the optimized structure for **1**.

Table S1. Calculated electronic transition energies of the low-lying singlet excited-states of **1**[a].

Electronic transition	**Energy(nm)**	**Contrib.**	**CI%**	**Character**
$S_0 \rightarrow S_1$	424	HOMO-1→LUMO+2	61.9	CCCT
		HOMO→LUMO+2	34.0	CCCT
$S_0 \rightarrow S_2$	422	HOMO-1→LUMO	82.0	CCCT
		HOMO→LUMO	14.2	CCCT
$S_0 \rightarrow S_3$	409	HOMO→LUMO+1	94.4	CCCT
$S_0 \rightarrow S_4$	408	HOMO-1→LUMO+2	34.2	CCCT
		HOMO→LUMO+2	61.9	CCCT
$S_0 \rightarrow S_5$	407	HOMO-1→LUMO	14.2	CCCT
		HOMO→LUMO	83.3	CCCT
$S_0 \rightarrow S_6$	395	HOMO-1→LUMO+1	96.4	CCCT
$S_0 \rightarrow S_7$	380	HOMO-1→LUMO+6	21.0	CCCT
		HOMO→LUMO+3	58.5	CCCT
		HOMO→LUMO+4	8.9	CCCT

[a]HOMO means highest occupied molecular orbital, and LUMO means lowest unoccupied molecular orbital. CCCT means coronene-to-cage charge transfer.

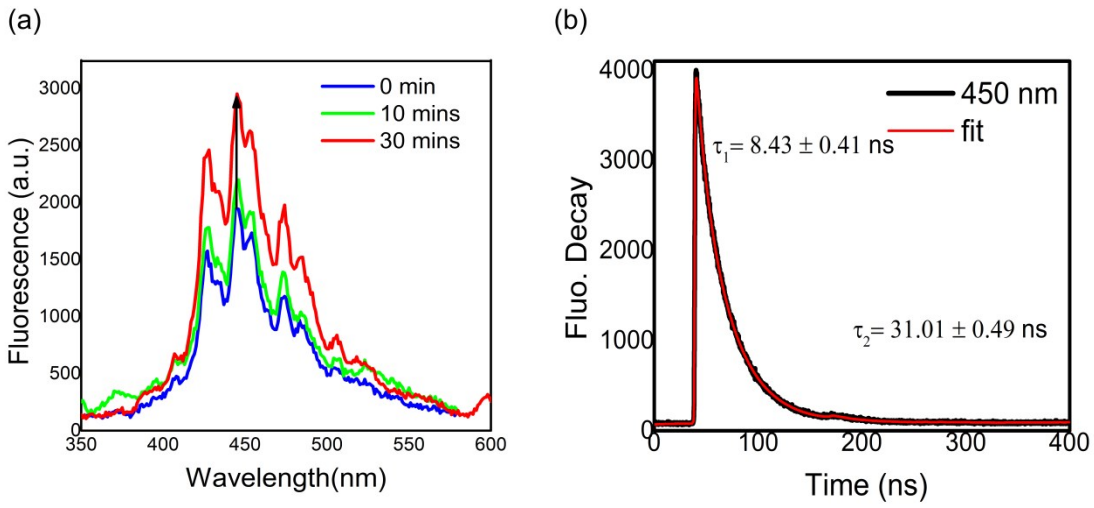

Figure S3. (a) Steady-state fluorescence spectra of coronene in DCM with different degassed time by N_2 bubbling. (b) Time-resolved fluorescence spectra of coronene in aerated solution of DCM.

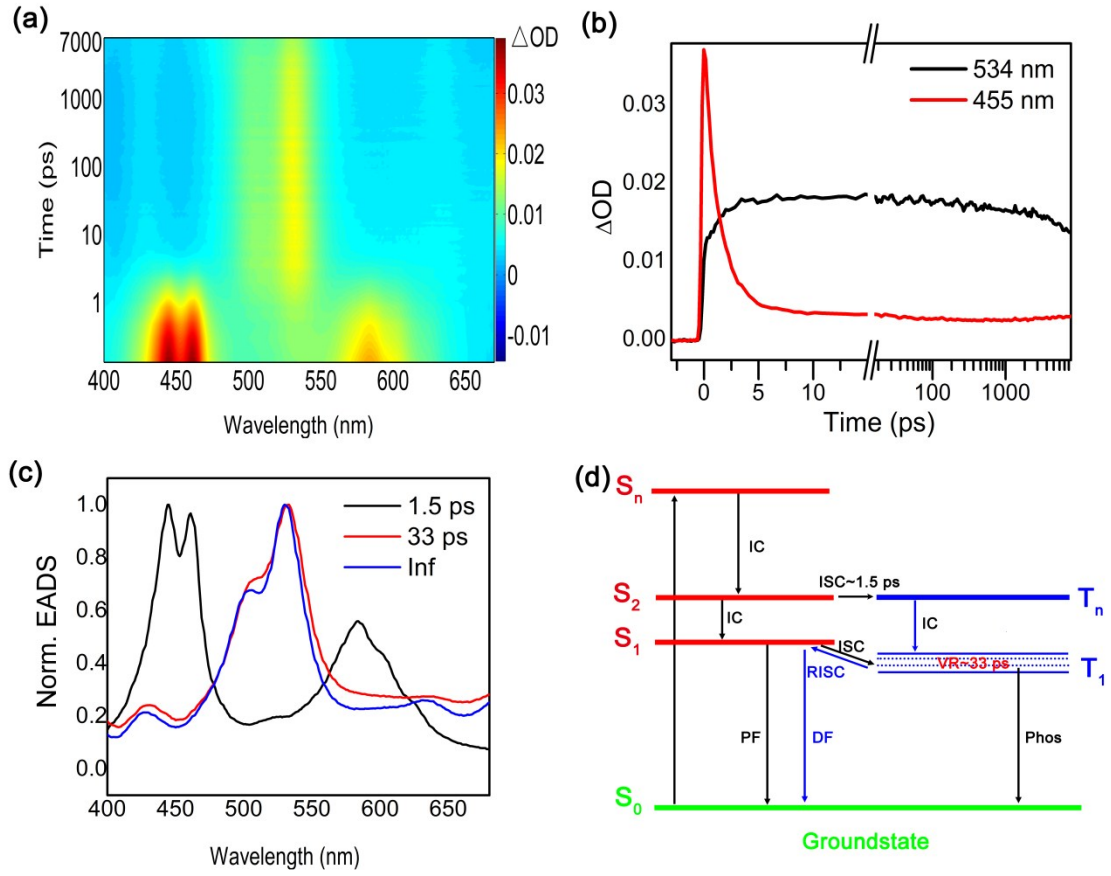

Figure S4. Fs TA spectra of coronene in DCM upon excitation at 340 nm; (a) contour plot of the fs TA spectra from 0 to 7800 ps; (b) kinetic profiles of 455 and 534 nm; (c) normalized EADS derived from global analysis; (d) excited-state decay pathways in coronene.

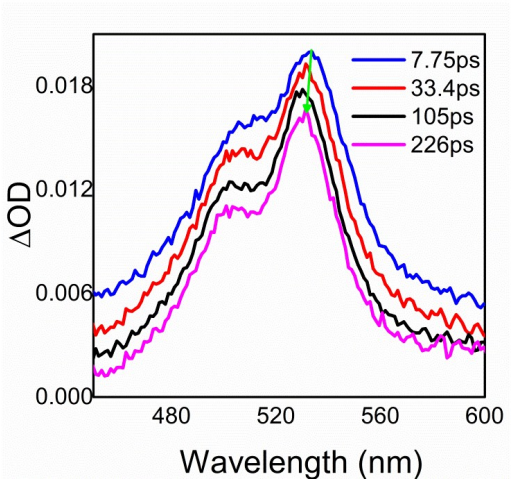

Figure S5. Fs TA spectra from 440 to 600 nm of coronene in DCM upon excitation at 340 nm

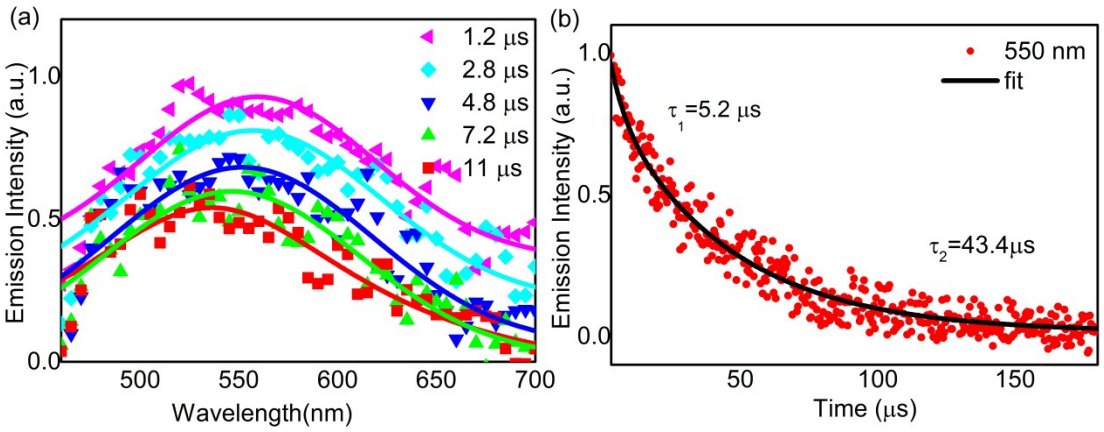

Figure S6. Ns TE spectra of **1** in water with excitation at 355 nm: (a) ns TE spectra at selected time decays with corresponding waveform fit; (b) kinetic profile (red dots) at 550 nm with singlet wavelength fit (black line).

Table S2. Global analysis results of **1** upon different excitation wavelengths (λ_{ex}) by Glotaran software: rate constant (k) and corresponding standard deviation (sd)

λ_{ex}/nm	k_1/ps^{-1}	sd_1/ps^{-1}	k_2/ps^{-1}	sd_2/ps^{-1}	k_3/ps^{-1}	sd_3/ps^{-1}
310	0.10502	0.00095	0.00716	0.00008	< 0.0005	–
450	–	–	0.00706	0.00004	< 0.0005	–