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Electronic Supplementary Information

High Contrast Mechanochromic and Thermochromic Luminescence Switching by a Deep Red Emitting Organic Crystal

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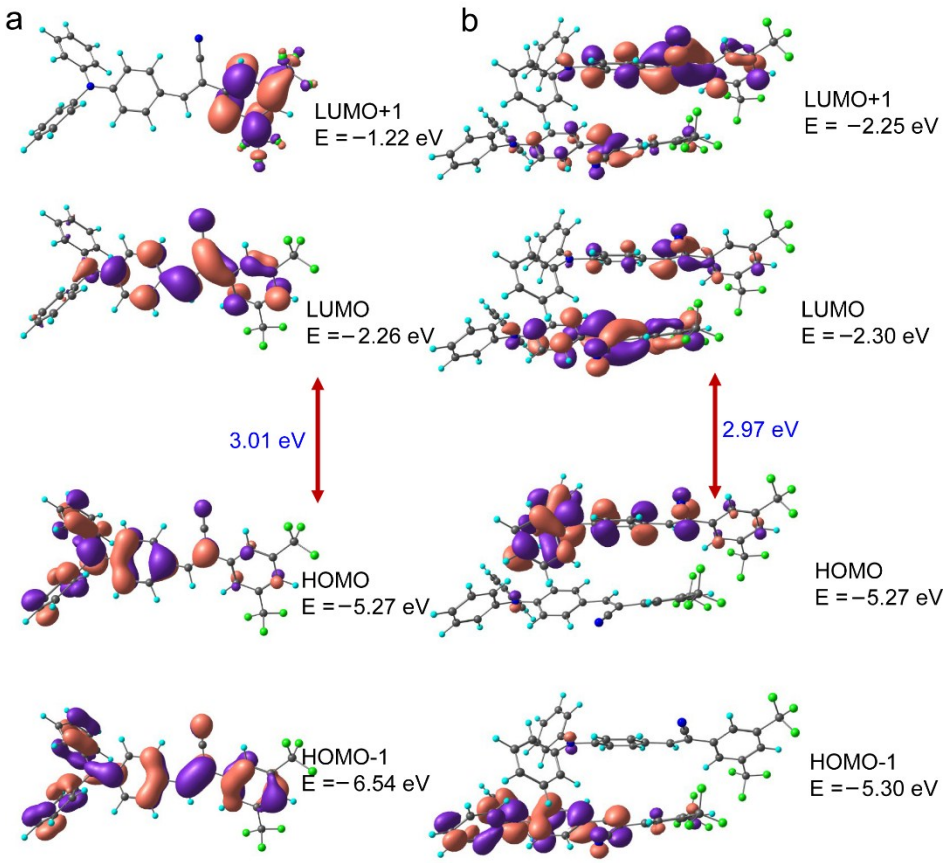

Figure S1. DFT calculated frontier molecular orbitals (FMO) of **1** as (a) monomer and (b) dimer.

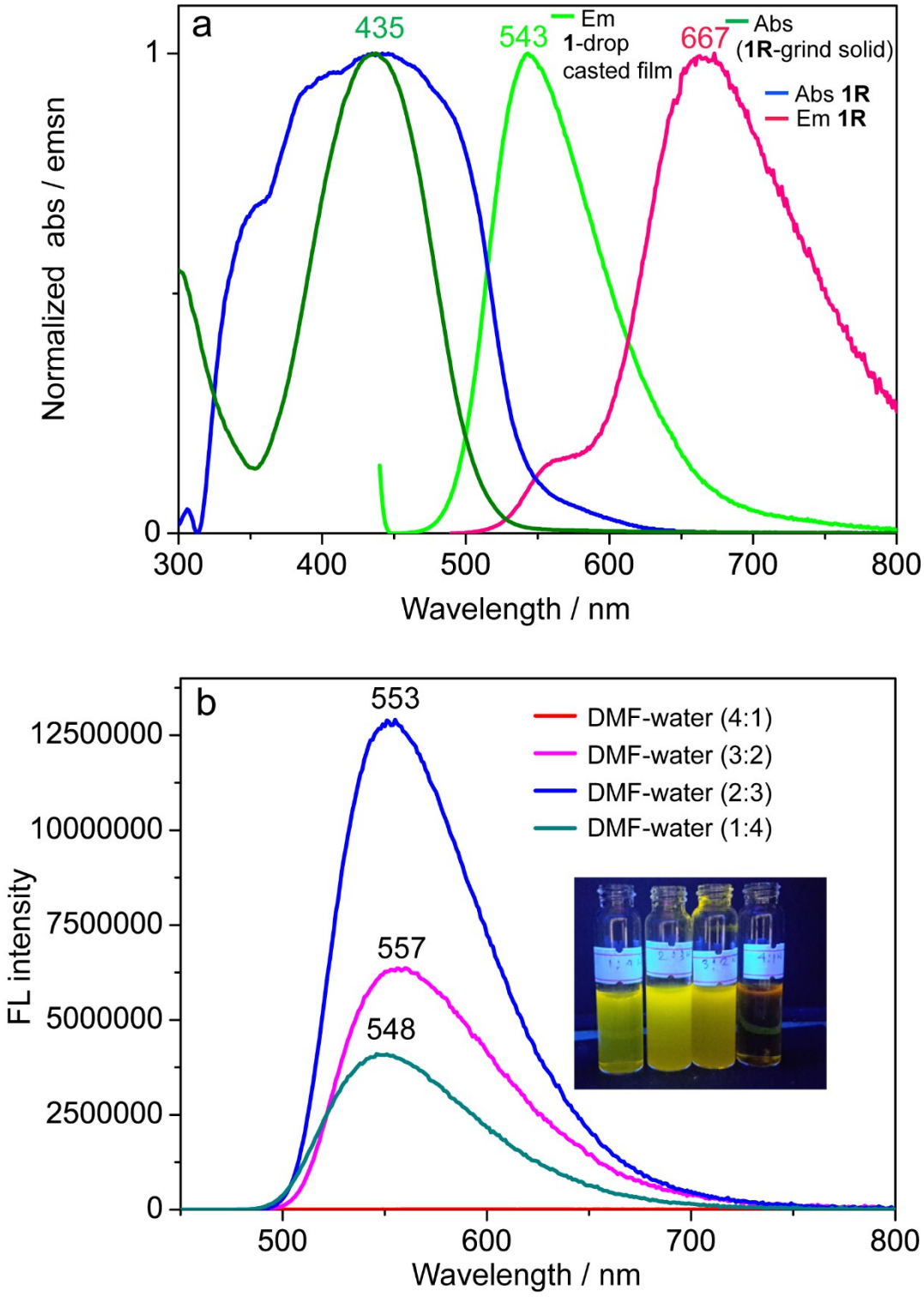

Figure S2. Solid-state absorption spectra (Abs) of pristine red emissive **1R** crystal, grinded powder (green emissive) and emission spectra (Em) of pristine **1R** crystal and drop casted film (green emissive). Drop-casted film was made from DCM solution (1 x 10^{-4} M). (b) Aggregation induced emission behavior of **1** in DMF-water mixture.

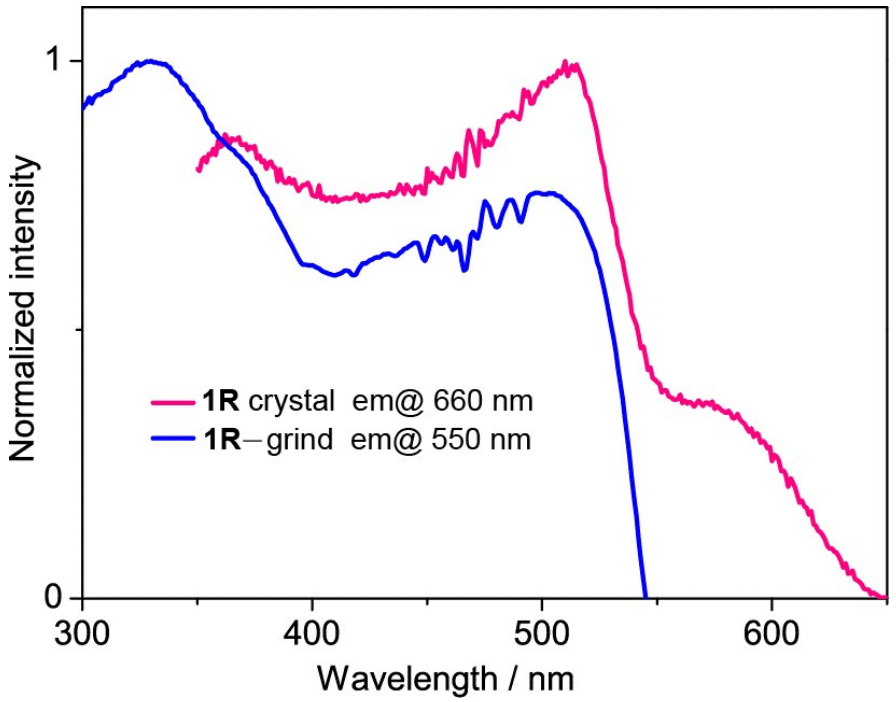

Figure S3. Fluorescence excitation profiles of **1R** crystal and grinded sample.

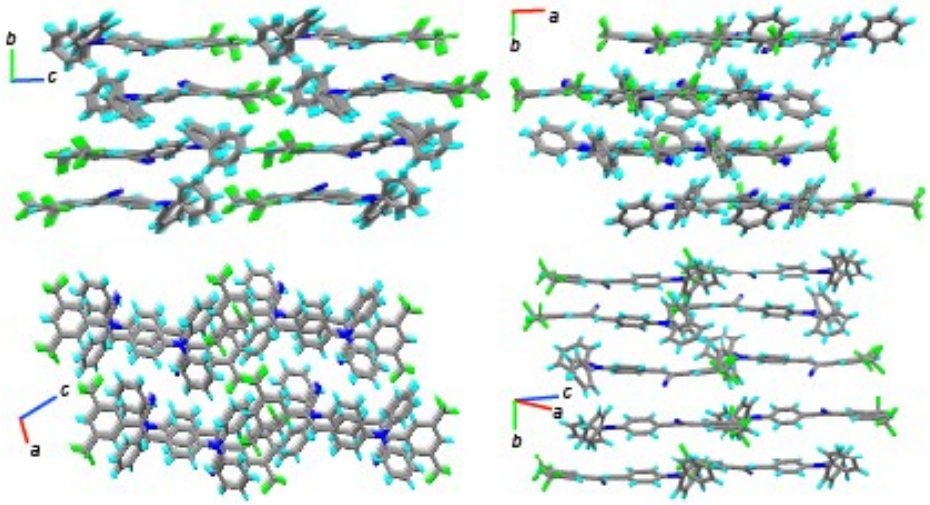

Figure S4. Packing diagrams of **1R**.

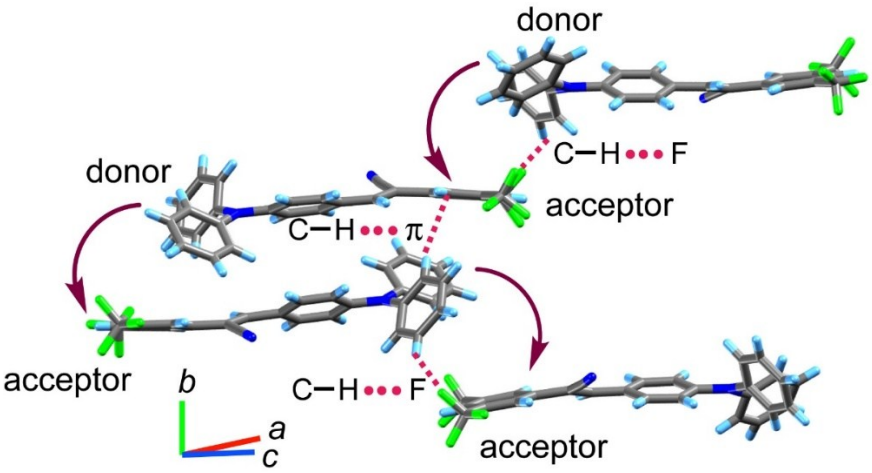

Figure S5. Intermolecular non-covalent interactions between the molecules in **1R** that facilitate intermolecular charge transfer delocalization.

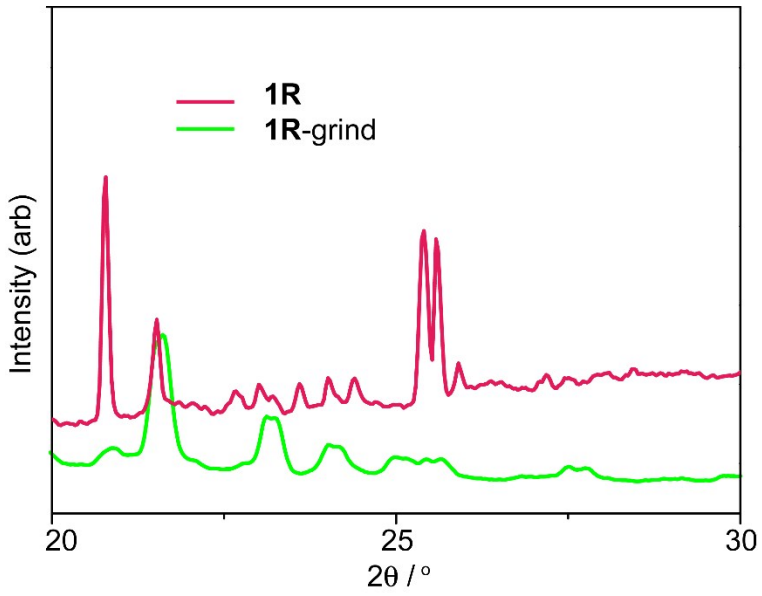

Figure S6. Expanded PXRD plots of **1R** and **1R**-grind powder.

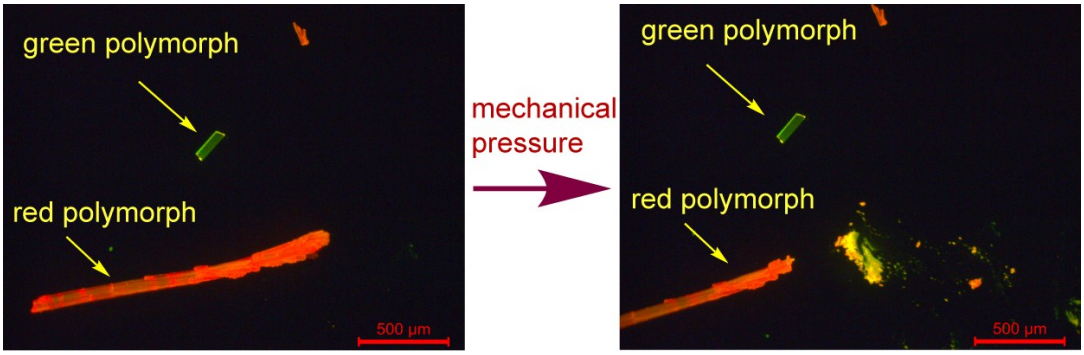

Figure S7. Red and green emissive polymorphs of **1**. Mechanochromic fluorescence change of red polymorph.

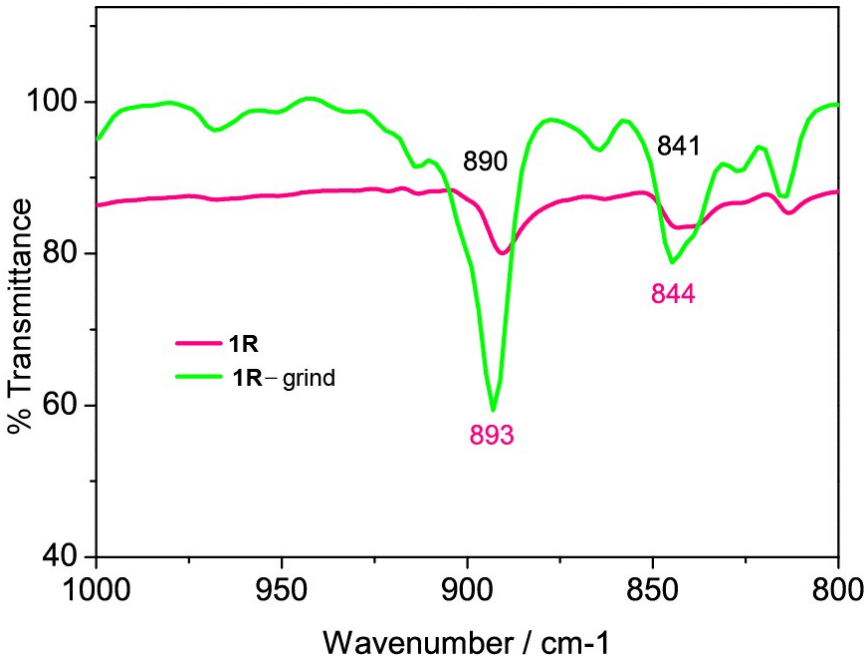

Figure S8. Expanded infrared spectra of the **1R** and **1R**-grind showing C–H out of plane frequencies.

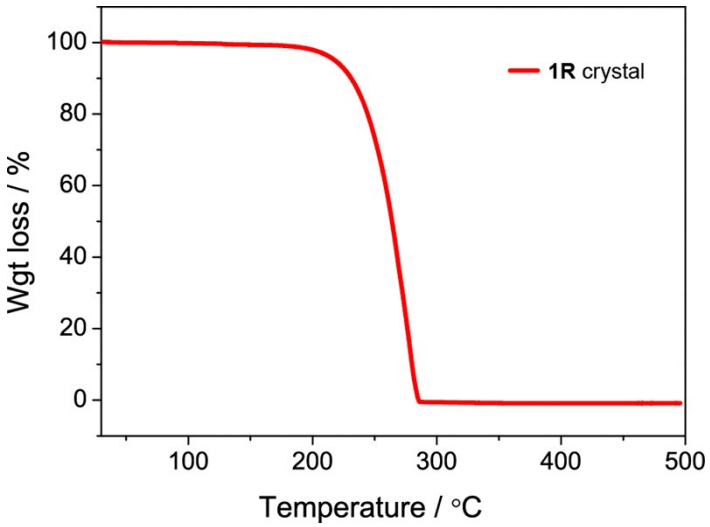

Figure S9. TGA plot of **1R** crystal.

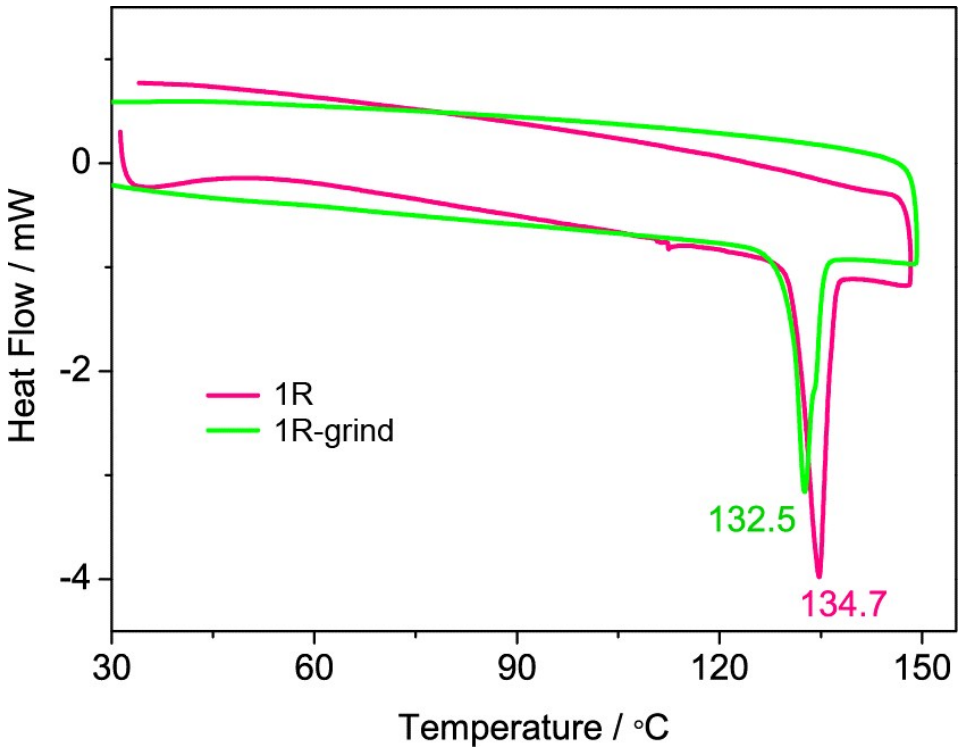

Figure S10. DSC plot for **1R** crystal and **1R**-grind.

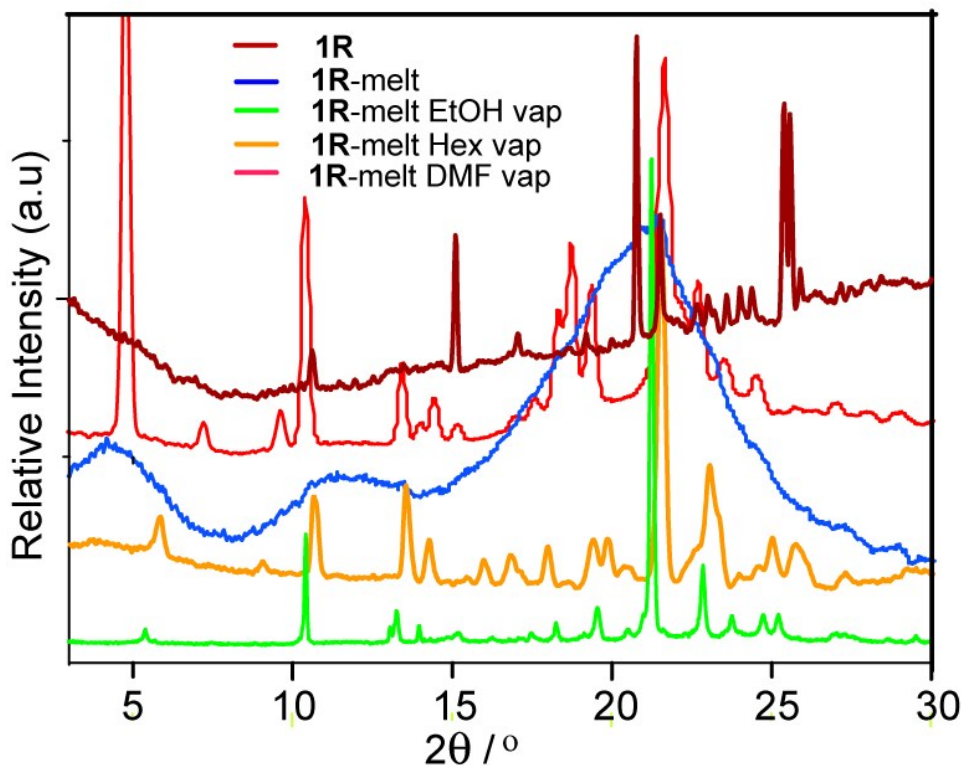

Figure S11. Overlapped PXRD plots of **1R** and vapour fumed crystalline solids.

Table S1. Photophysical parameters of **1** in solution and solid state.

Compound	Fluorescence	QY / %
1 (in toluene solution)	$\lambda_{em, max}$ = 523 nm	0.030
1 (DMF solution)	$\lambda_{em, max}$ = 612 nm	0.020
1R-crystal	$\lambda_{em, max}$ = 667 nm	0.50

Table S2. Fluorescence life time values of crystals and solution

	Life time values, τ (ns)
1 (in toluene solution) λ_{ex} = 418 nm, λ_{em} monitoring at 525 nm	τ = 0.304 χ^2 = 1.03
1 (in DMF solution) λ_{ex} = 418 nm, λ_{em} monitoring at 612 nm	τ_1 = 0.39 (85.18 %), τ_2 = 1.47 (14.8 %), χ^2 = 1.13
1R crystal λ_{ex} = 418 nm, λ_{em} monitoring at 660 nm	τ_1 = 7.27 (50.42 %) τ_2 = 0.48 (8.37 %) τ_3 = 25.5 (41.21 %) χ^2 = 1.18
1R-grind λ_{ex} = 418 nm, λ_{em} = 540 nm	τ_1 = 0.22 (35.04 %) τ_2 = 2.97 (64.96 %) χ^2 = 1.05

Table S3. Single crystal X-ray parameters of **1R** crystal (at 296 K)

Chemical formula	$C_{29}H_{18}F_6N_2$
M_r	508.45
Crystal system	Monoclinic
Space group	$P2_1$
a / Å	8.9164(6)
b / Å	16.6045(10)
c / Å	16.3908(11)
α / ° β / ° γ / °	90 101.409(3) 90
V / Å^3	2378.7(3)
Z	4
ρ_{calc} / (g cm^{-3})	1.420
μ / mm^{-1}	0.117
F_{000}	1040
θ_{min} / °	2.33
θ_{max} / °	26.26
Reflections collected	9593
Independent reflections	6086
GoF	1.045
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0836, wR_2 = 0.2499
R indices (all data)	R_2 = 0.1183, wR_2 = 0.2874

Table S4. Geometry optimized output coordinates of the monomer species.

9 7.076966000 -2.629371000 -0.245316000

7 -4.835917000 0.051162000 -0.033434000

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Table S5. Geometry optimized output coordinates of the dimer species.

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