Citric Acid: A Powerful Biomass-Derived Host Doped with Diverse Guests for Green Room-Temperature Phosphorescence Materials

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Materials and Instruments. Citric acid (99.5%), 9-phenanthreneboronic acid (99.9%) and 1-naphthaleneboronic acid (97%) were obtained from Machlin. 4-Biphenylboronic acid (98%), phenanthrene (99%), and 1-(bromomethyl)naphthalene (97%) were bought from Energy Chemical. 4-Biphenylmethanol (98%), 2-naphthalenemethanol (98%), 4-phenylphenol (99%), terephthalic acid (99%), 4-biphenylcarboxaldehyde (98%) and 2-naphthaldehyde (98%) were purchased from Shanghai D&B Biological Science and Technology Co. Ltd. 9-Formylphenanthrene (97%) was obtained from Alfa Aesar. Biphenyl (99.5%) was bought from Shanghai RHAWN Chemical Technology Co. Ltd. 4-Carboxyphenylboronic acid (98%) was purchased from J&K Scientific. Isophthalic acid (99.5%) was obtained from Shanghai Boer Chemical Reagents Co. Ltd. Naphthalene (99%) was bought from Meryer (Shanghai) Biochemical Technology Co. Ltd. All chemicals were directly used without further purification.

^{1}H NMR spectra were recorded on Bruker Avance 400 MHz spectrometer. X-ray powder diffraction patterns were measured by a Bruker D8 Focus diffractometer equipped with Cu K_α radiation. Luminescence steady and delayed spectra, fluorescence and phosphorescence decay curve and absolute quantum yield were all carried out on an Edinburgh Instruments FLS1000. For PA@CA and CPBA@CA, the fluorescence band is partially overlapped with itself phosphorescence band. The fluorescence and phosphorescence quantum yields are determined through peak-differentiation-imitating method according to the literature.[1] Solid-state absorption was measured on a Shimadzu UV-3600 Plus spectrophotometer in diffuse reflectance mode. High performance liquid chromatography (HPLC) analysis was recorded on a Shimadzu LC-20AT

system. FTIR spectra were recorded on a Shimadzu FTIR-8400S spectrophotometer.

Computational detail. For calculating the excited state energy level, the geometries of naphthalene (NP), citric acid (CA) and 4-biphenylboronic acid (BPBA) molecules were extracted from the crystal structure (CCDC 1216817, 1126301 and 1881839) without further optimization. The excited state energy levels were calculated at CAM-B3LYP/def2-TZVP level using Gaussian 09 software.[2]

For NP@CA guest-host aggregate, the calculation was simplified. First, eight adjacent CA molecules were extracted from the CA crystal structure. Then one NP was inserted into the central space formed by the eight CA molecules. This cluster is designated as NP@8CA. The ground-state geometries of NP@8CA cluster were optimized at CAM-B3LYP/6-31G(d) level. Based on the optimized structures, the hole-electron analysis was performed on Multiwfn,[3,4] and the spin-orbital coupling (SOC) matrix was calculated on Orca 5 at CAM-B3LYP/ZORA-def2-SV(P) level.[5] For comparison, the ground-state single NP molecule structure was also optimized and the SOC constants were calculated using the same methods. Frequency calculations were performed on the minima to check the absence of imaginary vibrational frequency.

Preparation of citric acid-based organic RTP system. The guest-host RTP systems (guest@CA) are prepared by doping citric acid (CA) host with different guests. Using 4-biphenylboronic acid (BPBA) as an example (BPBA@CA, mass ratio = 1:300), 453.5 mg CA and 1.5 mg BPBA were added in 6 mL methanol (or ethanol). The mixture was sonicated to dissolve the solid. Then the solvent was directly removed through a rotary evaporator. Other guest@CA doping materials were prepared by the same procedure.

Latent fingerprint collection and development. The collection and development process of fingerprint is according to the previous report.[6] After lightly touching his forehead with finger, the volunteer pressed his finger on the glass and plastic surfaces. Then the ground guest-host powder was spread over the fingerprint impression using a brush, and the excess powder was blown off gently with a rubber suction bulb. The latent fingerprint image was directly captured with an Apple smart phone.

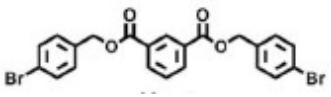
Table S1. The typical biomass-derived hosts and their corresponding guests for organic RTP. To simplify comparison, only bicomponent host-guest solid-state systems are listed. Our study also adopts bicomponent system. **Note**: some biomass-derived hosts such as microcrystalline cellulose and cyclodextrin are also used in multicomponent guest-host systems (Adv. Optical Mater. 2025, 13, e01631; Angew. Chem. Int. Ed. 2025, 64, e202505192; Adv. Optical Mater. 2024, 12, 2302928).

Host	Guest	Reference
silk fibroin	arylboronic acids	Adv. Mater. 2025, DOI: 10.1002/adma.202512659, e12659.
konjac glucomannan	arylboronic acids/aromatic carboxylic acids	Adv. Mater. 2024, 36, 2402666.
starch	coumarin derivatives fluorone dyes riboflavin and lumiflavin 4-carboxyphenylboronic acid	ACS Appl. Mater. Interfaces 2023, 15, 30717 J. Lumin. 2012, 132, 1055; Chem. Phys. 2010, 378, 58 Chem. Phys. 2012, 400, 142 Int. J. Biol. Macromol. 2025, 284, 138175
gelatin	fluorone dyes nitrilotribenzoic acid	Chem. Phys. 2010, 378, 58; Nat. Commun. 2019, 10, 3986; J. Photochem. Photobiol. A: Chem. 2009, 208, 131 CCS Chem. 2024, 6, 2727
chitosan	fluorone dyes polyhydroxy galactose-modfied phosphors	Chem. Phys. 2010, 378, 58 ACS Appl. Mater. Interfaces 2020, 12, 52059
microcrystalline cellulose	arylboronic acids/arenes bisdibenzoic acid derivative phenanthrene and coronene	Adv. Mater. 2023, 35, 2305126 Chem. Sci. 2024, 1517600 J. Phys. Chem. 1985, 89, 3026
α-cyclodextrin	diphenylacetylene and its derivatives polyhydroxy galactose-modfied phosphors linear brominated aromatic aldehyde polymer benzene/naphthalene-modified polyethylene glycol phorsphor-modified chitosan	Adv. Optical Mater. 2021, 9, 2101337; J. Phys. Chem. C 2023, 127, 12375 ACS Appl. Mater. Interfaces 2020, 12, 52059 Adv. Optical Mater. 2019, 7, 1900589 Adv. Optical Mater. 2022, 10, 2102169 Small 2023, 19, 2207403
β-cyclodextrin	polyhydroxy galactose-modfied phosphors benzoic acid derivatives dibenzothiophene	ACS Appl. Mater. Interfaces 2020, 12, 52059 Adv. Funct. Mater. 2024, 34, 2400898; ACS Appl. Mater. Interfaces 2025, 17, 24351 Sci China Chem. 2018, 61. 397

	biphenylboronic acid	ACS Nano 2023, 17, 12895
γ-cyclodextrin	arylboronic acids 4-bromo-1,8-naphthalic anhydride polymer	J. Colloid Interf. Sci. 2025, 687, 345; Adv. Mater. 2025, 37, 2418506 Polym. Chem., 2016, 7, 3989
citric acid	simple arenes aromatic boronic acids aromatic carboxylic acids aromatic aldehydes phenols aromatic alcohols aromatic halohydrocarbon alkaloid	this study

Table S2. The frequently-used/powerful small molecule host and its corresponding guests for organic RTP.

Host	Guest	Reference
β-estradiol	secondary amino-substituted deuterated carbon *N,N*′-dimethyl-1,1′-binaphthyldiamine hexa-peri-hexabenzocoronene	Adv. Funct. Mater. 2013, 23, 3386; Chem. Phys. Lett. 2014, 591, 119; J. Phys. Chem. Lett. 2016, 7, 1539; Adv. Opt. Mater. 2017, 5, 1600996.
carbazole	benzo[*f*]indole 6*H*-dibenzo[*b,h*]carbazole 5*H*-benzo[*b*]carbazole	Nat. Mater. 2021, 20, 175; Angew. Chem. Int. Ed. 2023, 62, e202310335.
1,3-bis(N-carbazolyl)benzene	*N,N*′-bis(3-methylphenyl)-N,N′-bisphenyl-9,9-dimethylfluorene difluoroboron β-diketonate derivatives corannulene derivatives	Adv. Funct. Mater. 2017, 27, 1703902; Angew. Chem. Int. Ed. 2024, 63, e202400089; Angew. Chem. Int. Ed. 2023, 62, e202309718.
melamine	aromatic carboxylic acid	Adv. Funct. Mater. 2019, 29, 1807599; J. Am. Chem. Soc. 2018, 140, 10734.
cyanuric acid	aromatic carboxylic acid aromatic boronic acid	Nat. Commun. 2020, 11, 4802; Angew. Chem. Int. Ed. 2021, 60, 17094.
benzophenone	triphenylamine derivatives isoquinoline derivatives difluoroboron β-diketonate derivatives phenothiazine derivatives quinone polycyclic aromatic hydrocarbons benzo[*c*][2,1,3]thiadiazole derivatives pyrrole derivatives	J. Mater. Chem. C 2021, 9, 3391; Chem. - Eur. J. 2020, 26, 17376; J. Phys. Chem. Lett. 2021, 12, 1814; J. Phys. Chem. Lett. 2021, 12, 4600; Adv. Opt. Mater. 2021, 9, 2100353; Nat. Commun. 2021, 12, 3522; Angew. Chem. Int. Ed. 2025, 64, e202417426; J. Phys. Chem. Lett. 2023, 14, 6927; Angew. Chem. Int. Ed. 2025, 64, e202500847; Chem. Sci. 2023, 14, 9733; Angew. Chem. Int. Ed. 2024, 63, e202317431.
triphenylphosphine	phenothiazine derivatives triphenylamine derivatives difluoroboron β-diketonate derivatives	Nat. Commun., 2021, 12, 3522; Angew. Chem. Int. Ed. 2020, 59, 16054; Adv. Opt. Mater. 2022, 10, 2201684; J. Mater. Chem. C 2022, 10, 11607; J. Mater. Chem. C 2022, 10, 11634.
triphenylamine	phenothiazine derivatives triphenylamine derivatives	Nat. Commun. 2021, 12, 3522; Chem. Sci. 2021, 12, 6518; Adv. Optical Mater. 2024, 12, 2401660; Angew. Chem. Int. Ed. 2023, 62,

	N,N-diphenylnaphthylamine	e202315911.
dimethylaminopyridine	diarylamine naphthalene and its derivatives with -NH_2, -COOH or -COOEt group	J. Mater. Chem. C 2023, 11, 6290; Matter 2020, 3, 449; Angew. Chem. Int. Ed. 2025, 64, e202508587.
 DPOBP-Br	3,6-diaminoacridine hydrochloride dibenzofuran 1,8-naphthalic anhydride 1,8-naphthalimide 4,4',4",4"'-(ethene-1,1,2,2-tetrayl)tetrabenzaldehyde coumarin pyrene rhodamine B	Angew. Chem. Int. Ed. 2024, 63, e202317631.
phenyl benzoate	benzophenone derivatives triphenylamine derivatives difluoroboron β-diketonate derivatives benzo[*e,g*]indazole derivatives	ACS Materials Lett. 2024, 6, 1042; Angew. Chem. Int. Ed. 2025, 64, e202513685; Chem. Commun. 2023, 59, 1525; J. Phys. Chem. Lett. 2023, 14, 11142; J. Mater. Chem. C 2022, 10, 11607; Dyes and Pigments 2023, 219, 111643.
	polycyclic aromatic hydrocarbons benzaldehyde derivatives naphthalene derivatives 5*H*-naphtho[8,1,2-*cde*]chromen-5-one 5*H*-phenanthro[1,10,9-*cde*]chromen-5-one 2,3,6,7,10,11-hexamethoxytriphenylene	Chem. Sci. 2025, 16, 2819.
citric acid	simple arenes aromatic boronic acids aromatic carboxylic acids aromatic aldehydes phenols aromatic alcohols aromatic halohydrocarbon alkaloid	this study

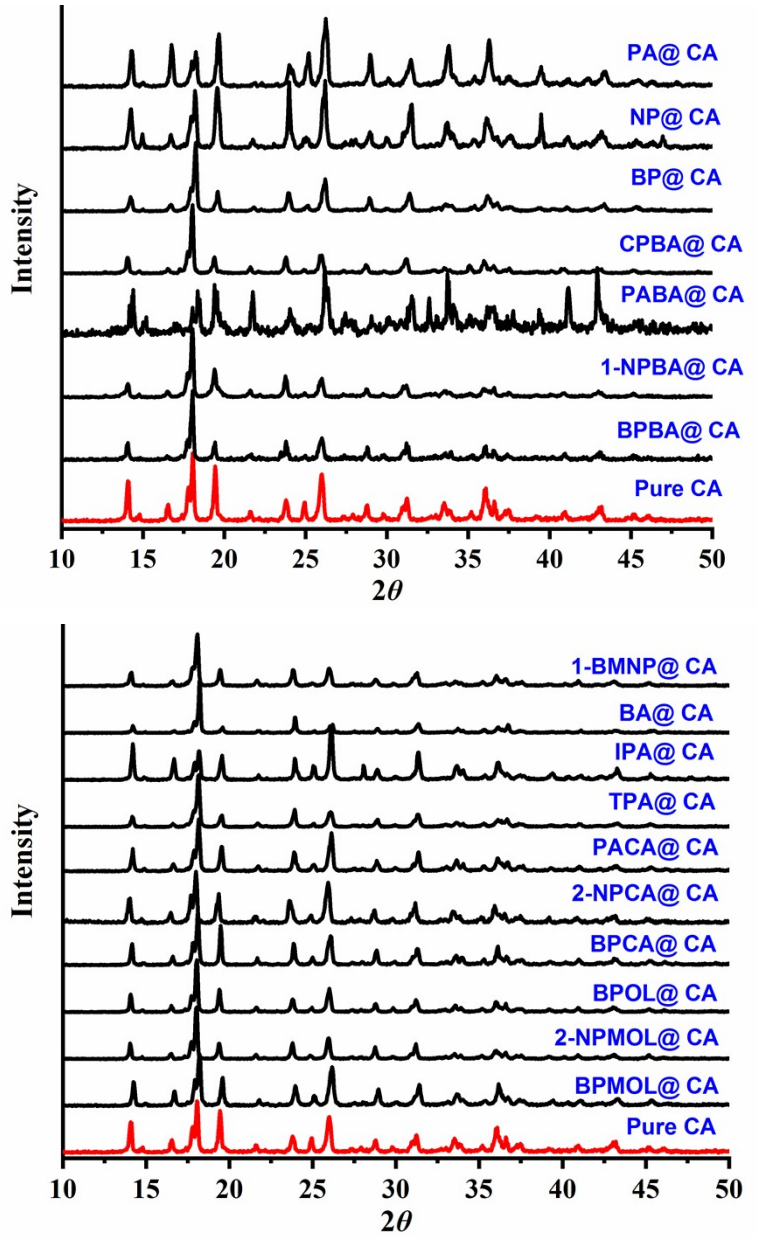


Figure S1. The X-ray diffraction patterns of pure CA and its 17 doped samples.

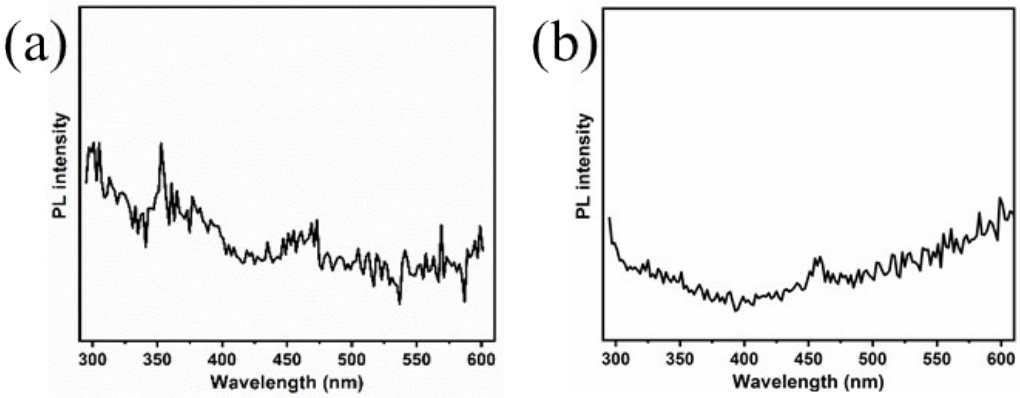


Figure S2. The steady-state (a) and 0.5 ms-delayed (b) spectra of pure CA. The excitation wavelength is 260 nm.

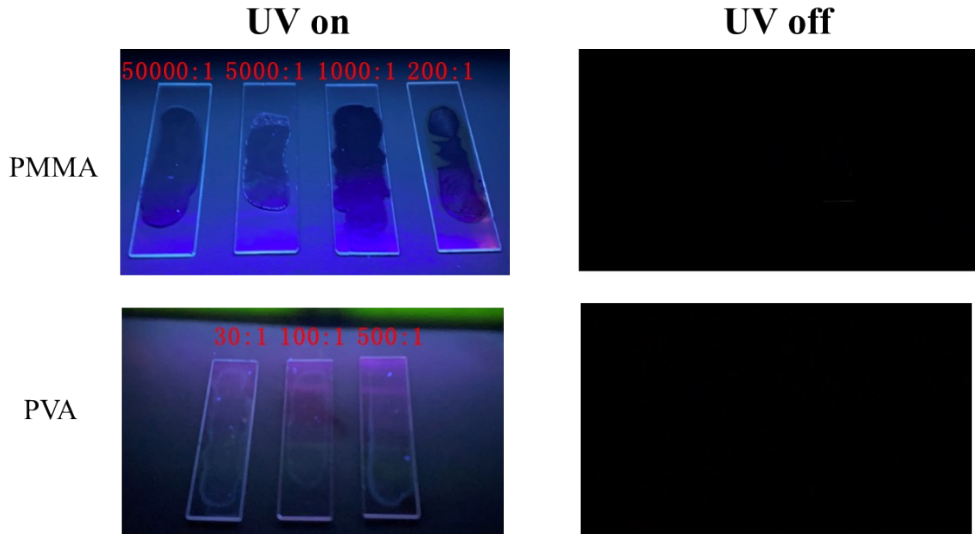


Figure S3. The photographs of naphthalene (NP)-doped PMMA/PVA films under 254 nm irradiation on (about 3 minutes) and off. The weight ratio of PMMA to NP is 50000:1, 5000:1, 1000:1 and 200:1, respectively. The weight ratio of PVA to NP is 30:1, 100:1, and 500:1, respectively.

NP-doped PMMA film preparation

NP (4.0 mg) was dissolved in 8 mL dichloromethane. 1.0 g PMMA was dissolved in 10 mL dichloromethane. Then 0.4 mL NP dichloromethane solution was added to the above PMMA solution and ultrasonic for about 5 min. This mixture was drop-cast on a quartz plate. After drying under natural condition, the NP-doped PMMA film (5000:1, w/w) was prepared. Other films with different mass ratio were made by the same method.

NP-doped PVA film preparation

90 mg PVA was added in 5 mL deionized water. The mixture was heated at 95 ºC for about 1 hour to obtain a clean solution. NP (9.3 mg) was dissolved in 9 mL ethanol. Then 3 mL NP ethanol solution was added into PVA solution under ultrasonic treatment. The NP-doped PVA film (30:1, w/w) was obtained by drop-casting the solution on a quartz plate. Other films with different mass ratio were made by the same method.

Table S3. The reported organic RTP lifetimes of doping systems using simple arene as the guest.

Host	Guest	RTP lifetime (s)	Reference
polymethyl methacrylate	biphenyl	0.90	J. Phys. Chem. A 2020, 124, 479
polymethyl methacrylate (*in situ* polymerization)	naphthalene	0.90	J. Mater. Chem. C 2022, 10, 17620
	phenanthrene	1.27	
1,4-dichlorobenzene	naphthalene	0.76	Matter 2022, 5, 3499
microcrystalline cellulose	biphenyl	0.14	Adv. Mater. 2023, 35, 2305126
	naphthalene	0.07	
	phenanthrene	0.18	
konjac glucomannan	naphthalene	0.49	Adv. Mater. 2024, 36, 2402666
	phenanthrene	0.28	
dimethylaminopyridine	naphthalene	1.79	Angew. Chem. Int. Ed. 2025, 64, e202508587
citric acid	biphenyl	2.15	this study
	naphthalene	1.54	
	phenanthrene	2.07	

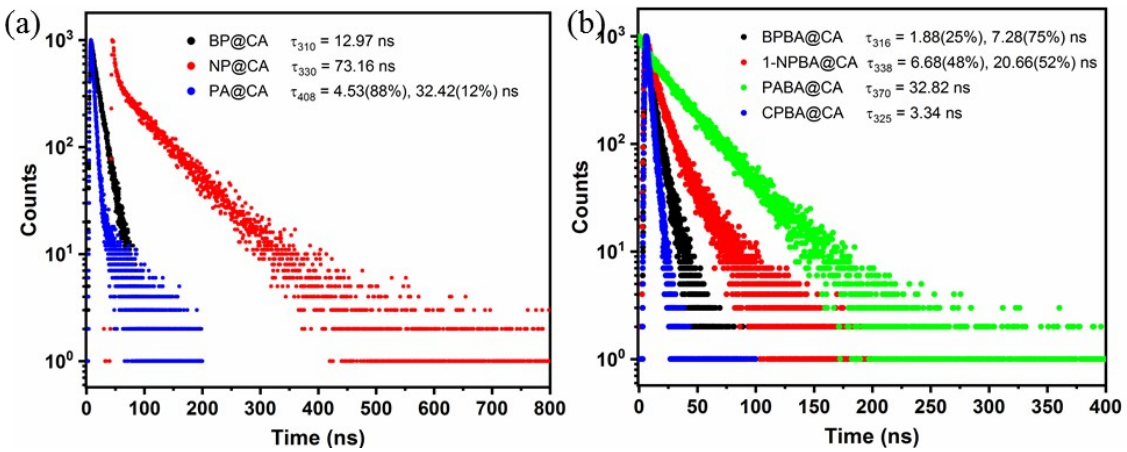


Figure S4. The fluorescence decay curves of arene and arylboronic acid-doped CA samples.

Table S4. The RTP lifetimes of 4-biphenylboronic acid (BPBA) doped in different hosts from the literature.

Guest	Host	RTP lifetime (s)	Reference
BPBA	poly(vinylidene fluoride)	1.27	Angew. Chem. Int. Ed. 2023, 62, e202314273
	cellulose	1.34	Adv. Mater. 2023, 35, 2305126
	carboxymethyl cellulose sodium	1.85	Mater. Today Chem. 2024, 40, 102211
	reconstructed cellulose	1.46	Small 2024, 20, 2309131
	β-cyclodextrin	1.03/2.23	ACS Nano 2023, 17, 12895
	β-cyclodextrin and PAETC	1.1	Angew. Chem. Int. Ed. 2025, 64, e202505192
	poly(HEMA)	1.79	FlexMat 2024, 2, 107
	PU elastomers	1.21	Chin. Chem. Lett. 2025, 36, 110676
	citric acid	2.07	this study

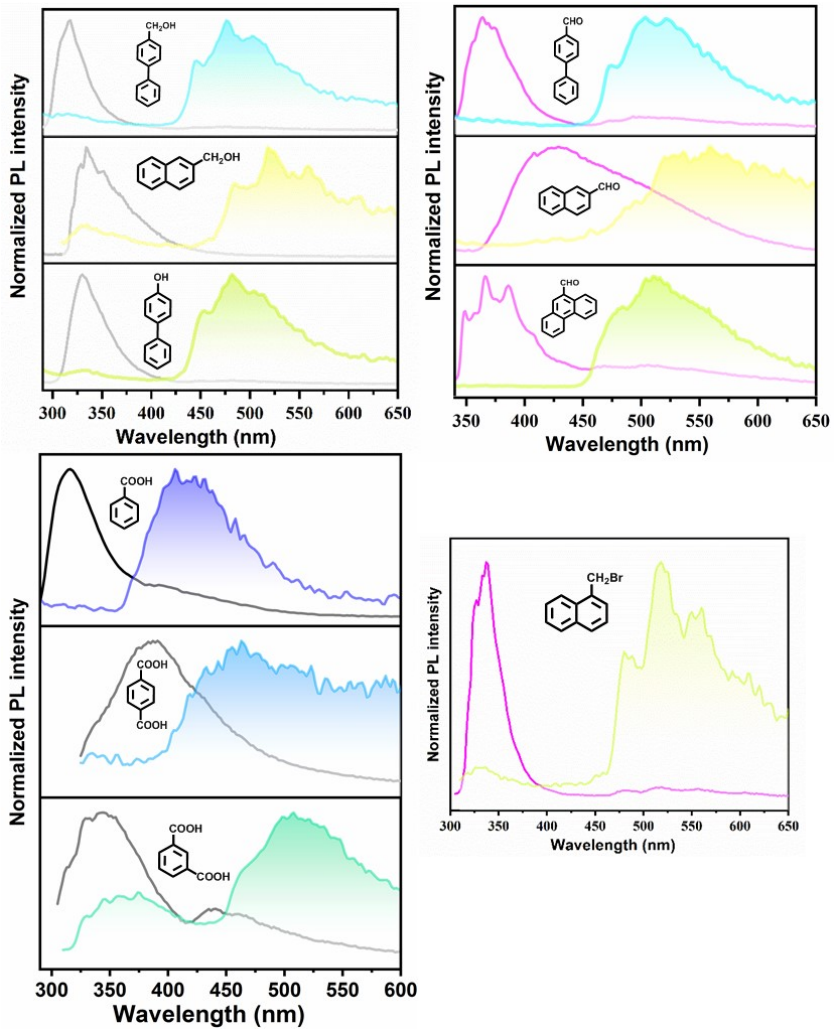


Figure S5. Steady-state and delayed emission spectra of CA samples doped with aromatic guest with different function group.

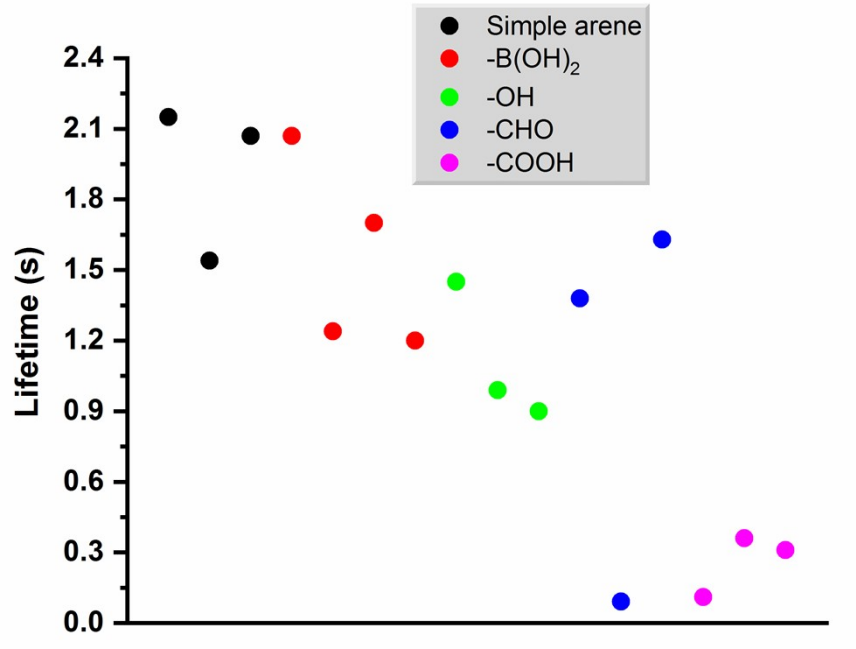


Figure S6. The distribution of RTP lifetimes with functional group.

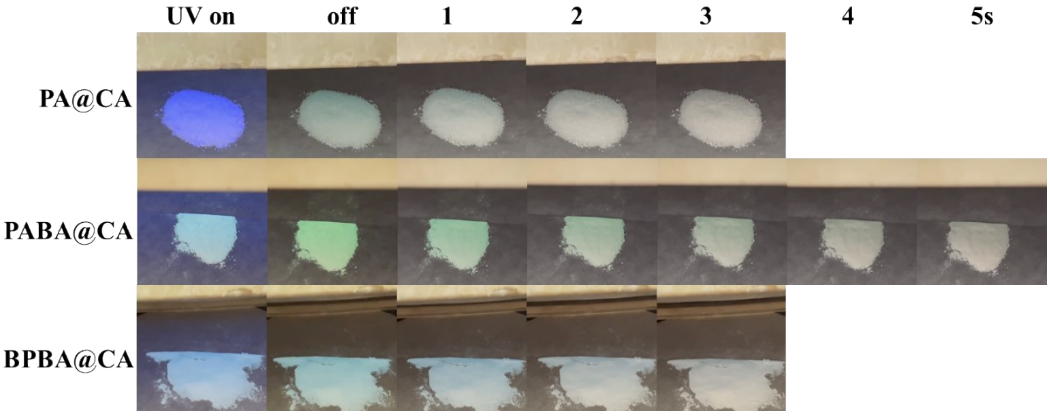


Figure S7. The afterglow observed under natural light condition.

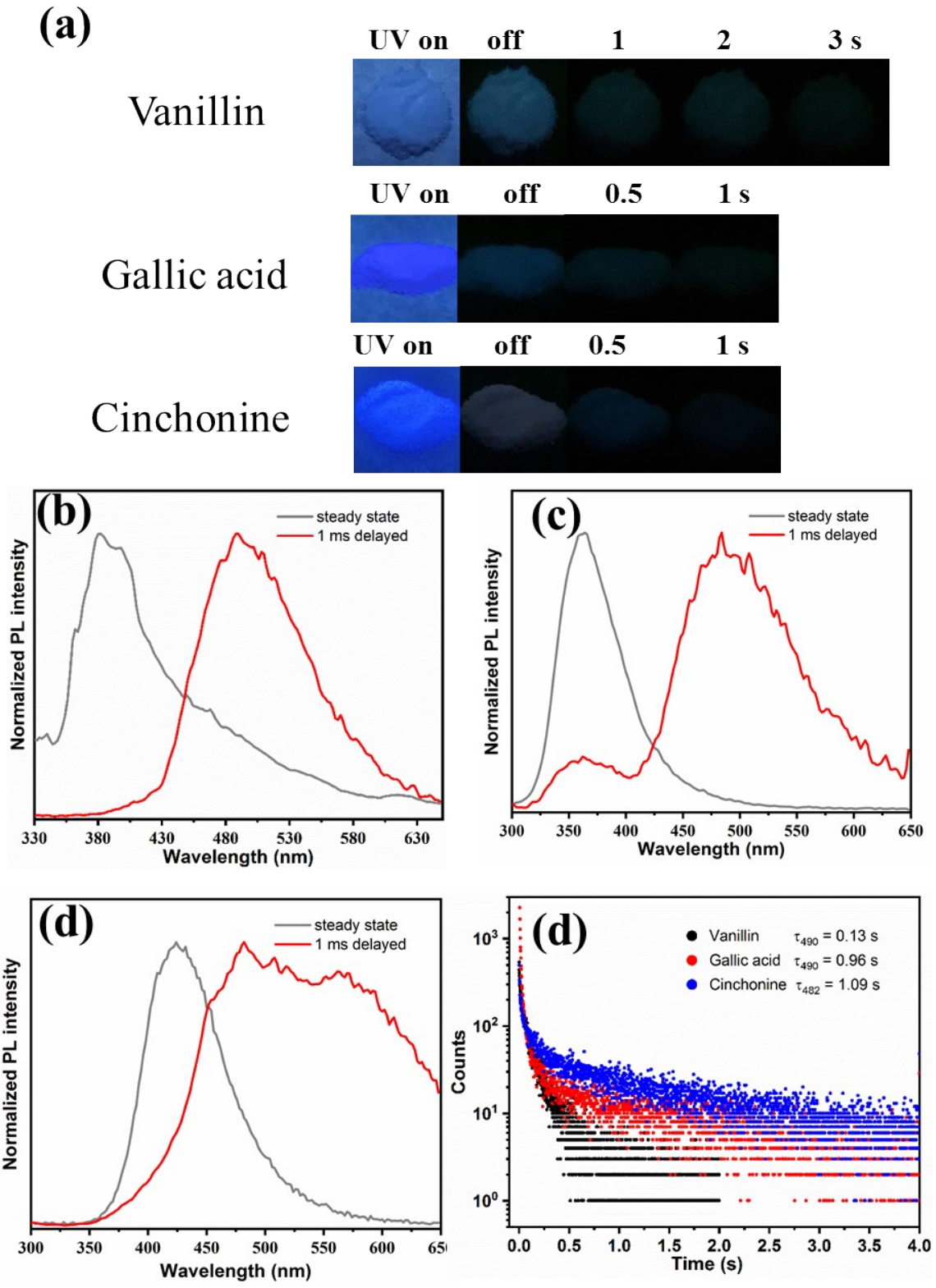


Figure S8. (a) Photographs of doped samples (host:guest ratio = 300:1, w/w) under 254 nm irradiation on and off. Steady-state (gray color) and 1 ms-delayed emission (red color) spectra of vanillin@CA (b), gallic acid@CA (c) and cinchonine@CA (d). (e) RTP decay curves.

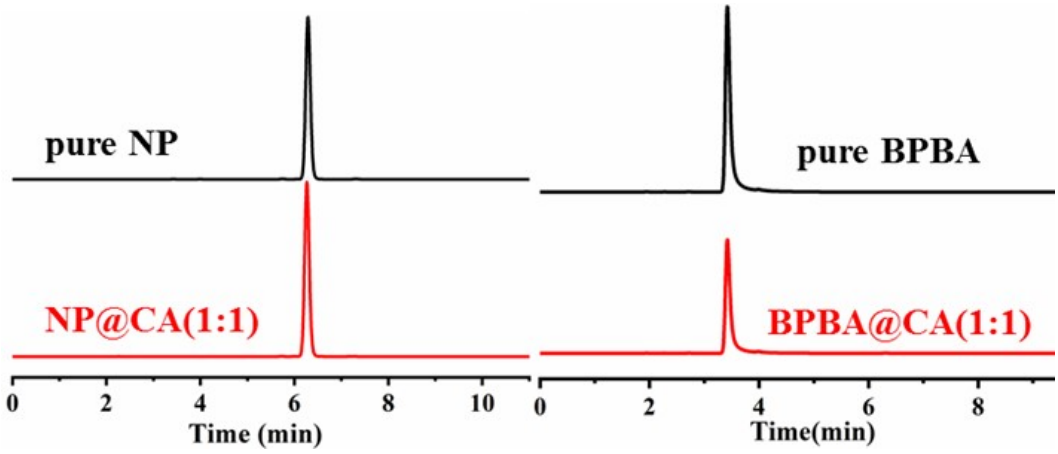


Figure S9. HPLC curves of NP, NP@CA (1:1, w/w), BPBA and BPBA@CA (1:1, w/w) monitored at 270 nm using acetonitrile-water mixture as eluent in a ratio of 80:20.

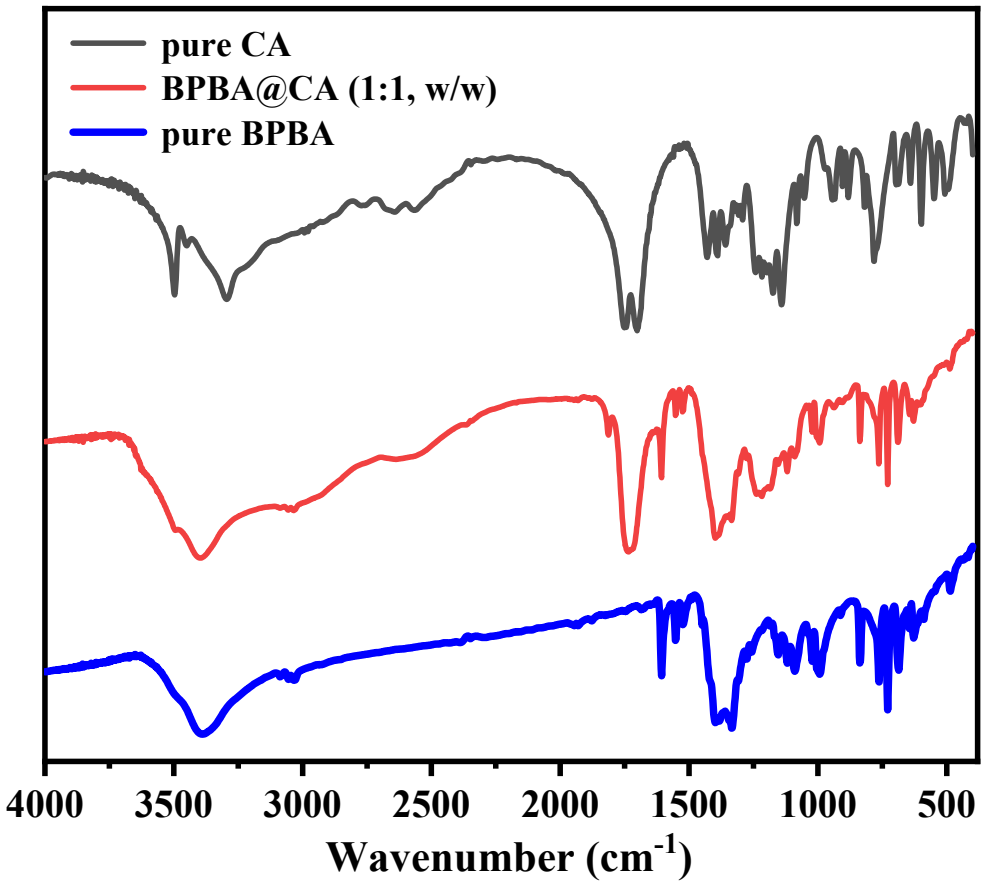


Figure S10. FTIR spectra of pure CA, BPBA@CA (1:1, w/w) and pure BPBA.

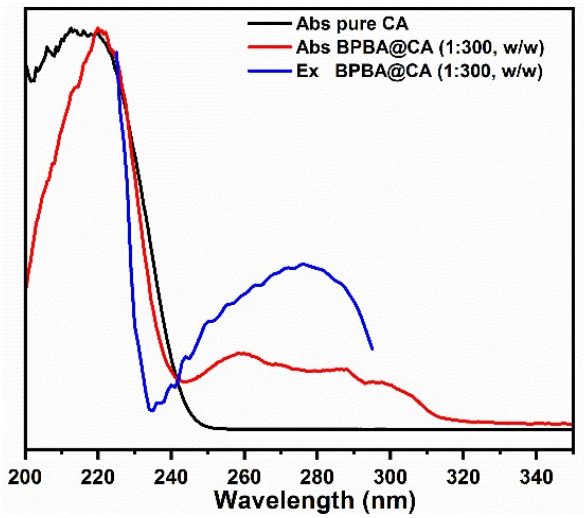


Figure S11. The absorption (Abs) and excitation (Ex, λ_{em} = 316 nm) spectra of pure CA and BPBA@CA samples.

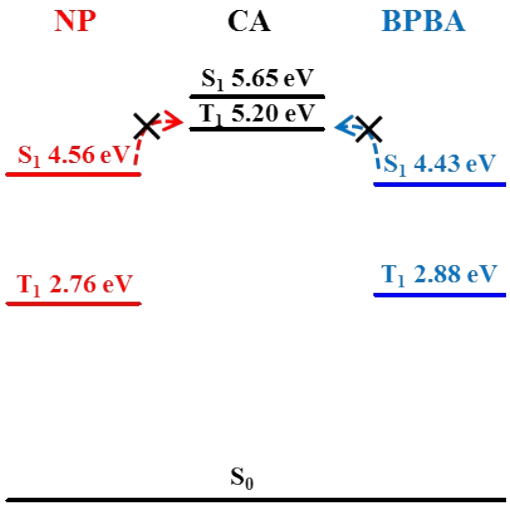


Figure S12. The calculated S_1 and T_1 energy levels of NP, CA and BPBA molecules.

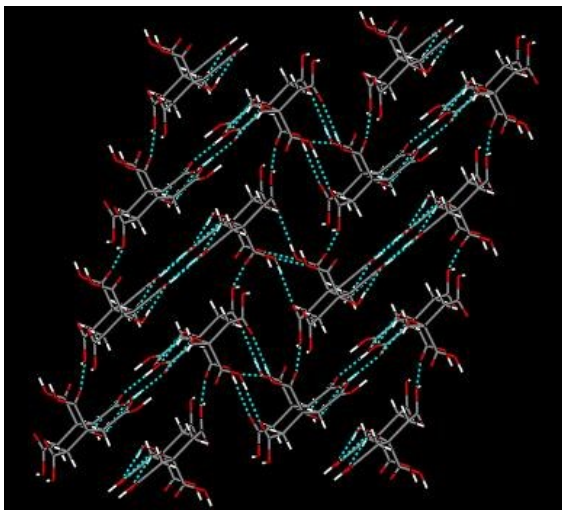


Figure S13. Packing motif of CA molecules. The blue dot line represents hydrogen bond.

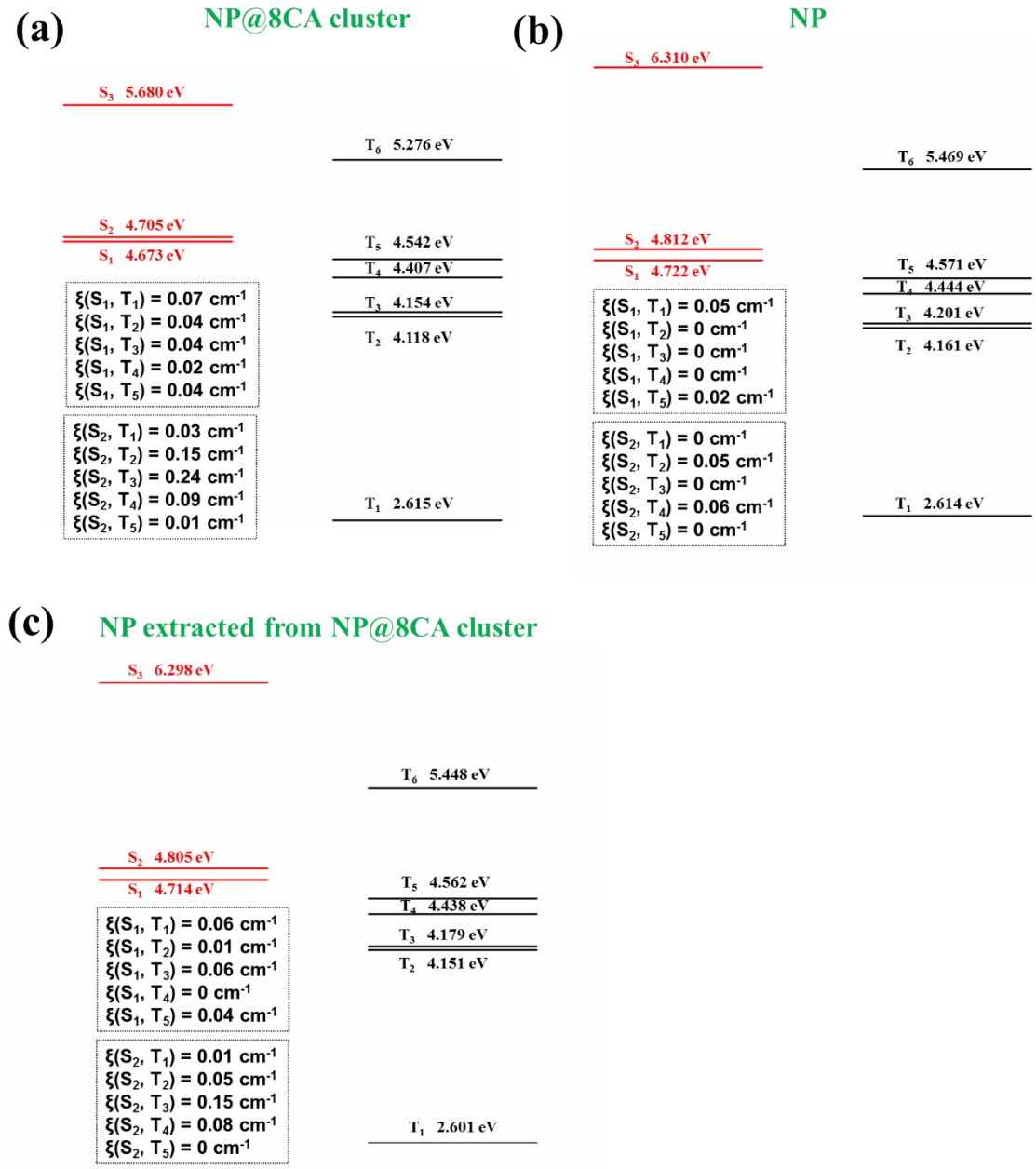


Figure S14. The calculated energy levels of NP@8CA cluster (a), NP single molecule (b) and NP directly extracted from NP@8CA (c). The SOC values (ξ) between interested S and T were listed.

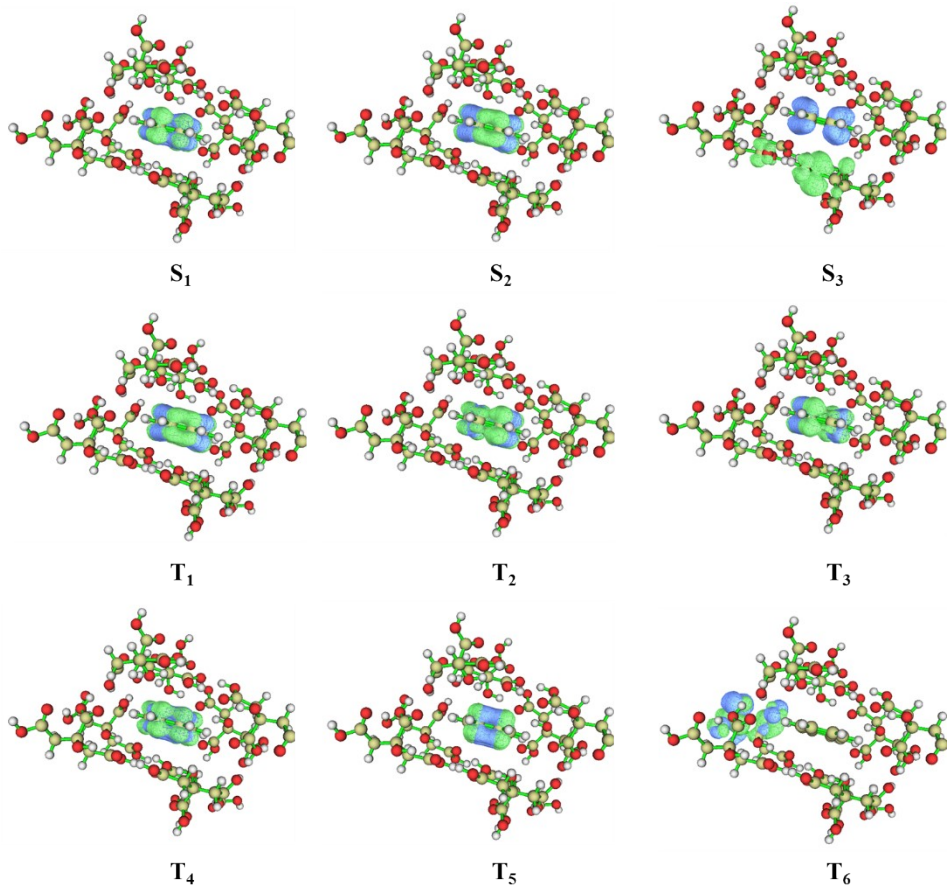


Figure S15. The hole-electron distribution of NP@8CA cluster upon excitation. Green and blue represents electron and hole distributions, respectively. The isosurface value is 0.002.

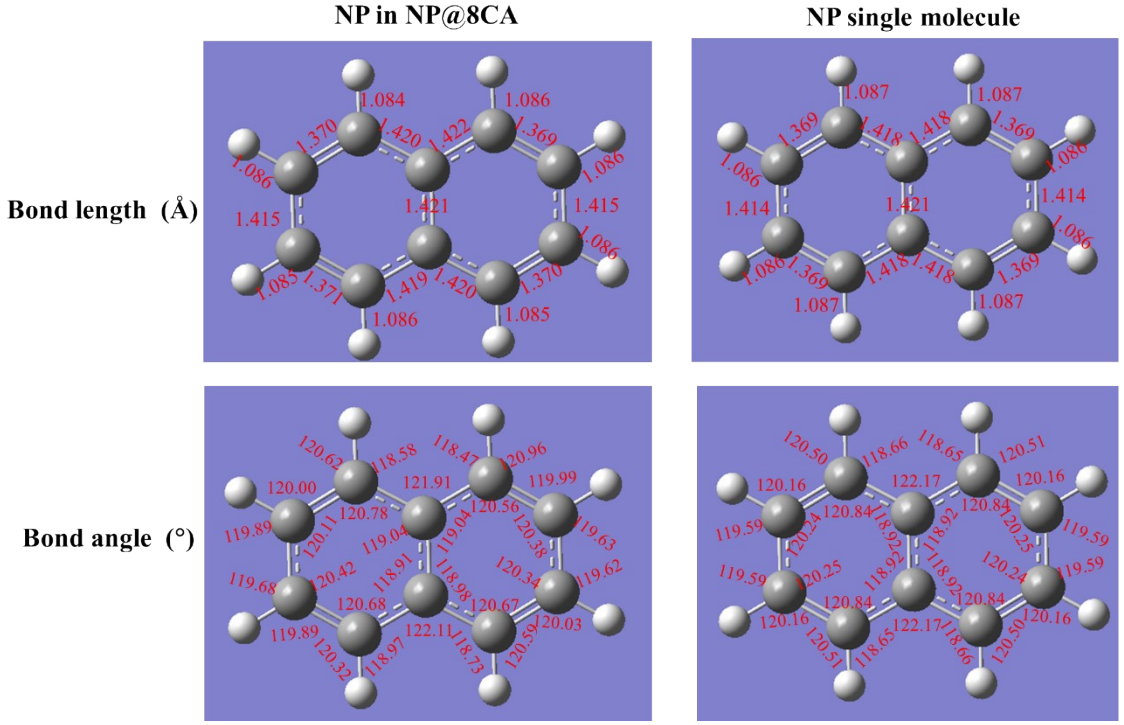


Figure S16. The distribution of bond lengths and bond angles.

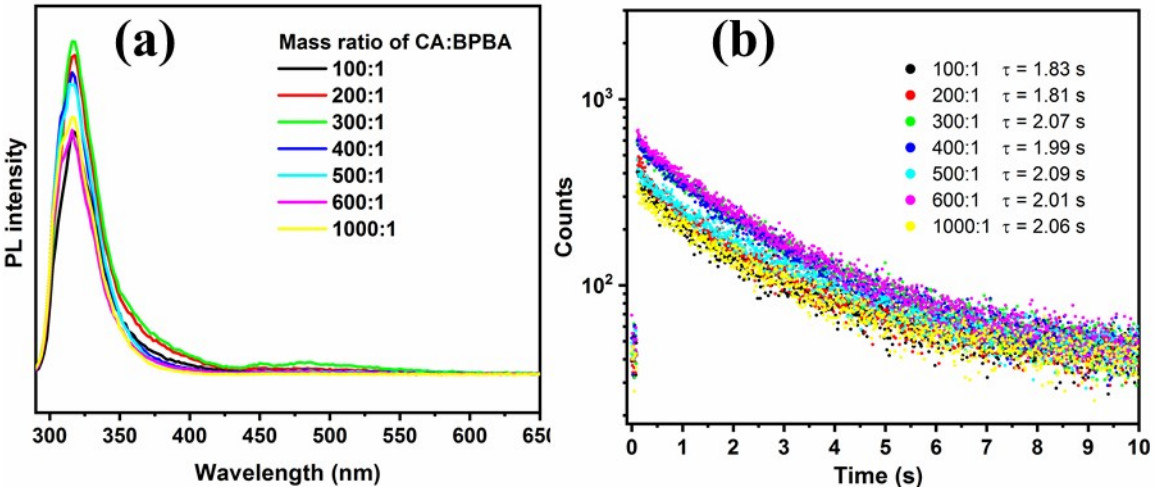


Figure S17. The changes of steady-state spectrum (a) and RTP lifetime (b) with the mass ratio of CA to BPBA. λ_{ex} = 270 nm, λ_{em} = 485 nm.

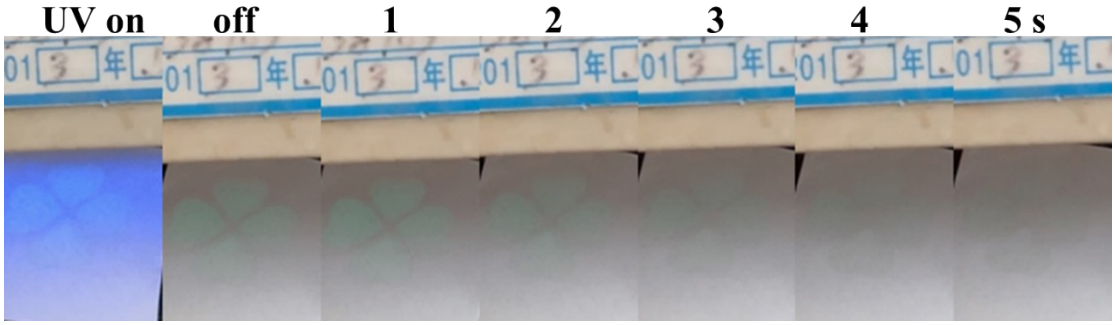


Figure S18. The afterglow of a four-leaf clover pattern observed under natural light condition. The four-leaf clover was painted by PABA@CA methanol solution.

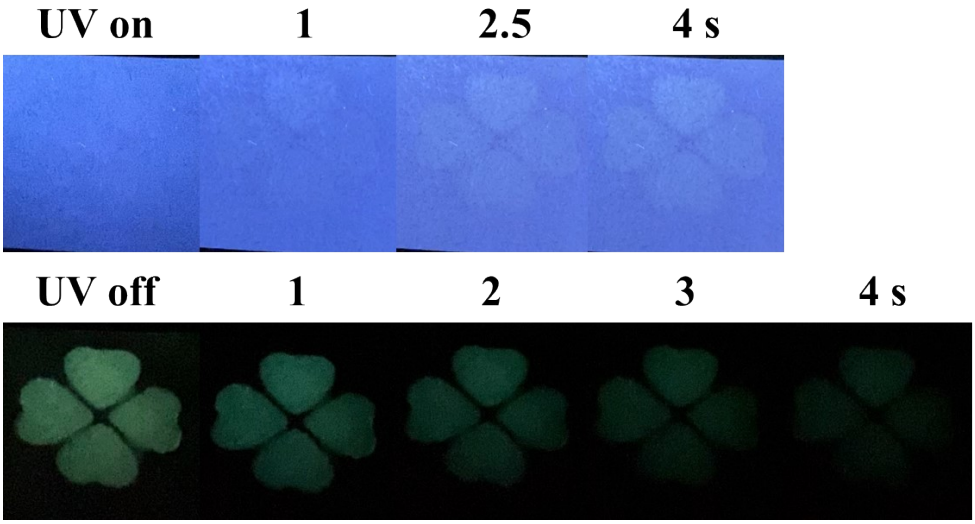


Figure S19. The photographs of the four-leaf clover pattern under 254 nm irradiation on and off after it is stored in natural condition for about 230 days.

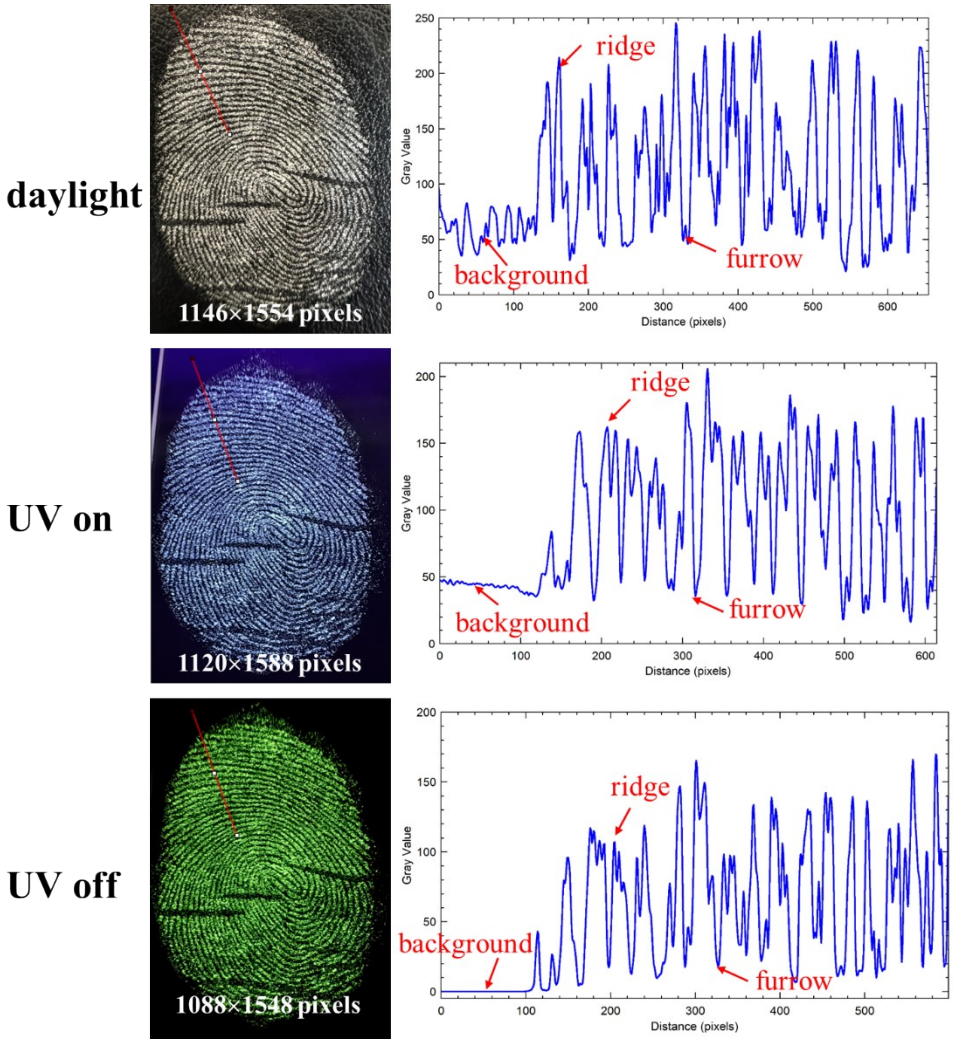


Figure S20. The change of gray value (right) for background, ridge and furrow across the red line (left) in the latent fingerprint images. The resolution is also present.

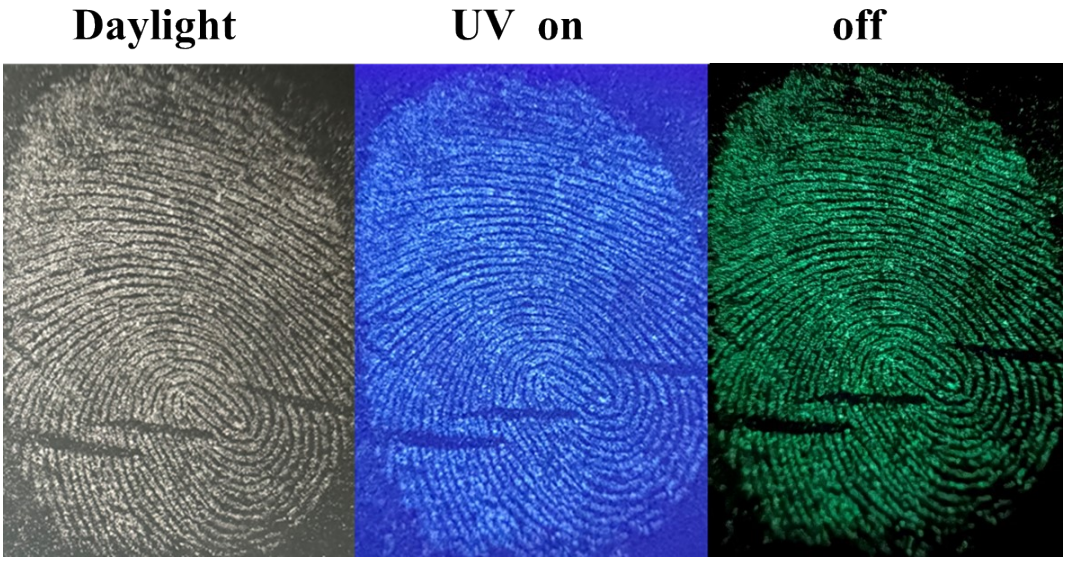


Figure S21. The latent fingerprint images developed by PABA@CA powder on plastic surface under daylight and 254 nm UV light on/off.

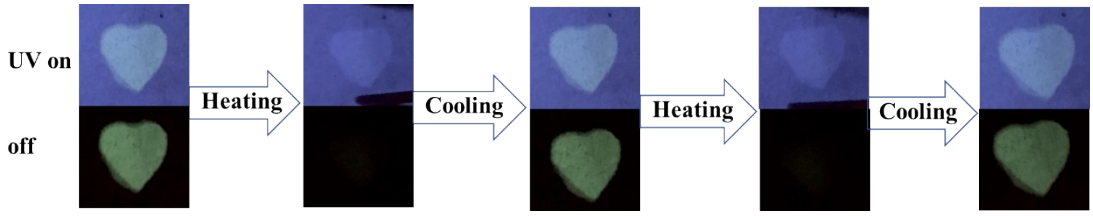


Figure S22. The successive luminescence change of a heart pattern made from PABA@CA methanol solution upon heating and cooling under 254 nm UV light on and off. The pattern was heated by a hairdryer.

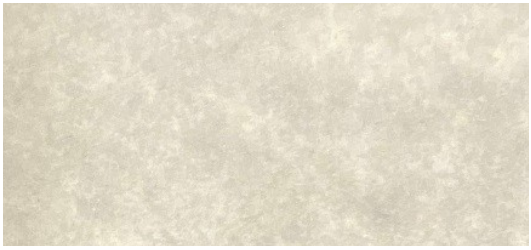


Figure S23. Photographs of "116" message on PABA@CA paper under natural light.

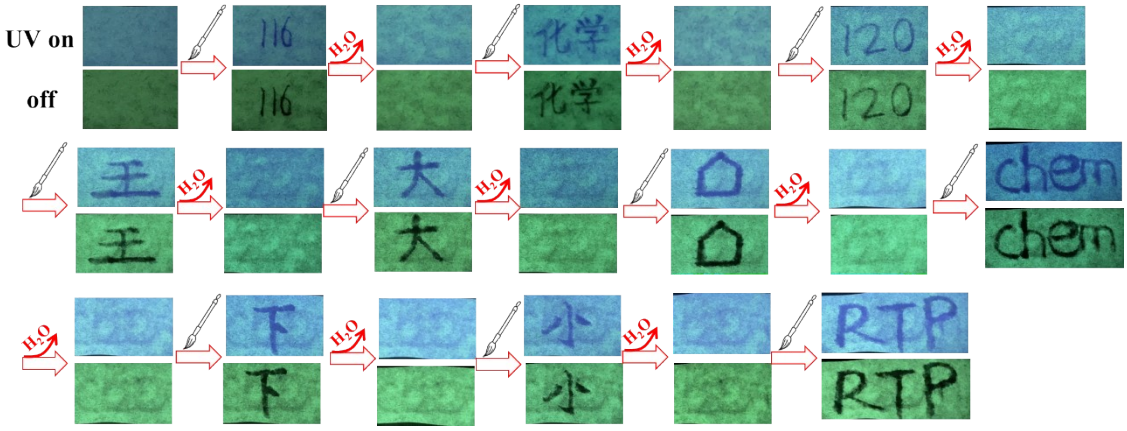


Figure S24. Ten-time recycling illustration of the luminescent paper made from PABA@CA. Water was used as the ink to write the information.

Table S5. Atom coordinates of NP molecule directly from crystal structure

C	-0.82500000	0.11200000	2.36300000
C	-1.29100000	-1.12200000	1.84700000
C	-0.09000000	0.95300000	1.59900000
C	-0.98600000	-1.48300000	0.57000000
C	0.22400000	0.61500000	0.25500000
C	-0.22400000	-0.61500000	-0.25500000
C	0.98600000	1.48300000	-0.57000000
C	0.09000000	-0.95300000	-1.59900000
C	1.29100000	1.12200000	-1.84700000

C	0.82500000	-0.11200000	-2.36300000
H	-1.05752398	0.38318150	3.37160953
H	-1.88208515	-1.76985083	2.46003152
H	0.25688042	1.87824410	2.00948426
H	-1.32183693	-2.42405024	0.18719719
H	1.32183693	2.42405024	-0.18719719
H	-0.25688042	-1.87824410	-2.00948426
H	1.88208515	1.76985083	-2.46003152
H	1.05752398	-0.38318150	-3.37160953

Table S6. Atom coordinates of BPBA molecule directly from crystal structure

O	12.42600000	1.40700000	3.52600000
H	11.60900000	1.53400000	3.66900000
O	12.35500000	3.72600000	3.80600000
H	12.81300000	4.40500000	3.62000000
B	13.07800000	2.59900000	3.52900000
C	14.61700000	2.63100000	3.26800000
C	15.26000000	1.61800000	2.55100000
H	14.74100000	0.90600000	2.19400000
C	16.62600000	1.62000000	2.34500000
H	17.02000000	0.92400000	1.83300000
C	17.43500000	2.62400000	2.87600000
C	16.79900000	3.63600000	3.59900000
H	17.32100000	4.33600000	3.97400000
C	15.43000000	3.64000000	3.78000000
H	15.03200000	4.35200000	4.26800000
C	18.91500000	2.61500000	2.68500000
C	19.54300000	1.63300000	1.92300000
H	19.01500000	0.96200000	1.50600000
C	20.92000000	1.61100000	1.75600000
H	21.32200000	0.93200000	1.22800000
C	21.70900000	2.57000000	2.35500000
H	22.65400000	2.55200000	2.25000000
C	21.10700000	3.56100000	3.10900000
H	21.64000000	4.23200000	3.51700000
C	19.73200000	3.58300000	3.27500000
H	19.33700000	4.26900000	3.79900000

Table S7. Atom coordinates of CA molecule directly from crystal structure

C	-0.51500000	-3.05500000	4.27000000
C	0.71900000	-3.15400000	3.42800000
C	1.00000000	-4.53300000	2.79200000
C	2.36100000	-4.45900000	2.09100000
C	2.82900000	-5.81300000	1.61900000
C	-0.11100000	-4.88100000	1.79000000
H	0.69700000	-2.43800000	2.73800000
H	1.41600000	-2.93800000	4.00500000
H	2.33400000	-3.87300000	1.29700000
H	3.02700000	-4.09700000	2.71100000
H	-1.67900000	-1.77200000	5.25600000
H	4.24800000	-6.88900000	1.75400000
H	-0.77000000	-4.32500000	0.14400000
H	0.32200000	-5.80400000	3.91100000
O	-0.80000000	-1.84800000	4.65100000
O	-1.19200000	-4.04500000	4.57600000
O	4.05600000	-6.05600000	2.00800000
O	2.18000000	-6.59600000	0.96500000
O	-0.09500000	-4.09900000	0.73100000
O	-0.90600000	-5.76300000	1.97300000
O	1.10800000	-5.54900000	3.75900000

Table S8. Atom coordinates of optimized NP molecule

C	-0.82500000	0.11200000	2.36300000
C	-1.29100000	-1.12200000	1.84700000
C	-0.09000000	0.95300000	1.59900000
C	-0.98600000	-1.48300000	0.57000000
C	0.22400000	0.61500000	0.25500000
C	-0.22400000	-0.61500000	-0.25500000
C	0.98600000	1.48300000	-0.57000000
C	0.09000000	-0.95300000	-1.59900000
C	1.29100000	1.12200000	-1.84700000
C	0.82500000	-0.11200000	-2.36300000
H	-1.05752398	0.38318150	3.37160953
H	-1.88208515	-1.76985083	2.46003152
H	0.25688042	1.87824410	2.00948426
H	-1.32183693	-2.42405024	0.18719719
H	1.32183693	2.42405024	-0.18719719
H	-0.25688042	-1.87824410	-2.00948426
H	1.88208515	1.76985083	-2.46003152
H	1.05752398	-0.38318150	-3.37160953

Table S9. Atom coordinates of NP@8CA molecules

C	3.41125100	-2.61822700	-2.75973600
C	4.74729900	-3.24510500	-2.44055200
C	5.97420300	-2.44240600	-2.93908900
C	7.22020100	-3.31501800	-2.80821500
C	8.48208700	-2.55292100	-3.12735600
C	6.05797600	-1.16367900	-2.09163800
H	4.80006300	-3.44210100	-1.36706300
H	4.74959400	-4.21510900	-2.95335300
H	7.31017900	-3.73263300	-1.80087800
H	7.12651100	-4.15457300	-3.50050000
H	1.56202000	-2.65719600	-2.27583100
H	10.22828400	-2.79979100	-3.74464700
H	6.28780000	-0.60820700	-0.28332600
H	5.06756600	-1.58744500	-4.40066500
O	2.44595600	-3.01517500	-1.96067400
O	3.23050400	-1.85514200	-3.70495300
O	9.44976100	-3.36437800	-3.58943600
O	8.64645200	-1.36924000	-2.96608400
O	6.51494400	-1.38591700	-0.85044900
O	5.63818100	-0.09480500	-2.46140400
O	5.87580200	-2.12091700	-4.29609700
C	1.26750500	-4.24091700	2.02350900
C	2.67194700	-4.60095400	2.43378400
C	3.70180400	-3.52357400	2.05948700
C	5.11482500	-4.00796400	2.45253600
C	6.12556400	-3.06547300	1.84707100
C	3.41164200	-2.20710900	2.80745900
H	2.68408100	-4.82032400	3.50206300
H	2.93257900	-5.52281800	1.90145100
H	5.22102800	-4.01257600	3.53931100
H	5.26240100	-5.01644900	2.06260200
H	-0.56670100	-4.68657100	2.27988300
H	7.15776600	-2.82805900	0.31303100
H	2.94828200	-1.57014700	4.54226600
H	2.84990100	-3.04530500	0.37821200
O	0.34495600	-4.93878600	2.62654200
O	1.03740700	-3.38411700	1.16926000
O	6.75839000	-3.58436500	0.79165700
O	6.31107700	-1.93539600	2.23999500
O	3.07172100	-2.42878200	4.07145500
O	3.50154700	-1.10485600	2.31412300
O	3.74196600	-3.30337700	0.67765500
C	-2.80747300	4.30319200	0.26242500

C	-4.18837900	4.56103700	-0.28848200
C	-4.30300300	4.51894100	-1.82961100
C	-5.58853600	5.23746800	-2.24349100
C	-5.83483600	5.16269200	-3.72995900
C	-4.30977000	3.06135700	-2.32097300
H	-4.86546100	3.85094700	0.19659400
H	-4.47971900	5.55764800	0.06008100
H	-6.45573400	4.80368000	-1.73561800
H	-5.51371400	6.28427400	-1.94288200
H	-1.86365400	4.14817900	1.91127300
H	-6.60670000	6.11589200	-5.13943900
H	-5.34387300	1.46515600	-2.32880500
H	-2.43654000	4.74447700	-2.21243300
O	-2.76611700	4.42139500	1.56590800
O	-1.82951800	4.02500700	-0.42866900
O	-6.46434000	6.25896300	-4.18634300
O	-5.54874000	4.23144900	-4.44087500
O	-5.44902200	2.40343000	-2.02897200
O	-3.38301500	2.52645900	-2.87294400
O	-3.25688400	5.21755000	-2.44260300
C	-2.80725500	1.37651900	4.28854500
C	-4.29842800	1.24393400	4.08369200
C	-4.66737200	0.85038300	2.64206400
C	-6.18109200	1.02964200	2.41266600
C	-6.43109800	0.98046100	0.92834700
C	-4.26962100	-0.61155300	2.37854700
H	-4.69422900	0.52405100	4.80689700
H	-4.74281500	2.21558900	4.32063600
H	-6.73142900	0.23238200	2.91301700
H	-6.49466100	2.00082600	2.79797500
H	-1.52148600	2.03605500	5.52169900
H	-6.55681500	2.16715100	-0.55716200
H	-4.77507900	-2.40238800	2.81750000
H	-3.08096300	1.44823800	1.75225300
O	-2.49212700	1.81435900	5.48611600
O	-1.98925700	1.11685800	3.41703500
O	-6.68536700	2.17952000	0.41643200
O	-6.36899000	-0.04173900	0.26795000
O	-4.99749500	-1.46410700	3.08675300
O	-3.38140700	-0.92289300	1.61945900
O	-4.02649200	1.68258900	1.70950400
C	-0.13061800	-1.51511100	-3.87489800
C	-1.50107500	-1.06681200	-4.31036000
C	-2.65632000	-1.69028300	-3.50605500

C	-3.97733400	-1.01402500	-3.92421500
C	-5.03764500	-1.36084400	-2.90623800
C	-2.72207200	-3.20075500	-3.77285000
H	-1.60813500	-1.25846500	-5.38137700
H	-1.52551700	0.01884000	-4.17184600
H	-4.28983900	-1.35691900	-4.91297300
H	-3.82430500	0.06650900	-3.94298500
H	1.71601700	-1.29936900	-4.28104500
H	-6.03224700	-0.49042900	-1.47014800
H	-2.95667700	-4.43605500	-5.15984000
H	-1.77025300	-1.93749500	-1.78106200
O	0.82185800	-1.05204000	-4.64591400
O	0.06331400	-2.23040600	-2.89470200
O	-5.52481600	-0.26870900	-2.28726000
O	-5.40914100	-2.47847400	-2.64703000
O	-2.92513900	-3.46604300	-5.07918300
O	-2.57817100	-4.06761900	-2.95120400
O	-2.53365700	-1.44611100	-2.13759500
C	-2.29243500	-3.68177200	0.65547800
C	-3.66347900	-3.56086900	0.06086500
C	-4.77352700	-4.25082800	0.87518600
C	-6.12682000	-3.71625900	0.41750000
C	-7.28671900	-4.47408300	1.00577100
C	-4.65142700	-5.76849500	0.70343400
H	-3.62533900	-3.94696000	-0.96175800
H	-3.86631200	-2.49223200	-0.03018300
H	-6.19714000	-3.76036300	-0.67409500
H	-6.20897900	-2.65942800	0.68724400
H	-0.48192300	-3.12826900	0.41760200
H	-9.11232100	-4.31650300	1.36017400
H	-4.89864400	-7.12896000	-0.55145300
H	-3.86958000	-4.46177500	2.56747000
O	-1.36763600	-3.05061800	-0.03158000
O	-2.04289000	-4.31458000	1.68286200
O	-8.41458700	-3.73980400	1.00065300
O	-7.25747400	-5.60973300	1.41321700
O	-5.02448600	-6.16411200	-0.52341000
O	-4.18894800	-6.50645500	1.53338000
O	-4.66312700	-3.97842300	2.26580000
C	3.69158300	5.07736100	-2.08767600
C	4.84571900	4.19620700	-1.69196500
C	4.67028200	3.59841600	-0.28428500
C	5.77912500	2.55642200	-0.04721500
C	5.44069700	1.71745600	1.16298200

C	4.73957800	4.70257900	0.77963400
H	5.77441800	4.76854500	-1.77489300
H	4.90079600	3.37773600	-2.41523600
H	6.73804600	3.05493600	0.11633200
H	5.85429900	1.91261800	-0.92569100
H	2.99845500	6.03189500	-3.53472000
H	5.06623800	-0.12792200	1.62111700
H	5.86630100	6.05393300	1.41709700
H	2.71668500	3.52819800	-0.20354200
O	3.79503600	5.50012400	-3.35632000
O	2.76598600	5.38535200	-1.37225100
O	5.39125400	0.40661900	0.86192100
O	5.23083300	2.14734500	2.26983400
O	5.89979000	5.38692200	0.70830400
O	3.88115300	4.96733500	1.57895500
O	3.46488400	2.90325300	-0.17581800
C	0.55002300	3.25982500	1.88386500
C	1.77151200	2.67948500	2.52827400
C	1.52127800	2.08749000	3.92262500
C	2.88277300	1.63929000	4.48928100
C	2.69916100	1.01398900	5.84256800
C	0.90218000	3.12405000	4.86880000
H	2.53209300	3.46641800	2.55113900
H	2.16404700	1.89476800	1.87899900
H	3.55239500	2.49522900	4.58922000
H	3.32365200	0.93257700	3.78713200
H	-0.19088200	3.75109600	0.19472400
H	2.79629900	-0.62398100	6.77125400
H	1.17335700	4.83582700	5.56105900
H	-0.19357900	1.14079300	3.64747600
O	0.67923900	3.47656500	0.59254800
O	-0.47011000	3.52577700	2.51525100
O	2.96571900	-0.32240700	5.85982700
O	2.35965200	1.58568900	6.84526600
O	1.61458300	4.24984700	4.92004300
O	-0.09833800	2.97288200	5.53625500
O	0.73232800	0.93293100	3.89616800
C	-0.45801000	0.25256300	-0.01777700
C	-0.78263000	0.99667600	-1.12121300
C	0.21528600	1.39159400	-2.05057200
C	1.55719300	0.97249600	-1.84183400
C	1.86666200	0.21401400	-0.68277400
C	0.88606200	-0.12689600	0.21240800
H	-1.11356600	2.52373400	-3.32528600

H	-1.23483800	-0.06109100	0.67335700
H	-1.81094300	1.28145600	-1.31209200
C	-0.08968300	2.19016000	-3.18687900
C	2.54748800	1.33742800	-2.79173100
H	2.89986800	-0.06413400	-0.49653500
H	1.14177100	-0.68016300	1.10962800
C	2.22123700	2.09525100	-3.88532900
C	0.88986800	2.53282200	-4.08037900
H	3.56629300	0.99549600	-2.64071900
H	2.98591200	2.36289800	-4.60914400
H	0.64543200	3.13896700	-4.94814500

References

[1] G. Guo, H. Li, Y. Yan, W. Zhao, Z. Gao, H. Cao, X. Yan, H. Li, G. Xie, R. Chen, Y. Tao, W. Huang, *Adv. Mater.*, **2024**, *36*, 2412100.

[2] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09*, Revision A.02; Gaussian, Inc.: Wallingford, CT, **2009**.

[3] T. Lu, F. Chen, *J. Comput. Chem.*, **2012**, *33*, 580.

[4] Z. Liu, T. Lu, Q. Chen, *Carbon*, **2020**, *165*, 461.

[5] F. Neese, F. Wennmohs, U. Becker, C. Riplinger, *J. Chem. Phys.*, **2020**, *152*, 224108.

[6] X. Bi, Y. Shi, T. Peng, S. Yue, F. Wang, L. Zheng, Q.-E. Cao, *Adv. Funct. Mater.*, **2021**, *31*, 2101312.