Electronic Supplementary Information for

Tuning the Fluorescence Emission of DADQ Based Molecular Solids by Dielectric Environment Variation

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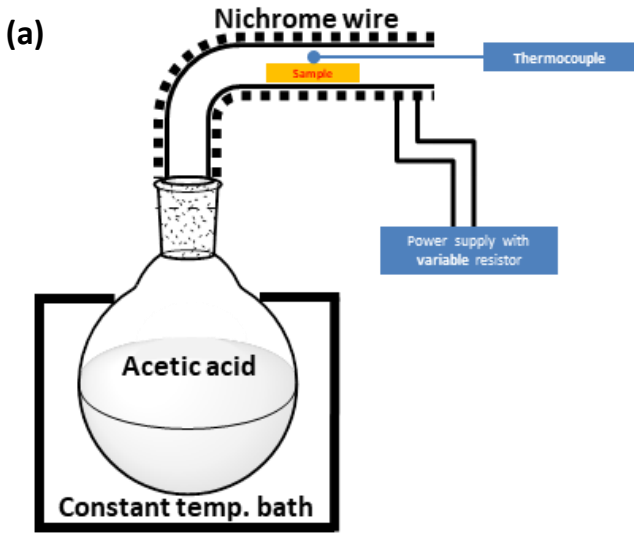
Figure S1. **(a)** Schematic diagram of the setup used for exposing the DADQ samples to acid vapors at a controlled temperature. **(b)** The structure and **(c)** optical images (under UV light) of the DADQs upon exposure to acetic acid vapor for different time periods (min) showing the fluorescence changes and the corresponding fluorescence emission spectra [BFPDQ (λ_{exc} = 380 nm), BMPDQ (λ_{exc} = 395 nm), BNMPDQ (λ_{exc} = 400 nm), BPPDQ (λ_{exc} = 400 nm), and BBADQ (λ_{exc} = 395 nm)].



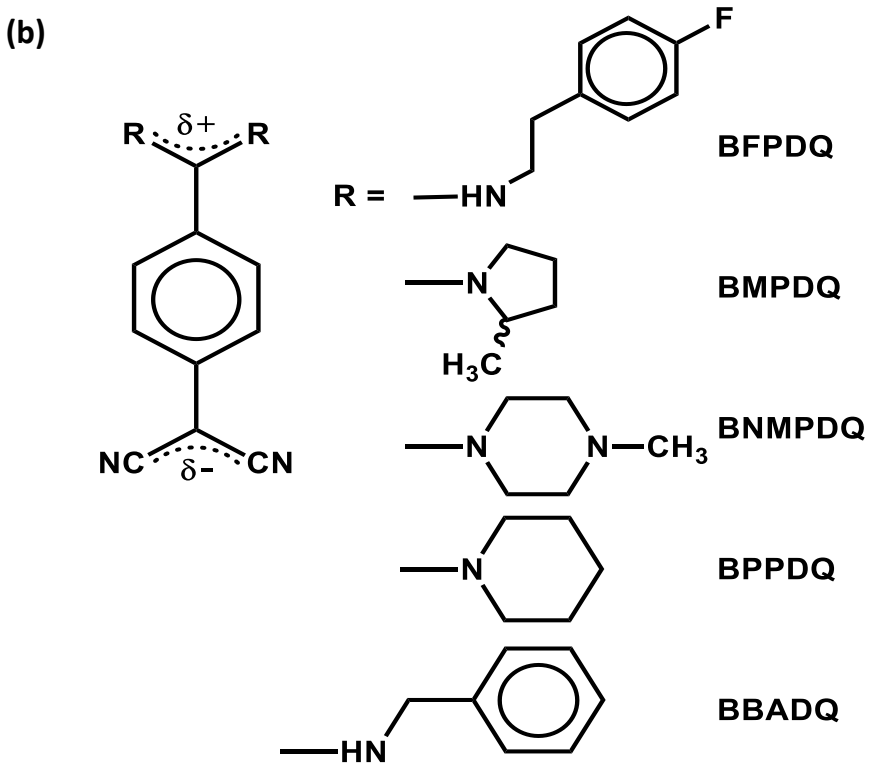
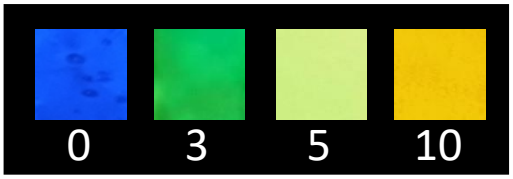
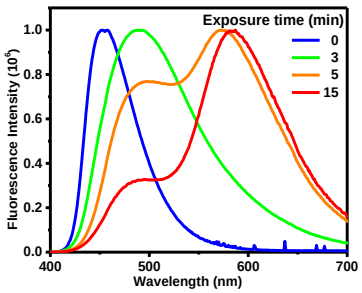
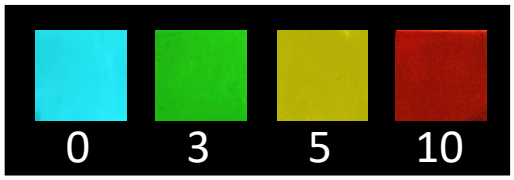
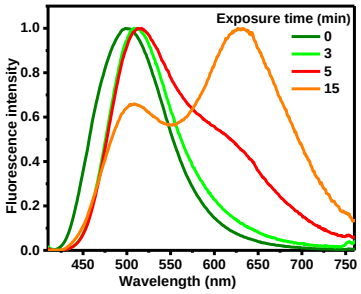
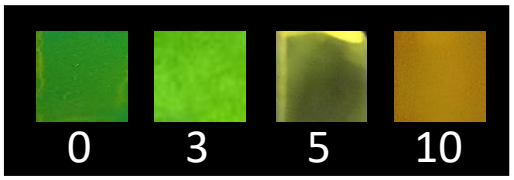
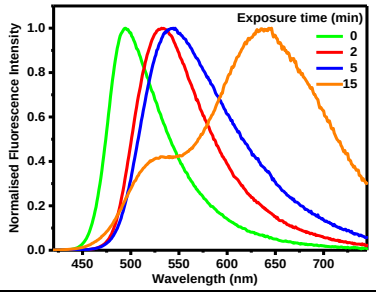
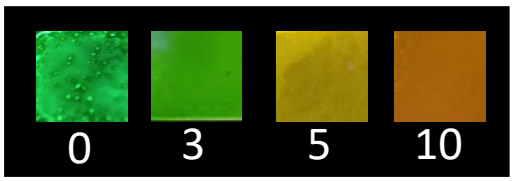
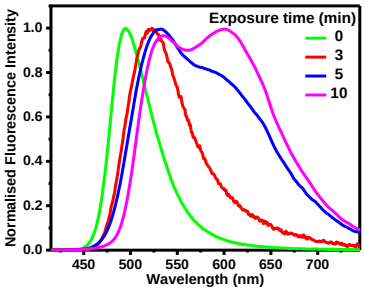
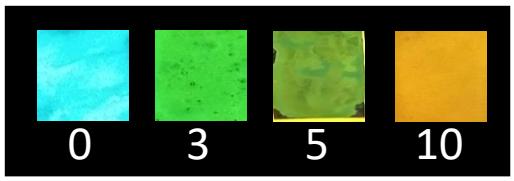
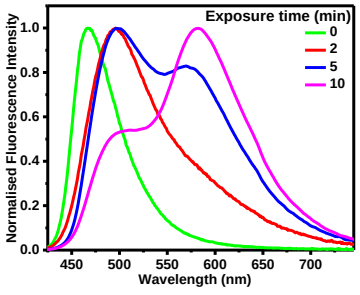


Figure 1 (contd…)

Figure 1(c)

	Optical images of the sample under UV (365 nm) light	Fluorescence spectra
BFPDQ		
BMPDQ		
BNMPDQ		
BPPDQ		
BBADQ		

Crystallographic details

Table S1. Crystallographic data of BFPDQ and BMPDQ.

	BFPDQ	**BFPDQ-Ac***	**BMPDQ**
Empirical Formula	$C_{26}H_{22}N_4F_2$	$C_{26}H_{22}N_4F_2$	$C_{20}H_{24}N_4$
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	C2/c
a /Å	9.555(3)	9.5002(4)	13.2460 (12)
b / Å	15.114(5)	15.0682(8)	11.8421 (9)
c / Å	15.708(5)	15.6698(8)	11.3670 (12)
β / º	102.466(11)	102.424(5)	97.842 (9)
V / $Å^3$	2215.0(12)	2190.62(19)	1766.4 (3)
Z	4	4	4
ρ_{calc} (g cm^{-3})	1.285	1.299	1.205
μ (mm^{-1})	0.089	0.090	0.073
Temperature (K)	293	293	100
λ (Å)	0.71073	0.71073	0.71073
No. of reflections	5430	4651	1532
No. of parameters	289	289	113
Max., Min. transmission	0.990, 0.981	0.991, 0.986	0.990, 0.985
GOF	1.0332	1.1132	0.969
R [for $I \geq \sigma_1$]	0.0554	0.0583	0.0684
wR^2	0.1555	0.1977	0.2204
Largest difference peak and hole /e $Å^{-3}$	0.37/-0.32	0.32/-0.35	0.35/-0.38
CCDC deposition number	2350446	2350467	2350461

*BFPDQ treated with acetic acid and recrystallized

Figure S2. Molecular structure of **(a)** BFPDQ **(b)** BFPDQ treated with acetic acid, and **(c)** BMPDQ from single crystal X-ray diffraction analysis. C (grey), N (blue), F (green) and H (white) atoms are shown with 90% thermal ellipsoids.

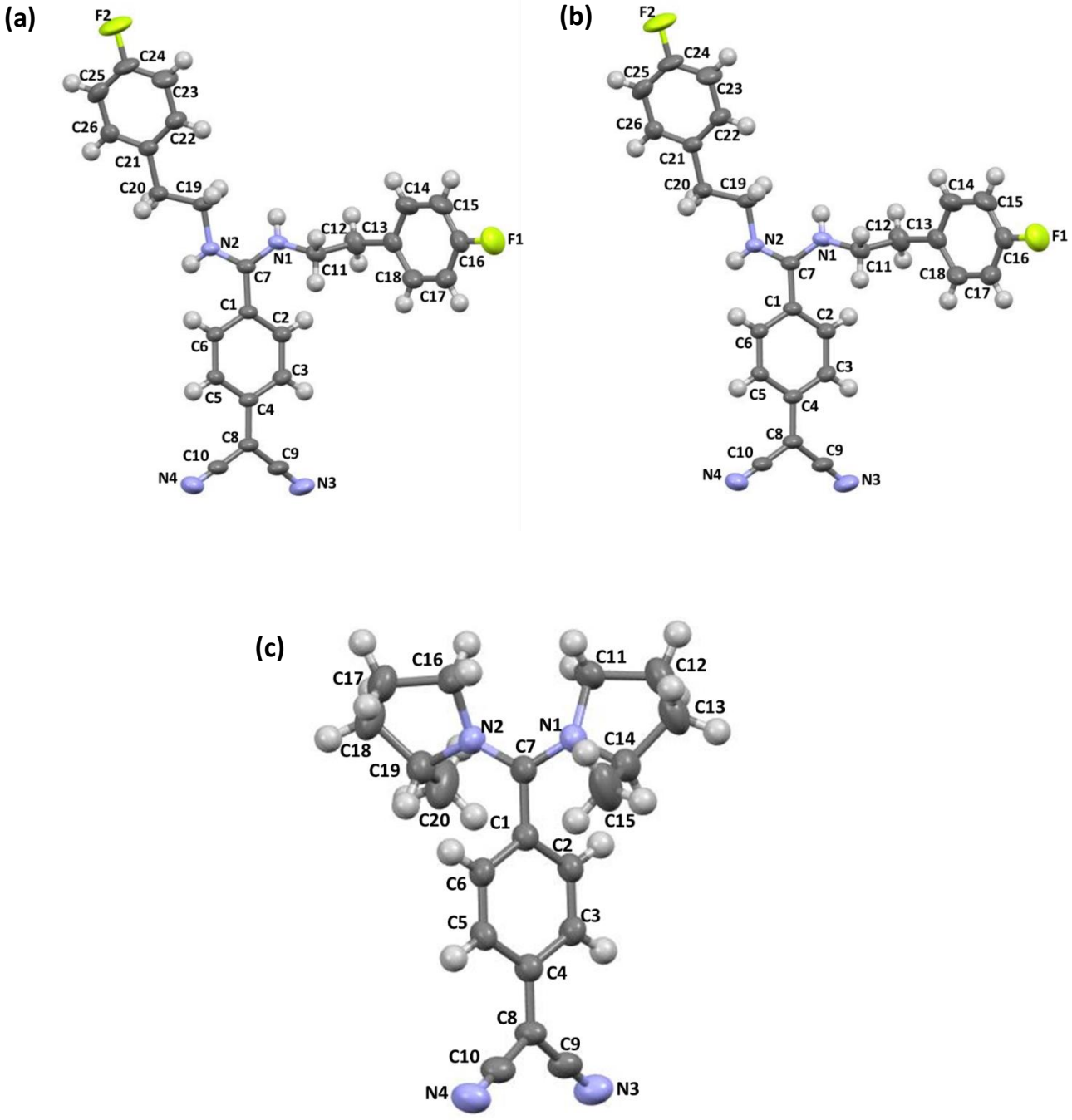


Table S2. Bond lengths, bond angles and relevant torsion angles in BFPDQ (Figure S2a).

Atoms	Bond Length (Å)
F2-C24	1.359 (3)
F1-C16	1.368 (3)
N1-C11	1.469 (3)
N1-C7	1.322 (3)
N2-C7	1.323 (3)
N2-C19	1.462 (3)
C2-C1	1.397 (3)
C2-C3	1.392 (3)
N3-C9	1.161 (2)
N4-C10	1.155 (4)
C16-C17	1.364(5)
C16-C15	1.364 (5)
C17-C18	1.390 (4)
C18-C13	1.384 (4)
C13-C12	1.522 (3)
C13-C14	1.391 (4)
C12-C11	1.497 (4)
C7-C1	1.464 (3)
C19-C20	1.546 (4)
C20-C21	1.513 (4)
C21-C26	1.403 (4)
C21-C22	1.395 (4)
C26-C25	1.380 (5)
C25-C24	1.371 (4)
C24-C23	1.386 (5)
C1-C6	1.410 (3)
C3-C4	1.413 (3)
C4-C5	1.422 (4)
C4-C8	1.446 (3)
C5-C6	1.377 (3)
C8-C9	1.407 (4)
C8-C10	1.400 (4)
C23-C22	1.375 (5)
C14-C15	1.392 (4)

Atoms	Torsion angle (^{o})
N2-C7-C1-C6	43.714 (2)
N1-C7-C1-C2	40.471 (5)
C3-C4-C8-C9	8.386 (2)
C5-C4-C8-C10	9.571 (2)

Atoms	Bond Angle (°)
C7-N1-C11	122.88 (19)
H1-N1-C11	118.56 (12)
H1-N1-C7	118.56 (12)
C19-N2-C7	128.4 (2)
H2-N2-C7	115.81 (13)
H2-N2-C19	115.81 (12)
C3-C2-C1	121.5 (2)
C17-C16-F1	118.5 (3)
C15-C16-F1	118.0 (3)
C15-C16-C17	123.4 (3)
C18-C17-C16	118.2 (3)
C13-C18-C17	120.9 (3)
C12-C13-C18	117.7 (2)
C14-C13-C18	118.6 (2)
C14-C13-C12	123.6 (2)
C11-C12-C13	113.6 (2)
C12-C11-N1	111.5 (2)
N2-C7-N1	118.4 (2)
C1-C7-N1	118.58 (19)
C1-C7-N2	123. (2)
C20-C19-N2	111.5 (2)
C21-C20-C19	110.3 (2)
C26-C21-C20	121.6 (3)
C22-C21-C20	120.60 (3)
C22-C21-C26	117.7 (3)
C25-C26-C21	121.5 (3)
C24-C25-C26	118.4 (3)
C25-C24-F2	119.1 (3)
C23-C24-F2	118.5 (3)
C23-C24-C25	122.4 (3)
C7-C1-C2	119.2 (2)
C6-C1-C2	118.1 (2)
C6-C1-C7	122.7 (2)
C4-C3-C2	120.6 (2)
C5-C4-C3	117.4 (2)
C8-C4-C3	121.1 (2)
C8-C4-C5	121.6 (2)
C6-C5-C4	121.4 (2)
C5-C6-C1	120.9 (2)
C9-C8-C4	121.0 (2)
C10-C8-C4	122.0 (2)
C10-C8-C9	117.0 (2)
C8-C9-N3	178.5 (3)
C8-C10-N4	178.6 (3)
C22-C23-C24	118.2 (3)
C23-C22-C21	121.7 (3)
C15-C14-C13	121.1 (3)
C14-C15-C16	117.7 (3)

Table S3. Bond lengths, bond angles and relevant torsion angles in BMPDQ (Figure S2c).

Atoms	Bond Length (Å)
N1-C7	1.314 (6)
N2-C7	1.314 (6)
N1-C11	1.508 (7)
N2-C16	1.508 (7)
N1-C14	1.518 (8)
N2-C19	1.518 (8)
C7-C1	1.459(10)
C1-C2	1.418 (7)
C1-C6	1.418 (7)
C2-C3	1.387 (8)
C6-C5	1.387 (8)
C5-C4	1.444 (6)
C4-C3	1.444 (6)
C4-C8	1.420 (10)
C8-C10	1.409 (8)
C8-C9	1.409 (8)
C11-C12	1.532 (9)
C12-C13	1.544 (10)
C13-C14	1.561 (9)
C14-C15	1.503 (11)
C16-C17	1.532 (9)
C17-C18	1.544 (10)
C18-C19	1.561 (9)
C19-C20	1.503 (11)
N3-C9	1.182 (8)
N4-C10	1.182 (8)

Atoms	Bond Angle (°)
C11-N1-C7	123.7 (5)
C14-N1-C7	124.1 (5) .
C14-N1-C11	111.3 (5)
N1-C7-N1	120.7 (7)
C1-C7-N1	119.6 (4)
C1-C7-N1	119.6 (4)
C1-C2-C3	121.5 (6)
C3-C4-C3	118.4 (7)
C8-C4-C3	120.8 (3)
C8-C4-C3	120.8 (3)
C4-C3-C2	119.9 (5)
C2-C1-C7	120.7 (4)
C2-C1-C7	120.7 (4)
C2-C1-C2	118.6 (7)
C10-C8-C4	121.9 (4)
C10-C8-C4	121.9 (4)
C10-C8-C10	116.3 (7)
C8-C10-N2	177.6 (6)
C12-C11-N1	102.2 (5)
C13-C14-N1	102.0 (5)
C15-C14-N1	111.2 (6)
C15-C14-C13	114.0 (6)
C13-C12-C11	102.3 (6)
C12-C13-C14	104.2 (6)

Atoms	Torsion angle (^{o})
N2-C7-C1-C6 N1-C7-C1-C2	56.947 (3)
C5-C4-C8-C10 C3-C4-C8-C9	15.316(3)

Figure S3. Absorption and fluorescence excitation spectra of **(a, b)** BFPDQ and **(c, d)** BMPDQ in acetonitrile solution (BMPDQ: 2.5 μM and BFPDQ: 4.0 μM) and the solid state.

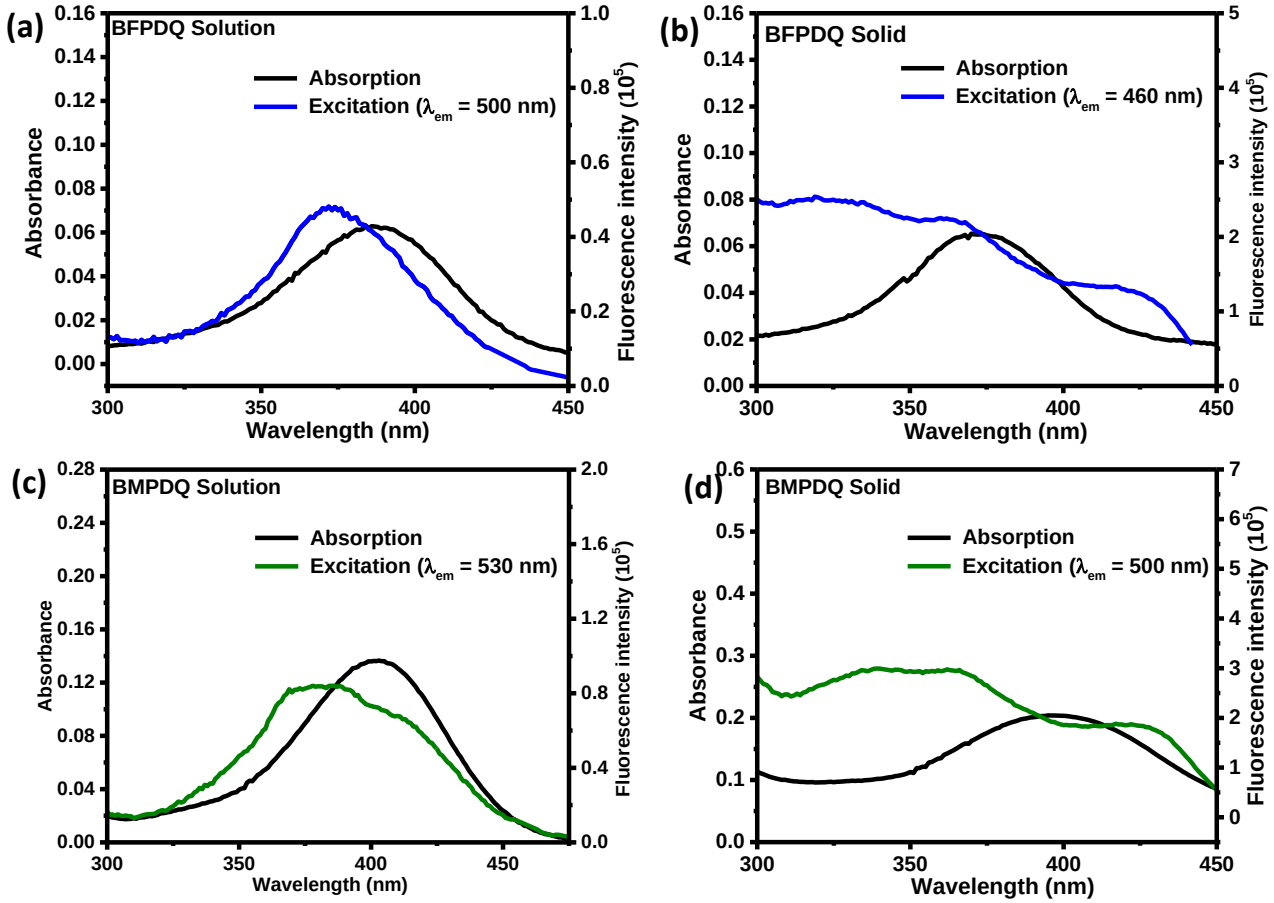


Figure S4. **(a)** Optical images (under UV light) of BFPDQ-PVDF upon exposure to acetic acid vapor for different time periods (min), showing the fluorescence changes and the corresponding fluorescence emission spectra (λ_{exc} = 380 nm). **(b)** Optical images (under UV light) of BMPDQ-PVDF upon exposure to acetic acid vapor showing the fluorescence changes and the corresponding fluorescence emission spectra (λ_{exc} = 395 nm).

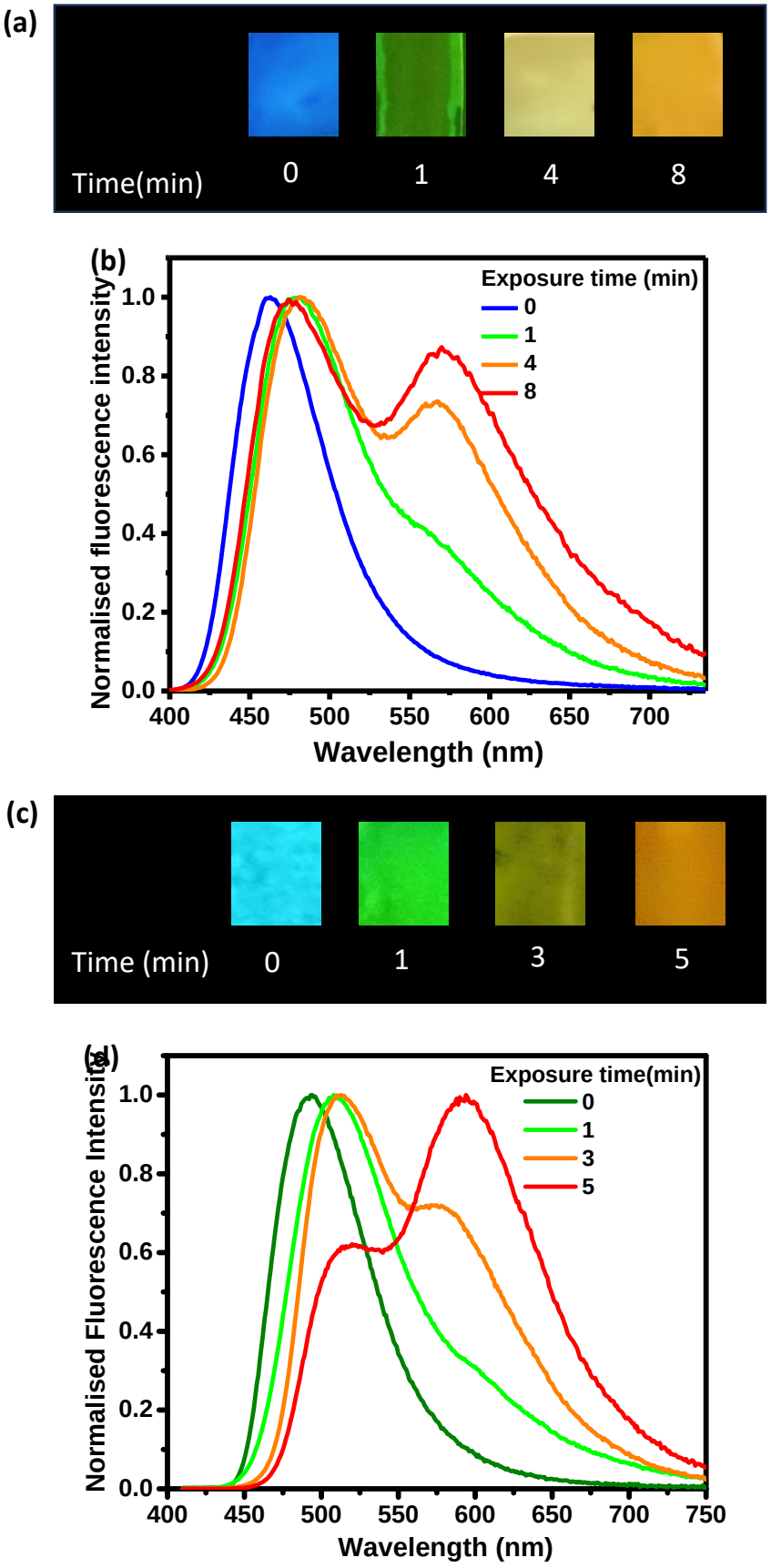


Figure S5. (a) Optical images (under UV light) of BMPDQ upon exposure to different acid vapors for 30 min showing the fluorescence changes and **(b)** the corresponding fluorescence emission spectra (λ_{exc} = 395 nm). A: acetic acid, B: trifluoroacetic acid, C: hydrofluoric acid, D: formic acid.

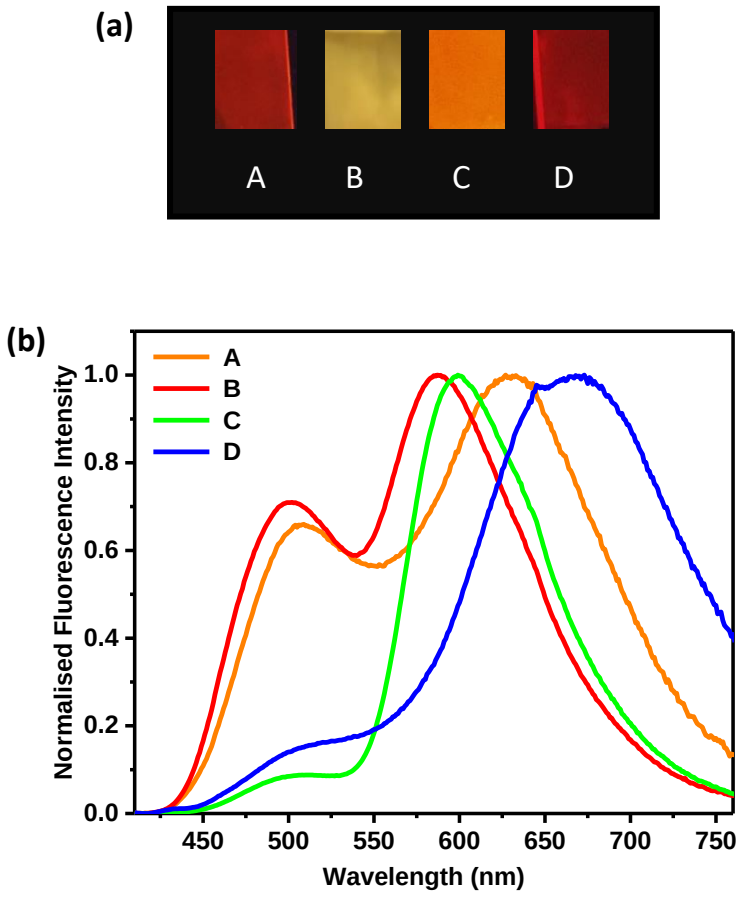


Figure S6. Optical images under ambient (left) and UV (right) light: BFPDQ **(a)** as prepared and **(b)** exposed to acetic acid vapor for 30 min followed by recrystallization in methanol. **(c, d)** Similar images of BMPDQ.

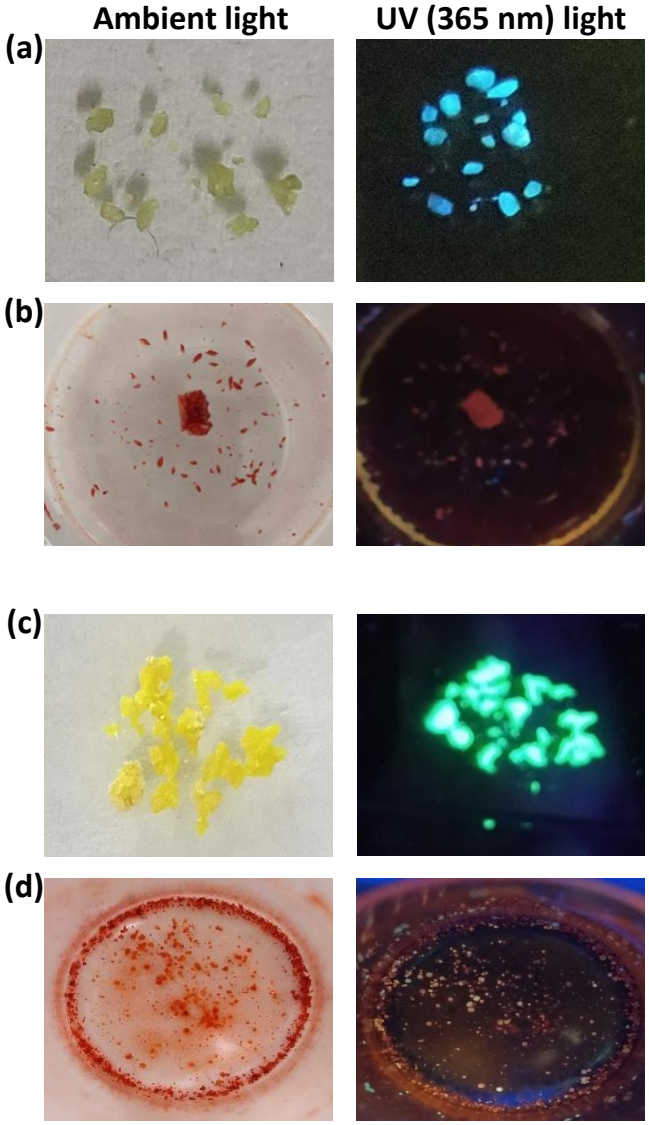


Figure S7. ^{13}C NMR spectra of **(a)** BFPDQ and **(b)** BMPDQ before (purple) and after (green) exposure to acetic acid vapor for 15 min; the new peaks are indicated (broken line box).

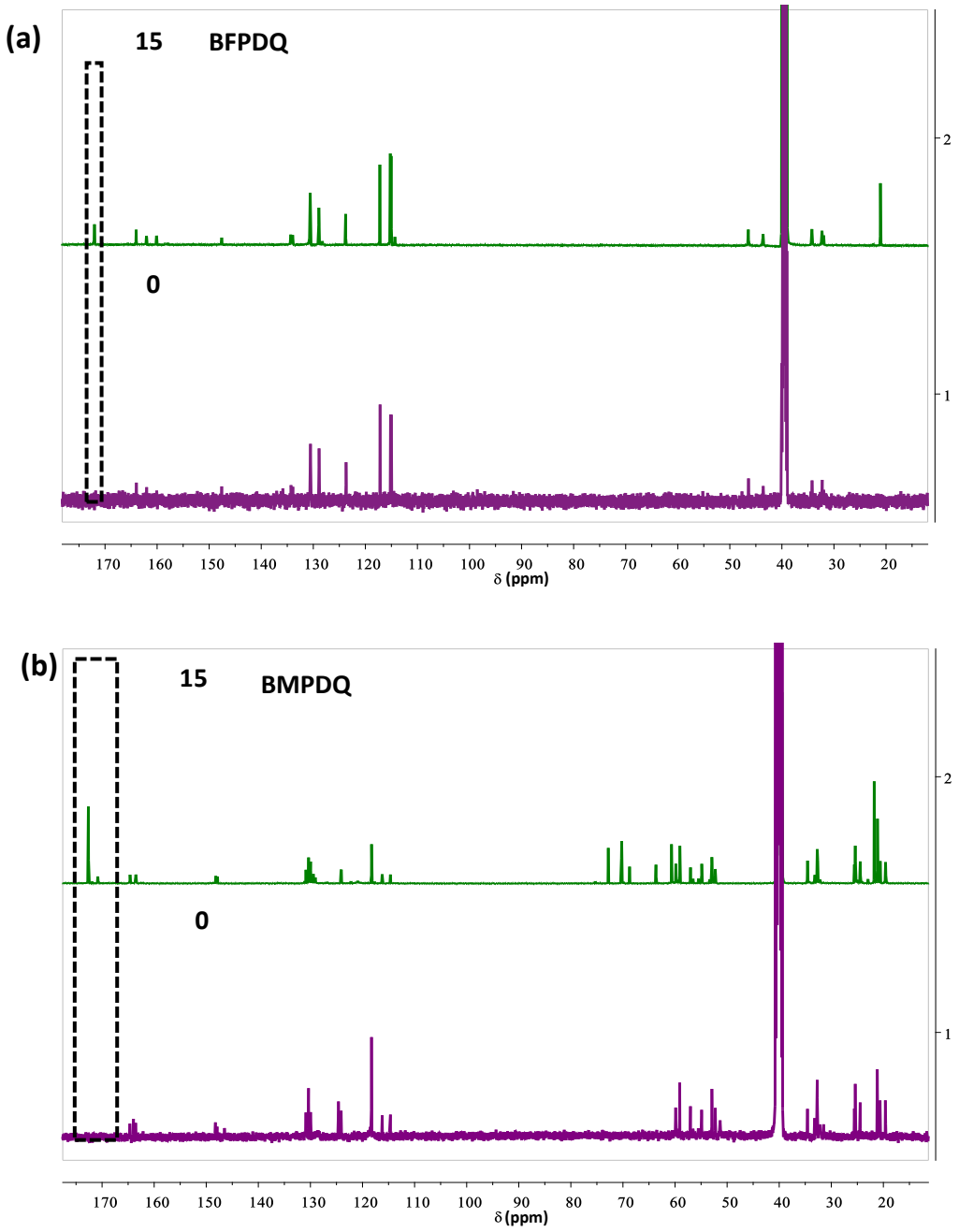


Figure S8. High resolution mass spectra of **(a)** BFPDQ and **(b)** BMPDQ as prepared and exposed to acetic acid vapor for different time periods (min) at 140 °C; ratio of the intensities of the M^+ and $M+H^+$ peaks $\left(\frac{I_{M+H^+}}{I_{M^+}} = x\right)$ are shown in (b). The spectra were recorded on a Bruker Maxis spectrometer, in ESI mode.

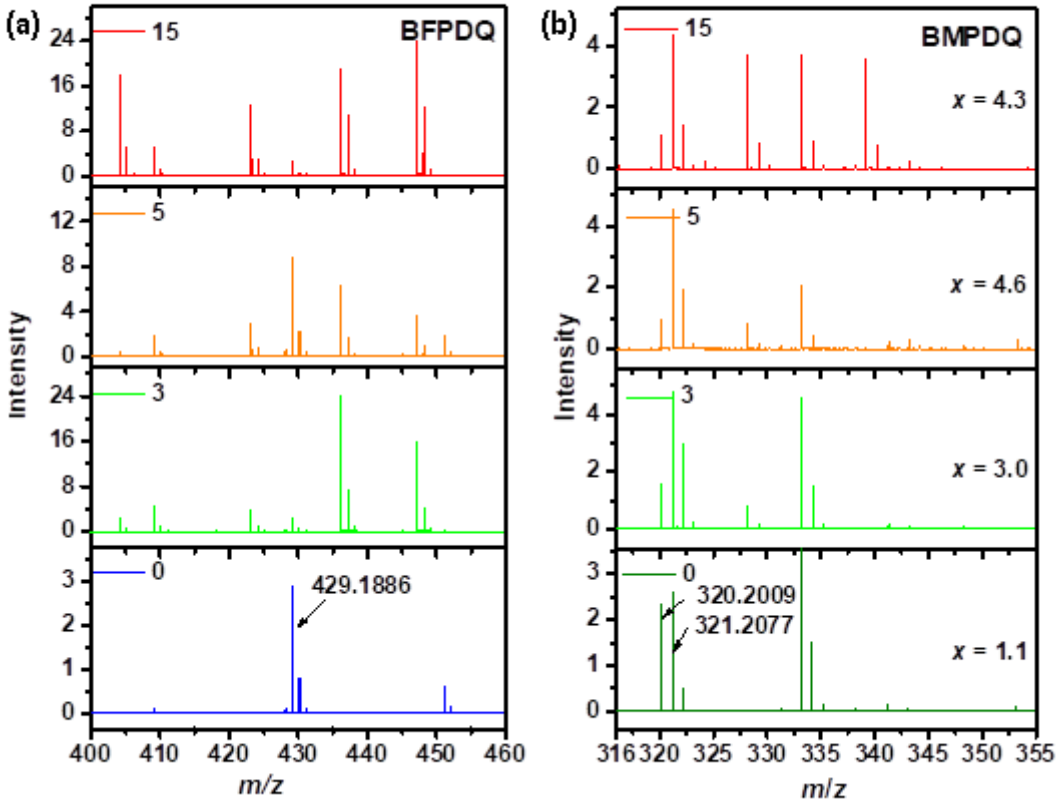


Table S4. Assignment of the prominent peaks in the HRMS of BFPDQ and BMPDQ.

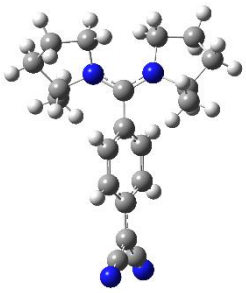
BFPDQ		
m/z	**Formula**	**Assignment**
429.1886	$C_{26}H_{22}N_4F_2 + H^+$	$]M + H]^+$
451.1694	$C_{26}H_{22}N_4F_2 + Na^+$	$[M + Na]^+$
436.1879*	$C_{24}H_{22}N_2F_2\ CH_3COO + H^+$	$[M\ [-\ 2(CN) + CH_3COO] + H^+]^+$
447.2033*	$C_{26}H_{21}N_4F + K^+$	$[M - (H) - (F)] + K^+$
BMPDQ		
m/z	**Formula**	**Assignment**
320.2009	$C_{20}H_{24}N_4$	$[M]^+$
321.2077	$C_{20}H_{24}N_4 + H^+$	$[M + H]^+$
333.1616	$C_{19}H_{24}N_3 + K^+$	$[M - CN] + [K]^+$
328.1996*	$C_{18}H_{24}N_2\ CH_3COO + H^+$	$[M\ [-2(CN) + CH_3COO] + H^+]^+$

*Arising as a consequence of the protonation

Computational Details

The salient results of the TD-DFT computation (B3LYP/6-31G*) using the electronic ground state (from the crystal structure) and optimized electronic excited state structures are provided below. The excited states with high oscillator strength (f) are listed; the corresponding energies (in eV and nm), MOs involved in the excitation, and their relative contributions are listed.

Ground state geometry



Ground state molecular structure: from single crystal diffraction study

ε = 0

Excited State 1: Singlet-A 2.9442 eV 421.11 nm f=0.6209 <S**2>=0.000
84 -> 87 -0.10922
86 -> 87 0.69432
Excited State 3: Singlet-A 4.6842 eV 264.69 nm f=0.2376 <S**2>=0.000
86 -> 89 0.69341
Excited State 7: Singlet-A 5.8159 eV 213.18 nm f=0.2465 <S**2>=0.000
82 -> 87 0.68541

ε = 1.6

Excited State 1: Singlet-A 3.0701 eV 403.84 nm f=0.7218 <S**2>=0.000
84 -> 87 -0.11207
86 -> 87 0.69142
Excited State 6: Singlet-A 5.6985 eV 217.57 nm f=0.2907 <S**2>=0.000
83 -> 87 0.68466
Excited State 12: Singlet-A 6.8267 eV 181.62 nm f=0.5296 <S**2>=0.000
77 -> 87 0.11518
84 -> 89 0.21904
85 -> 88 0.62735
86 ->101 -0.10641

ε = 1.8

Excited State 1: Singlet-A 3.1206 eV 397.31 nm f=0.7236 <S**2>=0.000
84 -> 87 -0.11228
86 -> 87 0.69095
Excited State 6: Singlet-A 5.6809 eV 218.25 nm f=0.2896 <S**2>=0.000
83 -> 87 0.68321
Excited State 10: Singlet-A 6.6694 eV 185.90 nm f=0.1926 <S**2>=0.000
82 -> 91 0.18673
84 -> 88 -0.20585
85 -> 89 0.22871
86 -> 93 -0.17487
86 -> 94 0.53918

ε = 2

Excited State 1: Singlet-A 3.1636 eV 391.91 nm f=0.7254 <S**2>=0.000
84 -> 87 -0.11234
86 -> 87 0.69057
Excited State 6: Singlet-A 5.6663 eV 218.81 nm f=0.2883 <S**2>=0.000
83 -> 87 0.68149
Excited State 9: Singlet-A 6.6542 eV 186.33 nm f=0.2063 <S**2>=0.000
82 -> 91 0.19220
84 -> 88 -0.11329
85 -> 89 0.15980
86 -> 93 0.60106
86 -> 94 0.15104

ε = 3

Excited State 1: Singlet-A 3.3086 eV 374.74 nm f=0.7329 <S**2>=0.000
84 -> 87 -0.11174
86 -> 87 0.68934
Excited State 9: Singlet-A 6.5952 eV 187.99 nm f=0.2217 <S**2>=0.000
82 -> 90 0.19354
84 -> 93 0.10067
86 -> 93 0.64681
Excited State 11: Singlet-A 6.8459 eV 181.11 nm f=0.5853 <S**2>=0.000
78 -> 87 -0.10637
84 -> 89 -0.19590
85 -> 88 0.63729

ε = 4

Excited State 1: Singlet-A 3.3910 eV 365.63 nm f=0.7382 <S**2>=0.000
83 -> 87 -0.11082
86 -> 87 0.68871
Excited State 6: Singlet-A 5.6027 eV 221.29 nm f=0.2571 <S**2>=0.000
83 -> 88 0.10121
84 -> 87 0.65123
85 -> 87 -0.20187
Excited State 11: Singlet-A 6.8527 eV 180.93 nm f=0.6046 <S**2>=0.000
79 -> 87 -0.11492
83 -> 89 -0.18716
85 -> 88 0.63529

ε = 5

Excited State 1: Singlet-A 3.4441 eV 359.99 nm f=0.7419 <S**2>=0.000
83 -> 87 -0.11000
86 -> 87 0.68833
Excited State 9: Singlet-A 6.5401 eV 189.58 nm f=0.2362 <S**2>=0.000
82 -> 90 0.18986
83 -> 92 0.10189
86 -> 92 0.65316
Excited State 11: Singlet-A 6.8573 eV 180.81 nm f=0.6171 <S**2>=0.000
79 -> 87 -0.12216
83 -> 89 -0.18126
84 -> 88 -0.12560
85 -> 88 0.63022

ε = 6

Excited State 1: Singlet-A 3.4811 eV 356.17 nm f=0.7446 <S**2>=0.000
83 -> 87 0.10930
86 -> 87 0.68809
Excited State 9: Singlet-A 6.5253 eV 190.00 nm f=0.2405 <S**2>=0.000
82 -> 90 0.18805
83 -> 92 -0.10215
86 -> 92 0.65425
Excited State 11: Singlet-A 6.8606 eV 180.72 nm f=0.6259 <S**2>=0.000
79 -> 87 -0.12537
83 -> 87 0.10384
83 -> 89 0.17699
84 -> 88 -0.15992
85 -> 88 0.62247

ε = 7

Excited State 1: Singlet-A 3.5083 eV 353.40 nm f=0.7466 <S**2>=0.000
83 -> 87 0.10873
86 -> 87 0.68792
Excited State 9: Singlet-A 6.5146 eV 190.32 nm f=0.2437 <S**2>=0.000

82 -> 90 0.18667
83 -> 92 -0.10234
86 -> 92 0.65496
Excited State 11: Singlet-A 6.8631 eV 180.65 nm f=0.6322 <S**2>=0.000
79 -> 87 -0.12751
83 -> 87 0.10882
83 -> 89 0.17375
84 -> 88 -0.19517
85 -> 88 0.61221

ε = 8
Excited State 1: Singlet-A 3.5292 eV 351.31 nm f=0.7482 <S**2>=0.000
83 -> 87 0.10826
86 -> 87 0.68780
Excited State 9: Singlet-A 6.5064 eV 190.56 nm f=0.2462 <S**2>=0.000
82 -> 90 0.18556
83 -> 92 -0.10249
86 -> 92 0.65543
Excited State 10: Singlet-A 6.8650 eV 180.60 nm f=0.6371 <S**2>=0.000
79 -> 87 -0.12912
83 -> 87 0.11281
83 -> 89 0.17121
84 -> 88 -0.23004
85 -> 88 0.59981

ε = 9
Excited State 1: Singlet-A 3.5457 eV 349.67 nm f=0.7495 <S**2>=0.000
83 -> 87 0.10786
86 -> 87 0.68771
Excited State 9: Singlet-A 6.4999 eV 190.75 nm f=0.2482 <S**2>=0.000
82 -> 90 0.18467
83 -> 92 -0.10260
86 -> 92 0.65576
Excited State 10: Singlet-A 6.8666 eV 180.56 nm f=0.6409 <S**2>=0.000
79 -> 87 -0.13039
83 -> 87 0.11607
83 -> 89 0.16916
84 -> 88 -0.26332
85 -> 88 0.58574

ε = 10
Excited State 1: Singlet-A 3.5592 eV 348.35 nm f=0.7505 <S**2>=0.000
83 -> 87 0.10752
86 -> 87 0.68763
Excited State 9: Singlet-A 6.4947 eV 190.90 nm f=0.2498 <S**2>=0.000
82 -> 90 0.18393
83 -> 92 -0.10268
86 -> 92 0.65599
Excited State 10: Singlet-A 6.8679 eV 180.53 nm f=0.6439 <S**2>=0.000
79 -> 87 -0.13142
83 -> 87 0.11879
83 -> 89 0.16747
84 -> 88 -0.29409
85 -> 88 0.57069

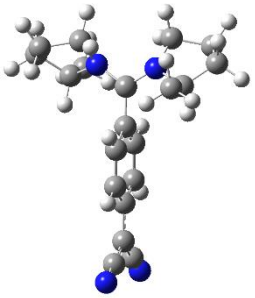
ε = 20
Excited State 1: Singlet-A 3.6217 eV 342.34 nm f=0.7556 <S**2>=0.000
83 -> 87 0.10575
86 -> 87 0.68733
Excited State 9: Singlet-A 6.4707 eV 191.61 nm f=0.2576 <S**2>=0.000

82 -> 90 0.18023
83 -> 91 -0.10294
86 -> 91 0.65510
Excited State 10: Singlet-A 6.8741 eV 180.36 nm f=0.6580 <S**2>=0.000
79 -> 87 0.13621
83 -> 87 -0.13235
83 -> 89 -0.15924
84 -> 88 0.45456
85 -> 88 -0.45124

ε = 30
Excited State 1: Singlet-A 3.6433 eV 340.31 nm f=0.7573 <S**2>=0.000
83 -> 87 0.10506
86 -> 87 0.68724
Excited State 9: Singlet-A 6.4625 eV 191.85 nm f=0.2605 <S**2>=0.000
82 -> 90 0.17880
83 -> 91 -0.10332
86 -> 91 0.65726
Excited State 10: Singlet-A 6.8763 eV 180.31 nm f=0.6625 <S**2>=0.000
79 -> 87 -0.13781
83 -> 87 0.13742
83 -> 89 0.15624
84 -> 88 0.49782
85 -> 88 0.40183

ε = 40
Excited State 1: Singlet-A 3.6543 eV 339.28 nm f=0.7583 <S**2>=0.000
83 -> 87 0.10470
86 -> 87 0.68720
Excited State 9: Singlet-A 6.4584 eV 191.97 nm f=0.2619 <S**2>=0.000
82 -> 90 0.17800
83 -> 91 -0.10341
86 -> 91 0.65750
Excited State 10: Singlet-A 6.8775 eV 180.28 nm f=0.6647 <S**2>=0.000
79 -> 87 -0.13857
83 -> 87 0.14007
83 -> 89 0.15468
84 -> 88 0.51511
85 -> 88 0.37870

Excited state geometry:



Excited state optimised molecular structure

ε = 0

Excited State 1: Singlet-A 1.0910 eV 1136.45 nm f=0.0006 <S**2>=0.000
84 -> 87 -0.16142
86 -> 87 0.68587
Excited State 4: Singlet-A 4.0500 eV 306.13 nm f=0.4911 <S**2>=0.000
84 -> 87 -0.42807
86 -> 87 -0.11478
86 -> 88 0.52511
Excited State 5: Singlet-A 4.0581 eV 305.52 nm f=0.3173 <S**2>=0.000
76 -> 87 0.12165
84 -> 87 0.49539
86 -> 87 0.12603
86 -> 88 0.45688

ε =2

Excited State 1: Singlet-A 1.7368 eV 713.86 nm f=0.0005 <S**2>=0.000
84 -> 87 -0.17360
86 -> 87 0.68281
Excited State 3: Singlet-A 4.0997 eV 302.43 nm f=0.8796 <S**2>=0.000
86 -> 88 0.69545
86 -> 88 0.69545
Excited State 13: Singlet-A 6.6149 eV 187.43 nm f=0.1891 <S**2>=0.000
82 -> 91 0.19563
84 -> 89 -0.12262
86 -> 97 0.62794

ε = 2.8

Excited State 1: Singlet-A 1.9689 eV 629.71 nm f=0.0005 <S**2>=0.000
84 -> 87 -0.17835
86 -> 87 0.68149
Excited State 3: Singlet-A 4.1597 eV 298.06 nm f=0.8698 <S**2>=0.000
86 -> 88 0.69491
Excited State 12: Singlet-A 6.5746 eV 188.58 nm f=0.2151 <S**2>=0.000
82 -> 91 0.18914
84 -> 89 -0.12828
86 -> 96 0.63043

ε = 3

Excited State 1: Singlet-A 2.0103 eV 616.76 nm f=0.0005 <S**2>=0.000
84 -> 87 -0.17916
86 -> 87 0.68124
Excited State 3: Singlet-A 4.1705 eV 297.29 nm f=0.8678 <S**2>=0.000
86 -> 88 0.69464
Excited State 12: Singlet-A 6.5675 eV 188.79 nm f=0.2189 <S**2>=0.000
82 -> 91 0.18573
84 -> 89 -0.13013
85 -> 88 -0.10302
86 -> 95 0.11884
86 -> 96 0.62448

ε = 4

Excited State 1: Singlet-A 2.1619 eV 573.50 nm f=0.0004 <S**2>=0.000
84 -> 87 -0.18047
86 -> 87 0.68031
Excited State 3: Singlet-A 4.2106 eV 294.46 nm f=0.8499 <S**2>=0.000
86 -> 88 0.68719
Excited State 12: Singlet-A 6.5421 eV 189.52 nm f=0.2320 <S**2>=0.000
82 -> 90 -0.10334

82 -> 91 -0.15750
84 -> 89 0.13687
85 -> 88 0.12920
86 -> 95 0.61332
86 -> 96 0.13990

ε = 5

Excited State 1: Singlet-A 2.2585 eV 548.98 nm f=0.0004 <S**2>=0.000
83 -> 87 -0.13136
84 -> 87 -0.13018
86 -> 87 0.67969
Excited State 4: Singlet-A 4.2379 eV 292.56 nm f=0.8003 <S**2>=0.000
83 -> 87 -0.13869
84 -> 87 0.12223
86 -> 88 0.66429
Excited State 13: Singlet-A 6.7259 eV 184.34 nm f=0.2314 <S**2>=0.000
77 -> 87 0.16292
78 -> 87 -0.17937
83 -> 88 -0.26286
84 -> 88 -0.26340
85 -> 89 0.50751

ε = 6

Excited State 1: Singlet-A 2.3254 eV 533.16 nm f=0.0004 <S**2>=0.000
83 -> 87 -0.18080
86 -> 87 0.67925
Excited State 4: Singlet-A 4.2554 eV 291.36 nm f=0.8502 <S**2>=0.000
86 -> 88 0.69196
Excited State 13: Singlet-A 6.7309 eV 184.20 nm f=0.2406 <S**2>=0.000
78 -> 87 0.18606
83 -> 88 -0.36242
84 -> 89 0.11402
85 -> 89 0.51657

ε = 7

Excited State 1: Singlet-A 2.3747 eV 522.11 nm f=0.0004 <S**2>=0.000
83 -> 87 -0.18528
86 -> 87 0.67892
Excited State 4: Singlet-A 4.2687 eV 290.45 nm f=0.8526 <S**2>=0.000
86 -> 88 0.69391
Excited State 11: Singlet-A 6.5074 eV 190.53 nm f=0.2488 <S**2>=0.000
82 -> 90 0.16190
83 -> 89 -0.15009
85 -> 88 -0.16957
86 -> 93 0.61518

ε = 8

Excited State 1: Singlet-A 2.4124 eV 513.95 nm f=0.0004 <S**2>=0.000
83 -> 87 -0.18699
86 -> 87 0.67867
Excited State 4: Singlet-A 4.2789 eV 289.76 nm f=0.8525 <S**2>=0.000
86 -> 88 0.69444
Excited State 11: Singlet-A 6.5023 eV 190.68 nm f=0.2533 <S**2>=0.000
82 -> 90 -0.16110
83 -> 89 0.15413
85 -> 88 0.17692
86 -> 92 0.61461

ε = 9

Excited State 1: Singlet-A 2.4422 eV 507.67 nm f=0.0004 <S**2>=0.000

83 -> 87 -0.18803
86 -> 87 0.67846
Excited State 4: Singlet-A 4.2870 eV 289.21 nm f=0.8521 <S**2>=0.000
86 -> 88 0.69466
Excited State 11: Singlet-A 6.4982 eV 190.80 nm f=0.2561 <S**2>=0.000
82 -> 90 -0.15793
83 -> 89 0.15689
85 -> 88 0.18219
86 -> 92 0.61307

ε = 10
Excited State 1: Singlet-A 2.4664 eV 502.69 nm f=0.0004 <S**2>=0.000
83 -> 87 -0.18877
86 -> 87 0.67830
Excited State 4: Singlet-A 4.2936 eV 288.76 nm f=0.8515 <S**2>=0.000
86 -> 88 0.69478
Excited State 11: Singlet-A 6.4950 eV 190.89 nm f=0.2583 <S**2>=0.000
82 -> 90 -0.15341
83 -> 89 0.15902
85 -> 88 0.18608
86 -> 92 0.61133

ε = 12
Excited State 1: Singlet-A 2.5033 eV 495.29 nm f=0.0004 <S**2>=0.000
83 -> 87 -0.18980
86 -> 87 0.67804
Excited State 4: Singlet-A 4.3037 eV 288.09 nm f=0.8506 <S**2>=0.000
86 -> 88 0.69488
Excited State 11: Singlet-A 6.4901 eV 191.04 nm f=0.2614 <S**2>=0.000
82 -> 90 -0.14189
83 -> 89 0.16217
85 -> 88 0.19110
86 -> 92 0.60825

ε = 14
Excited State 1: Singlet-A 2.5300 eV 490.05 nm f=0.0004 <S**2>=0.000
83 -> 87 -0.19050
86 -> 87 0.67786
Excited State 4: Singlet-A 4.3110 eV 287.60 nm f=0.8499 <S**2>=0.000
86 -> 88 0.69492
Excited State 11: Singlet-A 6.4867 eV 191.14 nm f=0.2636 <S**2>=0.000
81 -> 90 0.10901
82 -> 90 -0.12928
83 -> 89 0.16442
85 -> 88 0.19387
86 -> 92 0.60576

ε = 16
Excited State 1: Singlet-A 2.5503 eV 486.15 nm f=0.0004 <S**2>=0.000
83 -> 87 -0.19102
86 -> 87 0.67772
Excited State 4: Singlet-A 4.3165 eV 287.23 nm f=0.8493 <S**2>=0.000
86 -> 88 0.69494
Excited State 11: Singlet-A 6.4842 eV 191.21 nm f=0.2651 <S**2>=0.000
81 -> 90 -0.12055
82 -> 90 -0.11757
83 -> 89 0.16612
85 -> 88 0.19537
86 -> 92 0.60374

ε = 18

Excited State 1: Singlet-A 2.5663 eV 483.13 nm f=0.0004 <S**2>=0.000
83 -> 87 -0.19142
86 -> 87 0.67761
Excited State 4: Singlet-A 4.3209 eV 286.94 nm f=0.8489 <S**2>=0.000
86 -> 88 0.69495
Excited State 11: Singlet-A 6.4822 eV 191.27 nm f=0.2663 <S**2>=0.000
81 -> 90 -0.12864
82 -> 90 -0.10764
83 -> 89 0.16744
84 -> 88 0.10581
85 -> 88 0.19612
86 -> 92 0.60209

ε =20

Excited State 1: Singlet-A 2.5791 eV 480.72 nm f=0.0004 <S**2>=0.000
83 -> 87 -0.19174
86 -> 87 0.67752
Excited State 4: Singlet-A 4.3244 eV 286.71 nm f=0.8485 <S**2>=0.000
86 -> 88 0.69496
Excited State 11: Singlet-A 6.4807 eV 191.31 nm f=0.2673 <S**2>=0.000
81 -> 90 -0.13428
83 -> 89 0.16850
84 -> 88 0.11222
85 -> 88 0.19644
86 -> 92 0.60071

ε = 30

Excited State 1: Singlet-A 2.6182 eV 473.55 nm f=0.0004 <S**2>=0.000
83 -> 87 -0.19268
86 -> 87 0.67724
Excited State 4: Singlet-A 4.3351 eV 286.00 nm f=0.8474 <S**2>=0.000
86 -> 88 0.69496
Excited State 11: Singlet-A 6.4761 eV 191.45 nm f=0.2701 <S**2>=0.000
81 -> 90 -0.14617
83 -> 89 0.17171
84 -> 88 0.13305
85 -> 88 0.19572
86 -> 92 0.59627

ε = 40

Excited State 1: Singlet-A 2.6380 eV 469.99 nm f=0.0004 <S**2>=0.000
83 -> 87 -0.19315
86 -> 87 0.67710
Excited State 4: Singlet-A 4.3405 eV 285.64 nm f=0.8468 <S**2>=0.000
86 -> 88 0.69496
Excited State 11: Singlet-A 6.4738 eV 191.52 nm f=0.2715 <S**2>=0.000
81 -> 90 -0.14959
83 -> 89 0.17332
84 -> 88 -0.14417
85 -> 88 0.19439
86 -> 92 0.59388

Table S5. Excited states computed for the ground state geometry (from crystal structure) of BMPDQ under different dielectric constants (ε); the wavelength (λ_{max}) and the corresponding oscillator strength (f) for the excitations with high oscillator strength are shown.

ε	Excitation 1		Excitation 2		Excitation 3	
	λ_{max} (nm)	f	λ_{max} (nm)	f	λ_{max} (nm)	f
0	421.11	0.62	264.69	0.23	213.18	0.24
1.6	403.84	0.72	217.57	0.29	181.62	0.52
1.8	397.31	0.72	257.49	0.19	218.25	0.28
2	391.1	0.72	218.81	0.28	186.33	0.20
3	374.4	0.73	187.9	0.22	181.11	0.58
4	365.63	0.73	221.29	0.25	180.93	0.60
5	359.99	0.74	189.5	0.23	180.81	0.61
6	356.17	0.74	190.00	0.24	180.72	0.62
7	353.4	0.74	190.32	0.24	180.65	0.63
8	351.31	0.74	190.56	0.24	180.60	0.63
9	349.67	0.74	190.75	0.24	180.56	0.64
10	348.35	0.75	190.90	0.24	180.53	0.64
20	342.34	0.75	191.61	0.25	180.36	0.65
30	340.31	0.75	191.85	0.26	180.31	0.66
40	339.3	0.75	191.97	0.26	180.28	0.66

Table S6. Excited states computed for the optimized excited state geometry of BMPDQ under different dielectric constants (ε); the wavelength (λ_{max}) and the corresponding oscillator strength (f) for the excitations with high oscillator strength are shown.

ε	Excitation 1		Excitation 2		Excitation 3	
	λ_{max} (nm)	f	λ_{max} (nm)	f	λ_{max} (nm)	f
0	1136.45	0.0006	306.18	0.49	305.52	0.31
2	713.86	0.0005	302.43	0.87	187.43	0.18
2.8	629.71	0.0005	298.06	0.86	188.58	0.21
3	616.76	0.0005	297.29	0.86	188.79	0.21
4	573.50	0.0004	294.46	0.84	189.52	0.23
5	548.98	0.0004	292.56	0.80	184.34	0.23
6	533.16	0.0004	291.36	0.85	184.20	0.24
7	522.11	0.0004	290.45	0.85	190.53	0.24
8	513.95	0.0004	289.76	0.85	190.68	0.25
9	507.67	0.0004	289.21	0.85	190.80	0.25
10	502.69	0.0004	288.76	0.85	190.89	0.25
12	495.29	0.0004	288.09	0.85	191.04	0.26
14	490.05	0.0004	287.60	0.84	191.14	0.26
16	486.15	0.0004	287.23	0.84	191.21	0.26
18	483.13	0.0004	286.94	0.84	191.27	0.26
20	480.72	0.0004	286.71	0.84	191.31	0.26
30	473.55	0.0004	286.00	0.84	191.45	0.27
40	469.99	0.0004	285.64	0.84	191.52	0.27

Capacitance Measurements

Figure S9. Construction of a parallel plate capacitor using FTO coated plates and BMPDQ microcrystalline powder sandwiched between the plates.

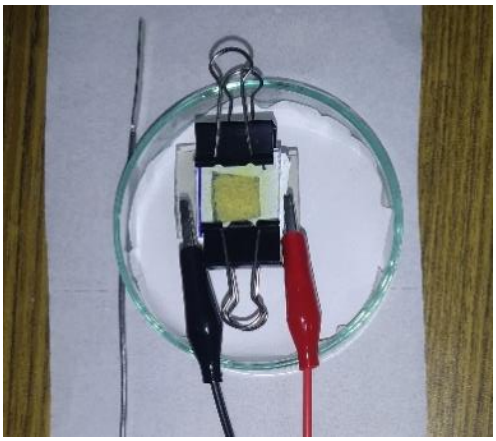
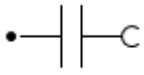
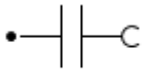
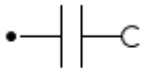
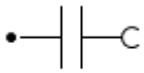
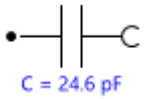
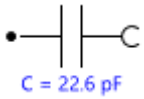


Table S7. Equivalent circuits used to simulate the impedance spectrum (at 1 V) of pristine and acetic acid exposed BMPDQ; the dielectric constant estimated* are also shown.

Time of exposure (min)	Equivalent circuit	ε
0		12.9
2		9.6
4		9.1
6		8.7
8		7.7
10		7.1

*Dielectric constant, $\epsilon = \frac{Cd}{\epsilon_0 A}$ where C is the capacitance, d and A are the thickness and area of the sample (400 µm, 1.44 cm^2 respectively), and ϵ_0 is the permittivity of free space (8.854×10^{-12} $CV^{-1}m^{-1}$).

Scanning Kelvin Probe Microscopy

Figure S10. SKPM topography and surface potential images of BMPDQ **(a)** before and **(b)** after exposure to acetic acid vapor for 15 min. Plots of the surface potential measured on the substrate and BMPDQ before and after exposure to acetic acid vapors corresponding to several points probed on 6 samples are shown in Figure 9 in the main text.