Supporting Information for Publication

Multi-stimuli Responsive Fluorochromic Organic Salt

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Table S1. Crystallographic Table of **1**.

Reaction Code	AAG-638
CCDC Number	2335128
Empirical Formula	C23 H20 N6 O5 S
Fw	492.51
Temperature [K]	0 K
Crystal System	Triclinic
Space Group	P -1
a, [Å]	7.2165(18)
b, [Å]	12.287(3)
c, [Å]	13.0501(14)
α, [°]	72.090(13)
β, [°]	80.149(14)
γ, [°]	83.652(19)
V, [Å3]	1082.8(4)
Z	2
D(calcd) [mg/cm3]	1.511
μ *[mm^{-1}]*	0.201
Θ range [o]	24.999
Reflns Collected	3727
Indep. Reflns	3727
GOF	1.062
R1(I0 >2σ(I0)	0.0368
wR2(all data)	0.1201

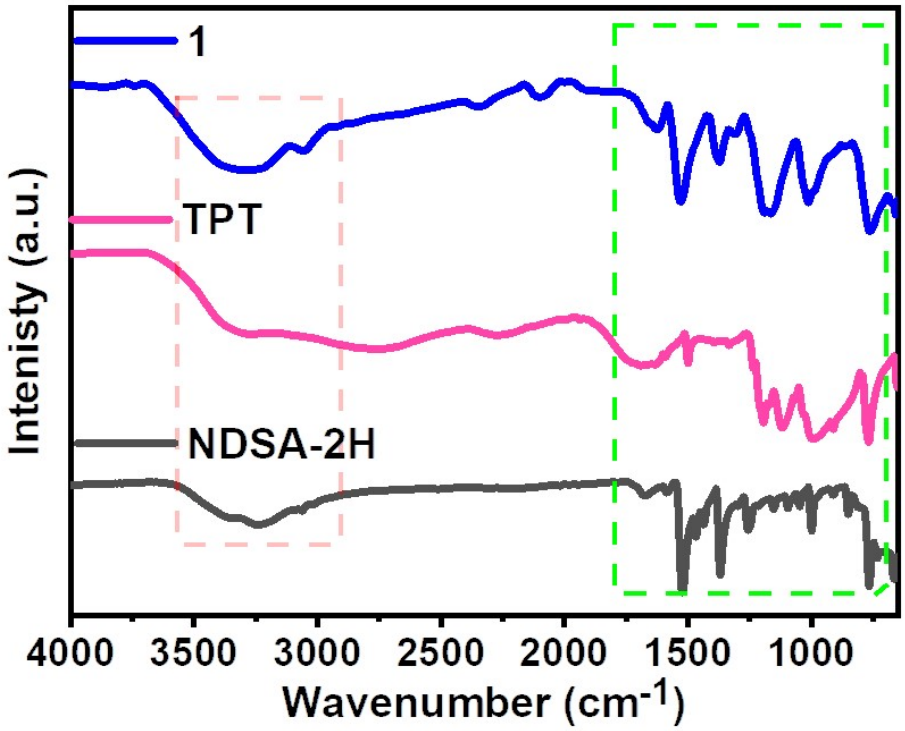

Figure S1. FT-IR spectra of **1** compared with TPT and NDSA-2H.

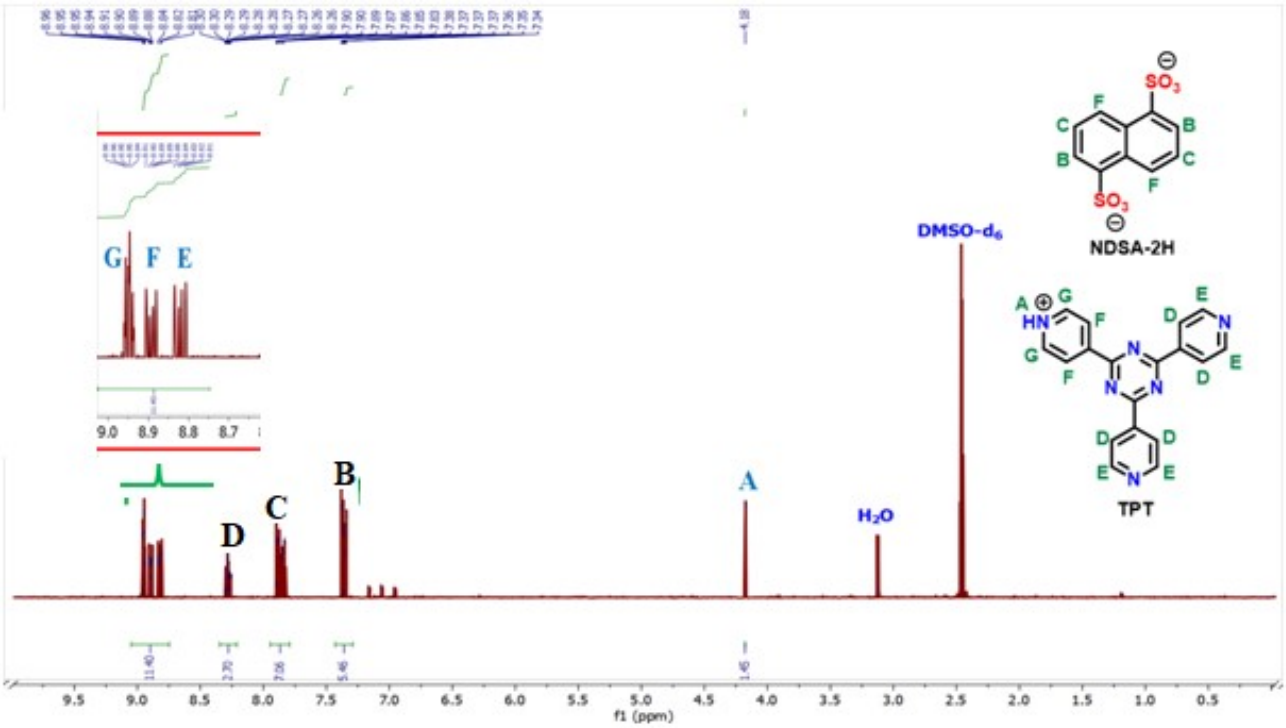

Figure S2.[1]HNMR Spectra of **1**, DMSO-d_6, 400 MHz.

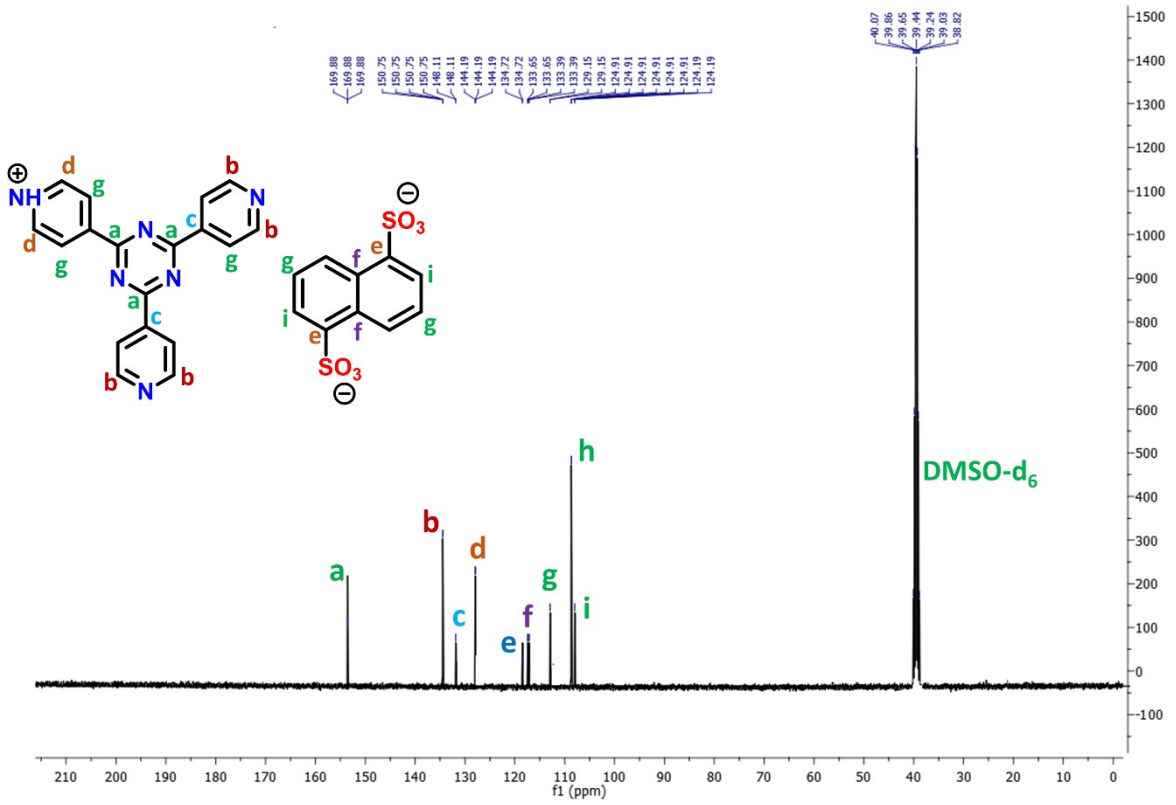

Figure S3. ^{13}C NMR of **1**.

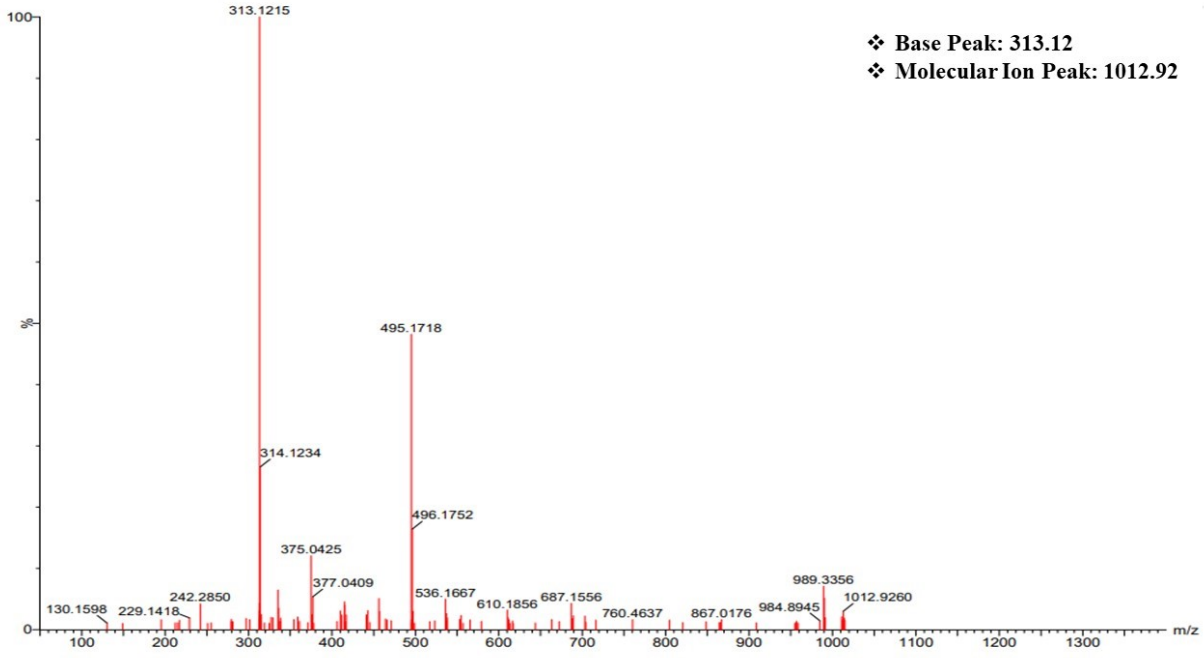

Figure S4.HR-MS of 1.

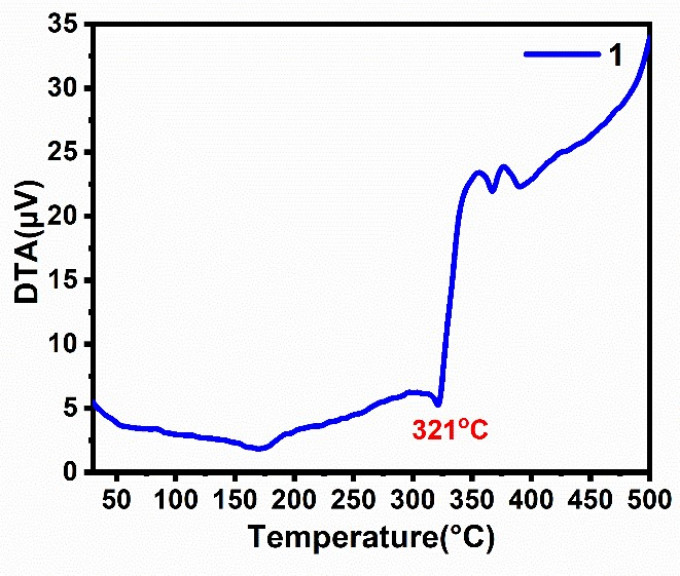

Figure S5.DTA Curves of **1**.

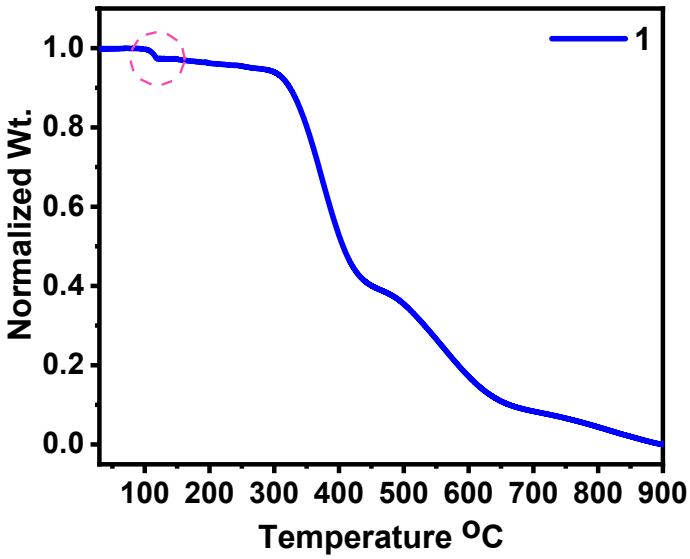

Figure S6.TGA Curves of **1**, **1-NH_3** and **1-NH_3-R**.

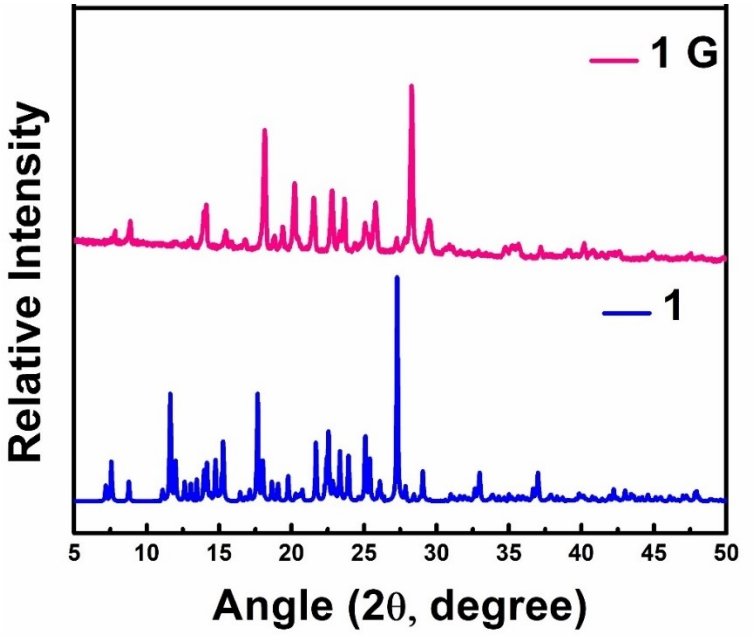

Figure S7. P-XRD of **1** compared with its ground form (**1 G**).

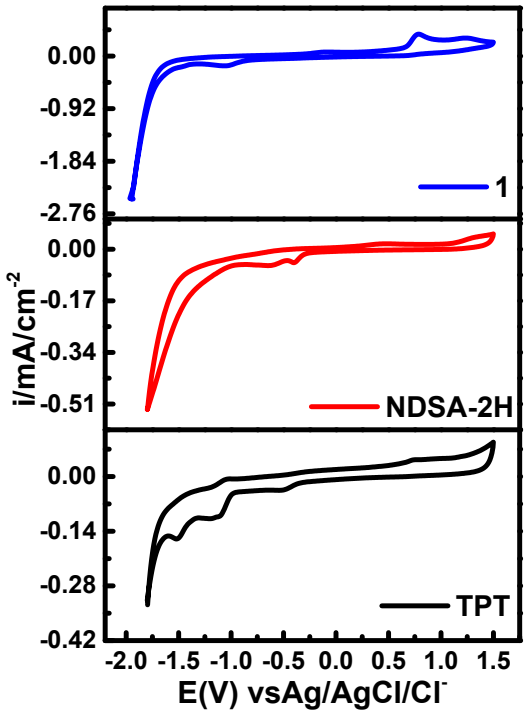

Figure S8. Cyclic voltammogram of **TPT**, **NDSA-2H,** and **1**.

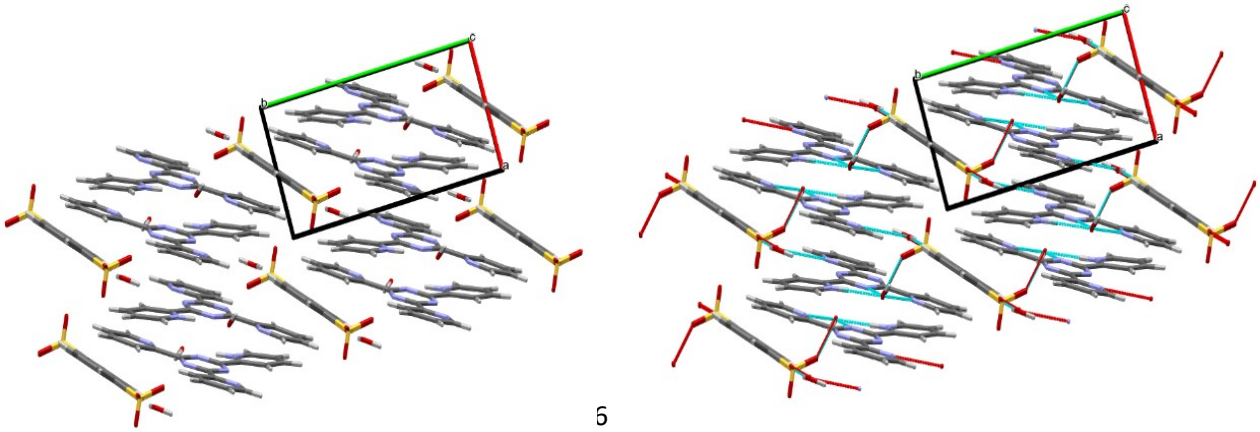

Figure S9. Hydrogen bonded 3-dimensional network of **1**.

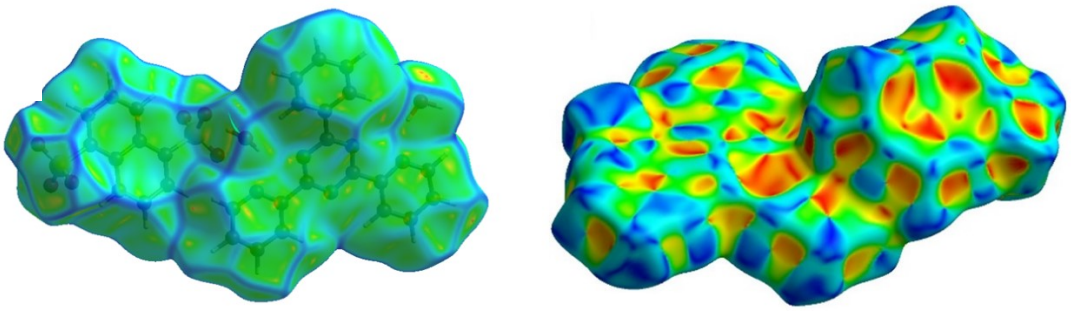

Figure S10. Curvedness and shape index of **1**.

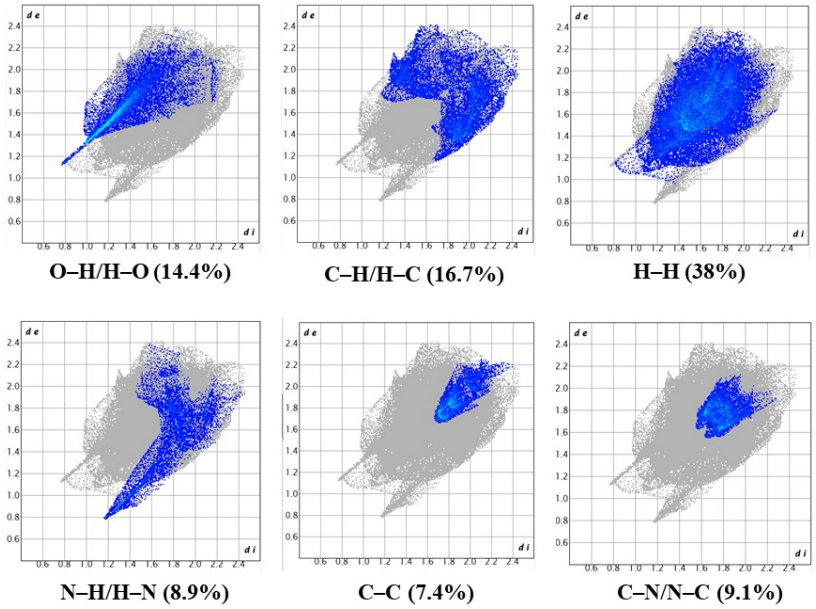

Figure S11. Fingerprint plots of **1**.

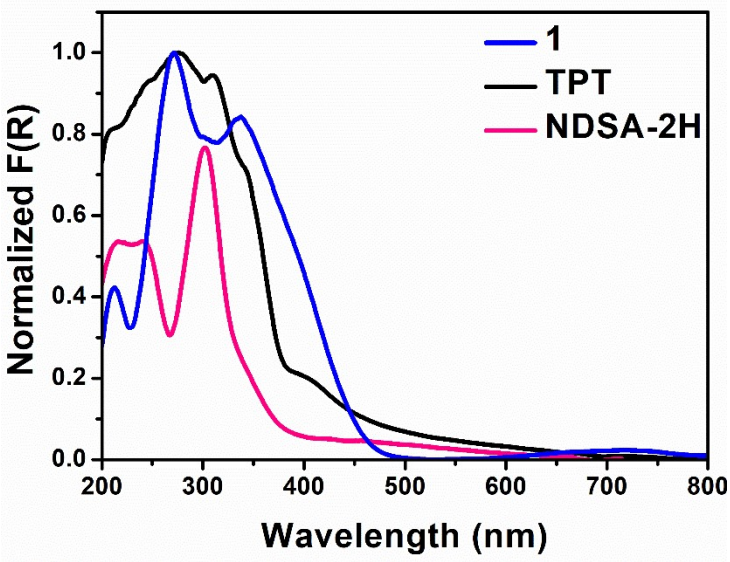

Figure S12. UV-DRS spectra of **TPT, NDSA-2H,** and **1**.

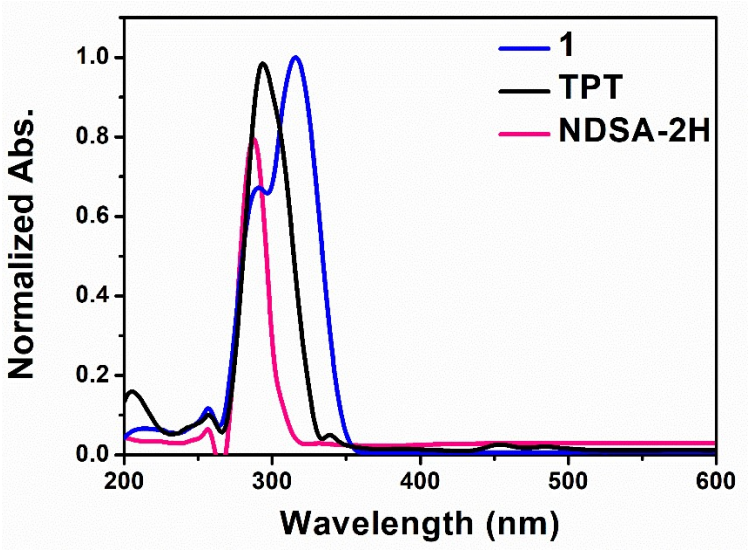

Figure S13. Solution phase Absorption of **1** compared with TPT and NDSA-2H

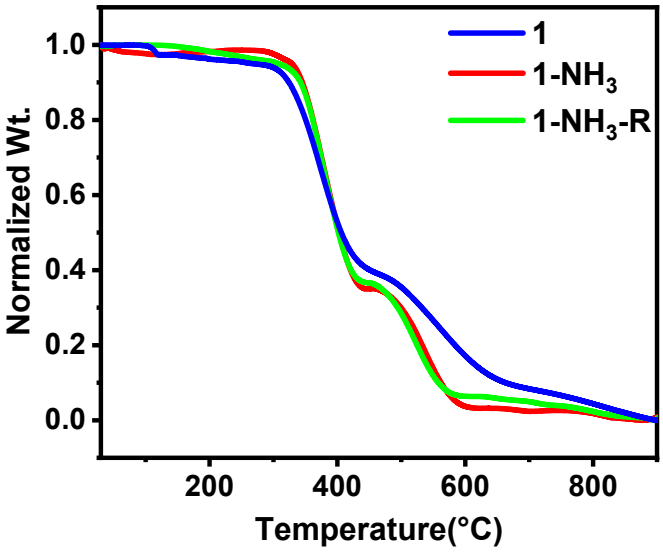

Figure S14.TGA Curves of **1**, **1-NH_3** and **1-NH_3-R**.

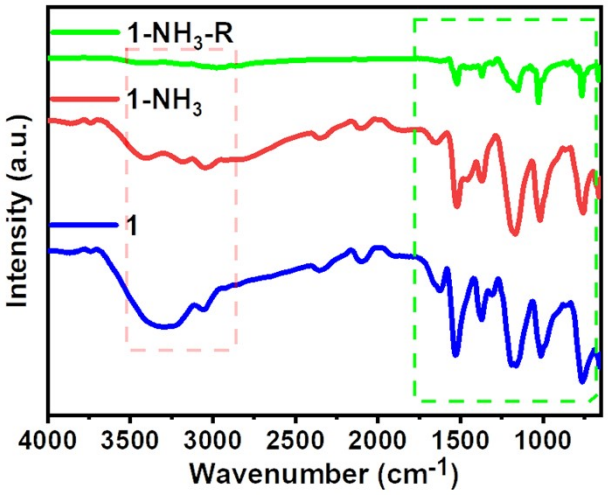

Figure S15. FT-IR spectra of **1**, **1-NH$_3$** and **1-NH$_3$-R**.

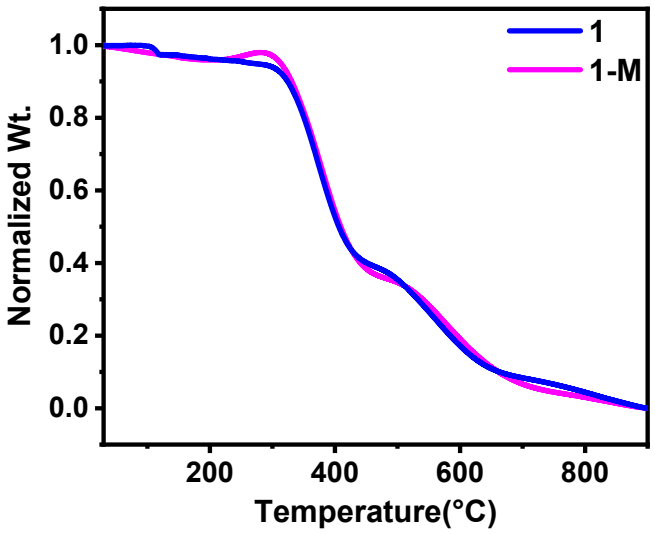

Figure S16.TGA Curves of **1**and **1-M**.

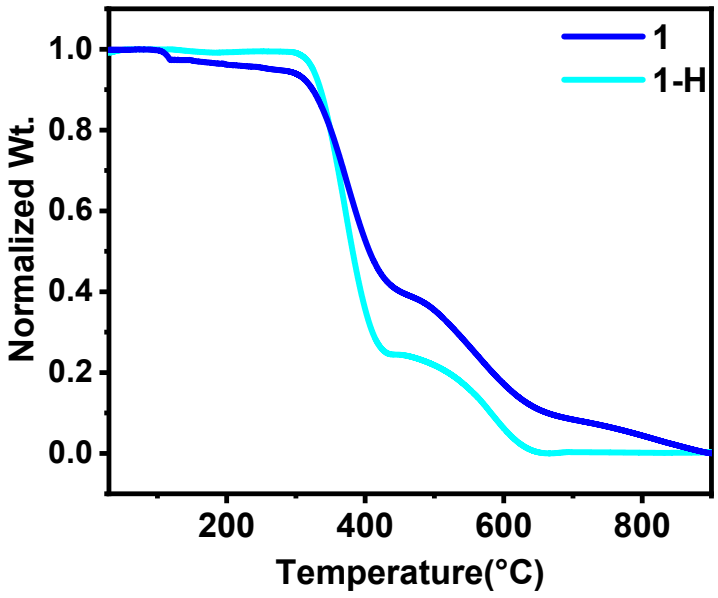

Figure S17.TGA Curves of **1** and **1-H**.

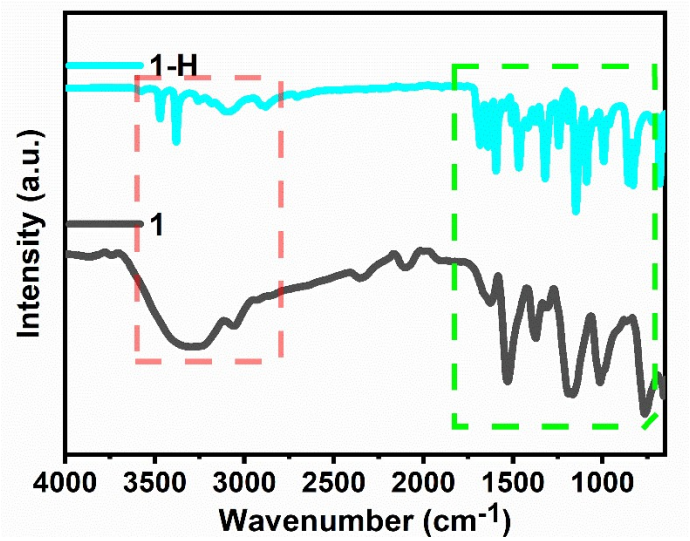

Figure S18. FT-IR spectra of **1** and **1-H**.

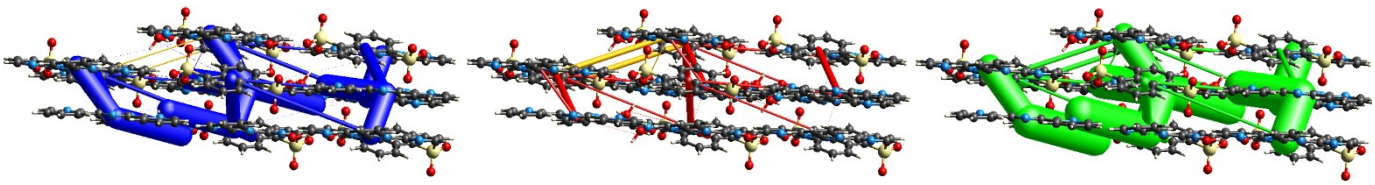

Figure S19. Total, coulomb and dispersion energy fragment of **1**.

Table S2. Interaction Energies (kJ/mol) of **1**.

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-	11.44	HF/3-21G	-6.2	-5.3	-9.9	7.8	-12.4
	1	-	6.16	HF/3-21G	0.0	nan	0.0	0.0	nan
	1	-x, -y, -z	3.42	HF/3-21G	-0.6	-6.1	-106.9	47.1	-62.7
	2	x, y, z	13.54	HF/3-21G	0.0	-0.2	0.0	0.0	-0.1
	1	-x, -y, -z	14.03	HF/3-21G	0.0	-0.5	0.0	0.0	-0.3
	1	-	7.38	HF/3-21G	-21.6	-13.4	-32.5	22.4	-41.8
	1	-	7.91	HF/3-21G	-20.3	-20.9	-28.9	25.3	-39.8
	1	-	9.15	HF/3-21G	0.0	nan	0.0	0.0	nan
	2	x, y, z	13.05	HF/3-21G	0.0	-0.3	0.0	0.0	-0.2
	1	-	9.17	HF/3-21G	17.1	-8.0	-15.6	7.0	3.9
	1	-	4.22	HF/3-21G	0.0	-0.3	0.0	0.0	-0.2
	1	-	6.59	HF/3-21G	0.0	-0.0	0.0	0.0	-0.0
	1	-	3.62	HF/3-21G	3.1	-0.5	-4.7	0.0	-1.5
	1	-x, -y, -z	4.75	HF/3-21G	-9.3	-6.4	-82.9	38.6	-57.0
	1	-x, -y, -z	11.24	HF/3-21G	0.8	-0.2	-6.1	0.4	-4.5
	1	-	7.32	HF/3-21G	-0.6	-6.1	-106.9	47.1	-62.7
	1	-	8.60	HF/3-21G	0.0	-0.5	0.0	0.0	-0.3
	1	-x, -y, -z	15.54	HF/3-21G	0.0	-0.0	0.0	0.0	-0.0
	1	-x, -y, -z	14.71	HF/3-21G	0.0	-1.0	0.0	0.0	-0.6
	1	-	11.72	HF/3-21G	-7.3	-4.2	-11.5	15.4	-8.1
	1	-	9.61	HF/3-21G	-20.5	-12.9	-17.8	12.3	-35.3
	1	-	7.61	HF/3-21G	0.0	-1.0	0.0	0.0	-0.6
	1	-	5.12	HF/3-21G	-0.6	-6.1	-106.9	47.1	-62.7

R is the distance between molecular centroids (mean atomic position) in Å.
Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below).

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618