Supporting information of

## A novel organic salt with water/humidity-induced fluorescence switching and heat-induced coloration performance

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**Figure S1.** The Oak Ridge Thermal Ellipsoid Plot (ORTEP) of the unsymmetrical unit of **1** with thermal ellipsoids at the 30% probability level.



Figure S2. Emission spectra of sulfuric acid solution of phen with different concentrations (the mole ratio of phen and  $H_2SO_4$  is 1:1,  $\lambda_{ex} = 360$  nm).



**Figure S3.** TG (green) and DSC (red) curve of compound **1**. This compound can be stable to 45 °C in nitrogen. Then it decomposes till 83 °C with a weight loss of 2.69 % (Calc. 2.88 %), attributed to the release of the lattice water molecule. In addition, there is an exothermic peak in the range of 145 °C~230 °C, which can be attributed to the *in situ* hydrogenation reaction of **1**.



Figure S4. IR specturm of 1.



**Figure S5.** Green: PXRD pattern calculated from the single crystal data of **1**; Red: PXRD pattern of original dry compound **1**; Blue: PXRD pattern of **1** at 80% RH for 6 h, then at 30% RH for 24 h.



**Table S6.** PXRD data of the calculated result from the single crystal data of **1** (calc), original compound **1** (ori) and restored compound **1** (res, at 80% RH for 6 h, then at 30% RH for 24 h). [I = intensity (a.u.)]

	-					-			
			The calculated result						
			from th	ne single	The	original	The	restored	
h	k	1	crystal d	ata of 1	compound	<b>1</b> (ori)	compound	<b>1</b> (res)	
			(calc)						
			$2 heta_{calc}$ (°)	<i>I</i> <sub>calc</sub>	$2\theta_{ori}$ (°)	I <sub>ori</sub>	$2\theta_{res}$ (°)	Ires	
0	1	1	9.54	6388	9.56	1222	9.50	203	
1	1	-1	11.26	498	11.22	19	11.24	33	
1	1	2	14.70	530	14.66	25	14.68	28	
1	0	-3	15.14	1820	15.12	83	15.04	416	
2	1	0	15.44	532	15.42	44	15.44	33	
0	1	3	16.58	10000	16.56	774	15.62	917	
1	2	0	17.78	363	17.78	21	17.76	20	
0	0	4	19.20	4849	19.16	1538	19.16	1443	
3	0	-1	19.70	693	19.70	158	19.68	43	
1	2	-2	19.88	2409	19.86	348	19.82	128	
1	2	2	20.56	2398	20.58	101	20.56	100	
3	0	1	20.72	2787	20.62	91	20.66	182	
1	1	-4	21.30	3948	21.22	156	21.24	507	
2	2	1	21.98	734	21.90	45	21.94	62	
1	1	4	22.56	2718	22.52	294	22.46	244	
3	0	-3	23.10	1386	23.06	542	23.04	90	
2	1	-4	23.60	892	23.52	137	23.50	94	
3	1	2	24.28	2259	24.20	221	24.24	107	
2	0	4	24.44	833	24.44	37	24.34	127	
0	2	4	25.44	3564	25.38	264	25.32	117	
2	1	4	25.84	1420	25.72	54	25.78	114	
4	0	0	26.26	5336	26.22	105	26.20	679	
3	2	1	26.62	1080	26.62	37	26.58	57	
3	2	-2	26.76	930	26.76	44	26.70	100	
4	0	-2	27.00	5163	26.92	197	26.92	109	
2	1	-5	27.48	7538	27.44	378	27.40	1284	
2	3	0	28.20	1780	28.18	124	28.14	108	
4	1	-2	28.26	2445	28.24	96	28.24	101	
3	2	-3	28.52	635	28.52	25	28.46	55	
0	0	6	28.98	509	28.92	65	28.96	55	
1	2	-5	29.50	1408	29.46	67	29.38	166	
2	1	5	29.94	1793	29.86	102	29.88	50	
0	1	6	30.18	824	30.12	38	30.10	96	
1	2	5	30.66	636	30.60	29	30.60	54	
2	3	3	32.46	211	32.48	18	32.46	169	
0	4	0	33.40	374	33.44	21	33.42	26	
5	0	1	33.90	495	33.90	41	33.92	37	
3	3	-3	34.22	619	34.18	42	34.14	71	

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3	1	-6	34.42	582	34.44	27	34.44	28
5	2	-2	37.46	442	37.48	16	37.48	29
4	2	-5	37.90	389	37.86	21	37.92	28
1	4	-4	39.02	343	39.00	44	39.04	28
4	2	5	41.58	360	41.60	18	41.58	65
0	3	7	42.54	474	42.52	28	42.50	74
2	5	1	44.72	347	44.72	22	44.72	21
3	5	1	47.38	471	47.40	28	47.38	47

Figure S7. <sup>1</sup>H NMR spectrum of compound 3a.







**Figure S9.** <sup>1</sup>H NMR spectrum of compound **3c**.







Figure S11. <sup>13</sup>C NMR spectrum of compound 3b.



Figure S12. <sup>13</sup>C NMR spectrum of compound 3c.



Figure S13. HRMS spectrum of compound 3a.



Figure S14. HRMS spectrum of compound 3b.



Figure S15. HRMS spectrum of compound 3c.

