SUPPORTING INFORMATION

Host-Guest Interactions Dictated Selective Adsorption and Fluorescent Quenching of Luminescent Lightweight Metal-Organic Framework Toward Liquid Explosives

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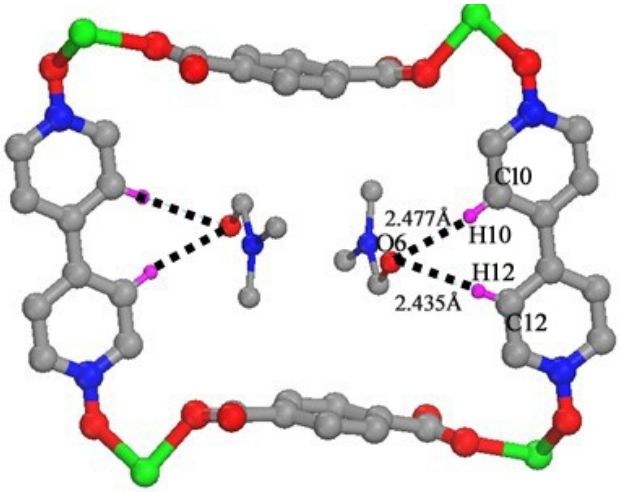
Table S1. Cell parameters, dimensions of channels and M–O distances of M^{II}-based MIL-53 (M = Mn, Co and Mg) in space group *C2/c*.

Compound	**Mn-MIL-53**	**Co-MIL-53**	**Mg-MIL-53**
a (Å)	18.2088(11)	18.191 (2)	18.510(5)
b (Å)	17.7065 (11)	17.177 (2)	16.894(4)
c (Å)	13.3781 (8)	13.6923 (17)	13.924(6)
β (deg)	128.438	129.7410 (10)	130.542(3)
v ($Å^3$)	3378.52 (34)	3289.8 (7)	3308.8(18)
dimensions of channel (Å)	13.24 × 17.71	13.69 × 17.17	13.92 × 16.89
M–O distances (Å)	2.110—2.263	2.051—2.172	2.023—2.196

Table S2 Crystal Data and Structure Refinement Parameters for **1**, **1a**, **2**, **2'**, **3**, **3'**, **4** and **4'**

Compound	**1**	**1a**	**2**	**3**	**4**	**2'**	**3'**	**4'**
Formula	$C_{32}H_{30}Mg_2N_4O_{12}$	$C_{26}H_{16}Mg_2N_2O_{10}$	$C_{28}H_{22}Mg_2N_4O_{14}$	$C_{30}H_{26}Mg_2N_4O_{14}$	$C_{38}H_{26}Mg_2N_4O_{14}$	$C_{32}H_{30}Mg_2N_4O_{12}$	$C_{32}H_{30}Mg_2N_4O_{12}$	$C_{32}H_{30}Mg_2N_4O_{12}$
Fw	711.22	565.03	687.12	715.17	811.25	711.22	711.22	711.22
space group	*C*2/*c* (No. 15)	*C*2/*c* (No. 15)	*C*2/*c* (No. 15)	*C*2/*c* (No. 15)	*C*2/*c* (No. 15)	*C*2/*c* (No. 15)	*C*2/*c* (No. 15)	*C*2/*c* (No. 15)
a (Å)	18.510(5)	17.608(8)	16.557(2)	17.3288(19)	19.2119(13)	18.0541(16)	18.1876(15)	18.1190(16)
b (Å)	16.894(4)	17.506(7)	18.311(3)	17.7491(19)	16.1935(11)	17.2527(14)	17.2441(14)	17.2294(15)
c (Å)	13.924(6)	12.967(5)	11.9349(17)	12.8570(14)	14.0617(17)	13.4128(11)	13.5313(11)	13.4780(12)
β (deg)	130.542(3)	127.619(6)	123.096(2)	126.530(2)	130.1130(1)	129.2740(10)	129.5050(10)	129.380(10)
v (Å^3)	3308.8(18)	3166(2)	3031.4(7)	3177.6(6)	3345.7(5)	3234.2(5)	3274.4(5)	3252.2(5)
Z	4	4	4	4	4	4	4	4
ρcalc (Mg/m^3)	1.428	1.185	1.506	1.495	1.611	1.461	1.443	1.453
μ (mm^{-1})	0.143	0.127	0.158	0.154	0.157	0.147	0.145	0.146
F (000)	1480	1160	1416	1480	1672	1480	1480	1480
*R*int	0.0366	0.0561	0.0541	0.0458	0.0333	0.0285	0.0422	0.0353
R_1, wR_2 [$I > 2\sigma(I)$]	R_1 = 0.0647, wR_2 = 0.1824	R_1 =0.0762, wR_2 = 0.2315	R_1 =0.0696, wR_2 = 0.1866	R_1 =0.0614, wR_2 = 0.1588	R_1 = 0.0930, wR_2 = 0.2772	R_1 =0.0631, wR_2 = 0.1862	R_1 = 0.0659 wR_2 = 0.1852	R_1 = 0.0666, wR_2 = 0.1886
R_1, wR_2 (all data)	R_1 = 0.0802, wR_2 = 0.1966	R_1 =0.1127, wR_2 = 0.2674	R_1 =0.0997, wR_2 = 0.2167	R_1 = 0.0883, wR_2 = 0.1804	R_1 =0.1069, wR_2 = 0.2933	R_1 =0.0713, wR_2 = 0.1962	R_1 = 0.0832, wR_2 = 0.2021	R_1 = 0.0799, wR_2 = 0.2005

Note: For the structures of 1, 1a and 2, there are several A or B technical section. In most cases, these A or B technical alerts are inevitable. (1) In structure of 1, since C15' and C16' are split atoms, we could not add the hydrogen on them. (2) In structure of 2, because benzene rings are largely distorted, the distances of C14 -C19 are smaller than the normal value 1.38.



Hydrogen bonding interactions in **Mg-MIL-53** complex

D—H…A	*d*(H…A) (Å)	*D*(D…A) (Å)	∠DHA (°)
C10—H10…O6	2.477	3.366	160.631
C12—H12…O6	2.435	3.329	160.977

Figure S1. Detail of Hydrogen bonding of guest-host interactions in **Mg-MIL-53** compound. The paired DMF molecules in three compounds (**Mn/Co/Mg-MIL-53**) are antiparallel and their packings along the 1D channels might be dictated by their dipole-dipole interactions complemented by C−H…O hydrogen bondings between DMF molecules and BPNO linkers.

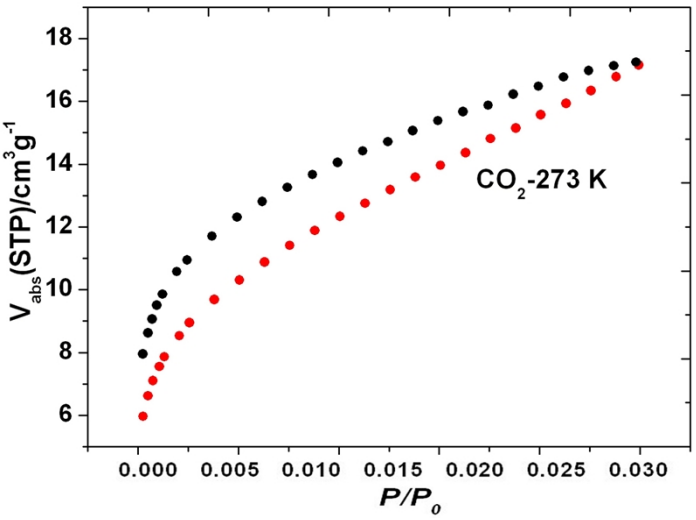


Figure S2. CO_2 adsorption isotherm of desolvated **1** at 273 K

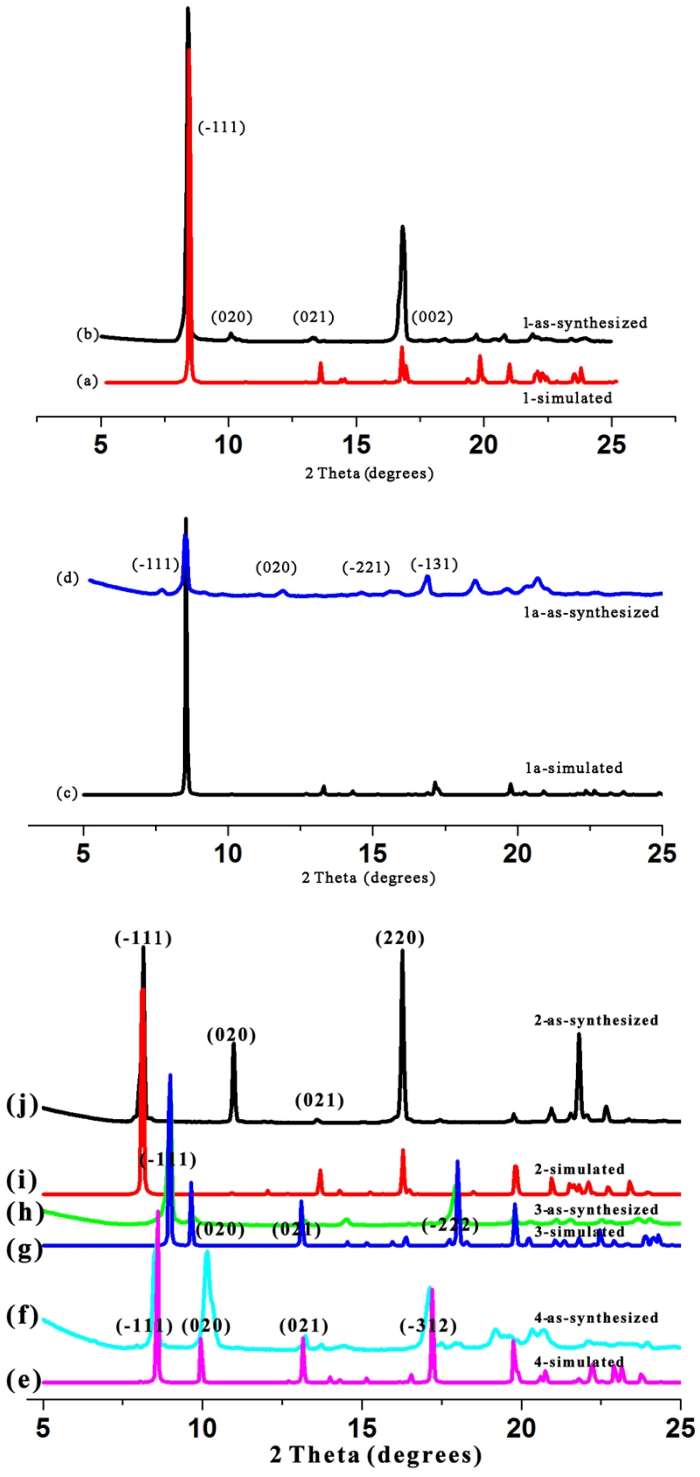


Figure S3. PXRD pattern of **1** in different states; (a) simulated from X-ray single crystal data of **1**, (b) as-synthesized **1**, (c) simulated from X-ray single crystal data of **1a**, (d) as-synthesized **1a**, (e) simulated from X-ray single crystal data of **4**, (f) as-synthesized **4**, (g) simulated from X-ray single crystal data of **3**, (h) as-synthesized **3**, (i) simulated from X-ray single crystal data of **2**, (j) as-synthesized **2**, respectively.

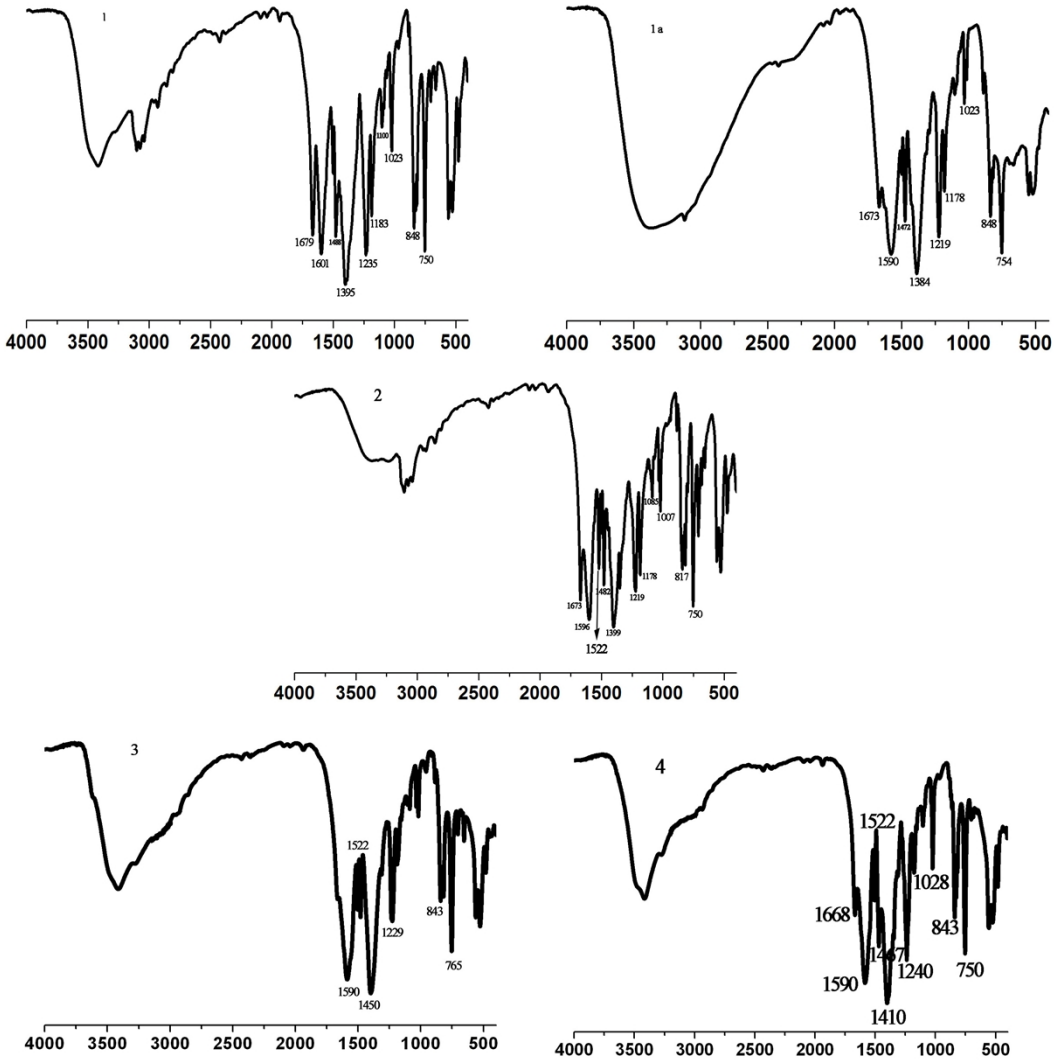


Figure S4. IR spectra of the complexes for **1**, **1a** (up) and **2, 3, 4** (down). FT-IR (KBr): The characteristic absorption peak at ν = 1522 (cm^{-1}) indicate the appearance of the N=O stretch.

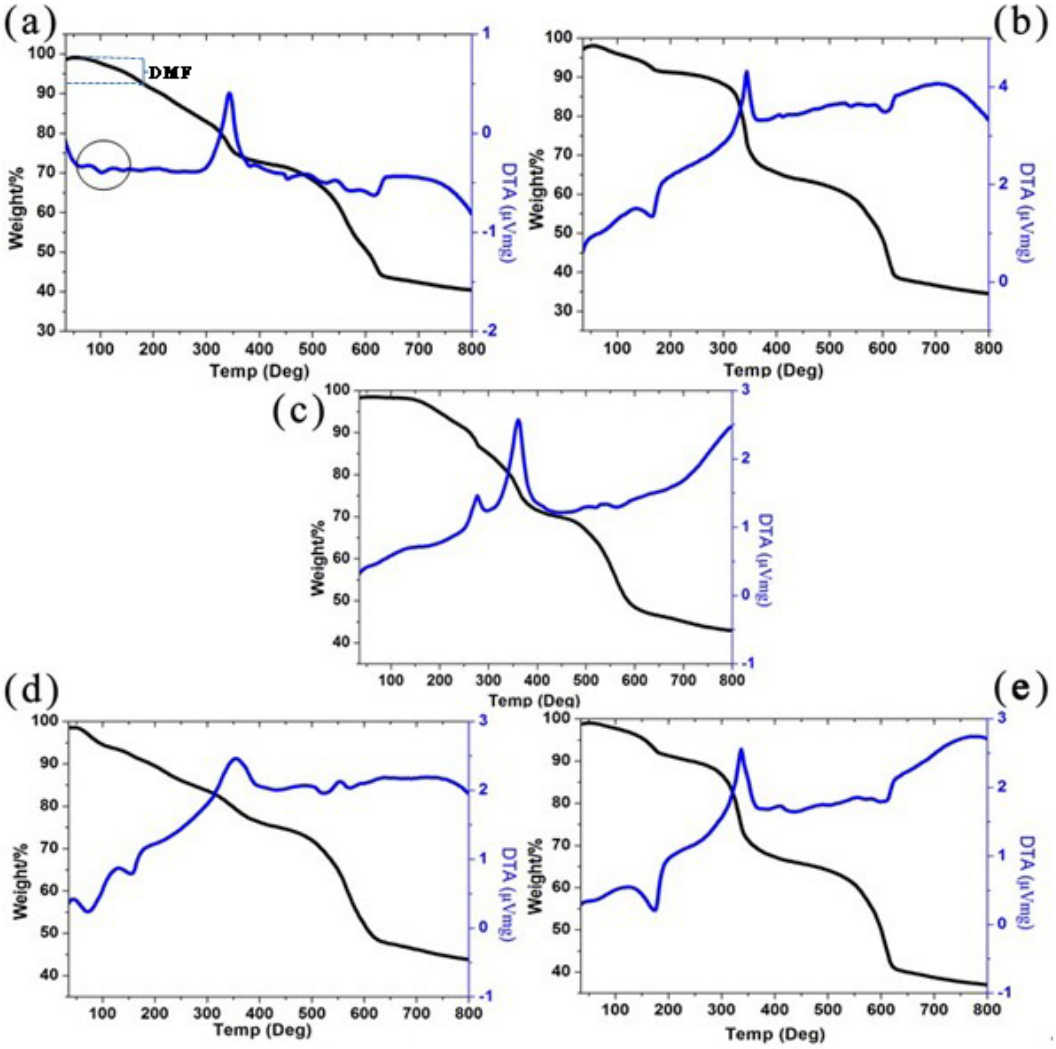


Figure S5. TG-DTA curves of **1** (a), **1a** (b), **2** (c), **3** (d) and **4** (e) at the heating rate of 10 °C/min. The endothermic peaks in (b), (d) and (e) between 150 and 200°C could be attributed to the release of remnant DMF molecules in (b) or guest NM and NE molecules in (d) and (e). The exothermic peak between 250 and 300°C is believed to be due to the self-oxidation of NB because of high evaporation point of NB and the presence of -NO_2 group within the molecule.

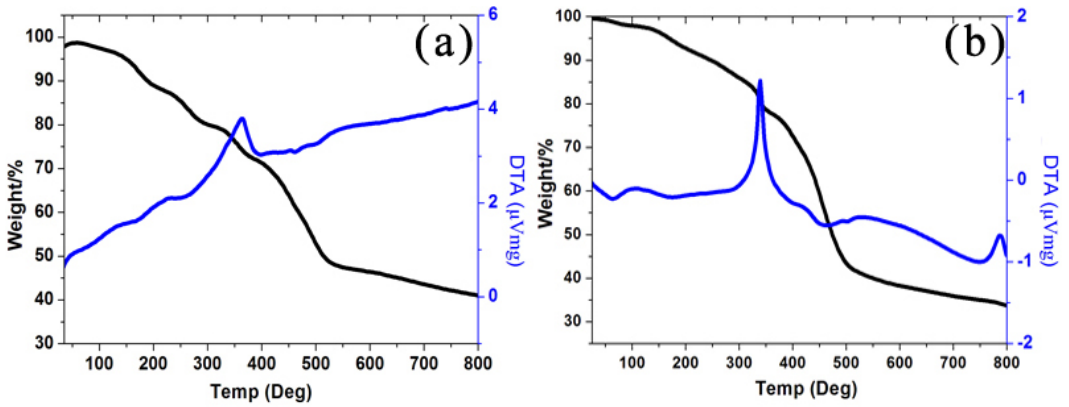


Figure S6. TG-DTA curves of **Mn-MIL-53** (a) and **Co-MIL-53** (b) at the heating rate of 10 °C per min.

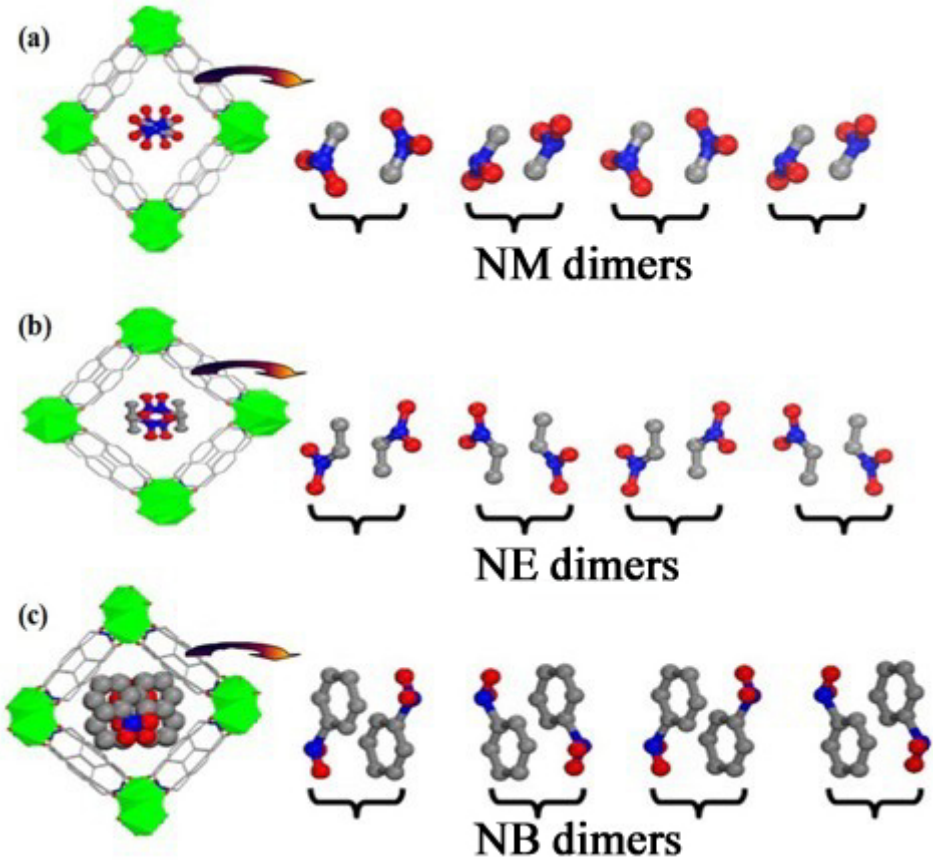


Figure S7. Columnar arrays of nitro guest molecules forming dimers in channels of **1a**: (a) NM, (b) NE and (c) NB, respectively.

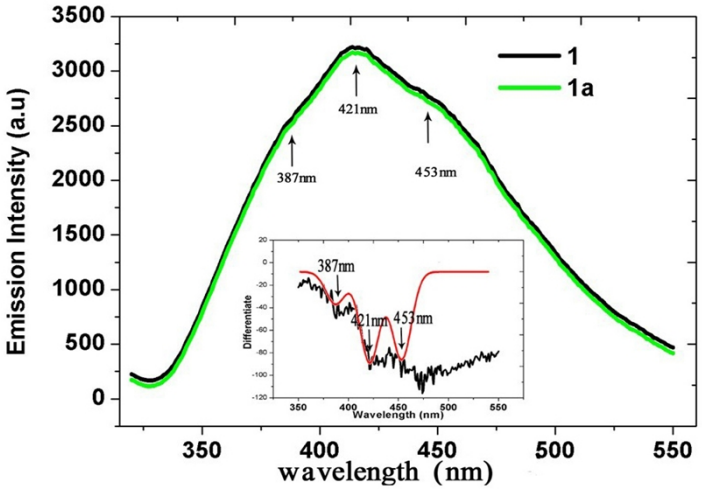


Figure S8. Fluorescence emission of as-made sample **1** (black), guest-free sample **1a** (green). Inset: its derivatives of **1a** with solid red lines showing the simulated fit to the experimental data.

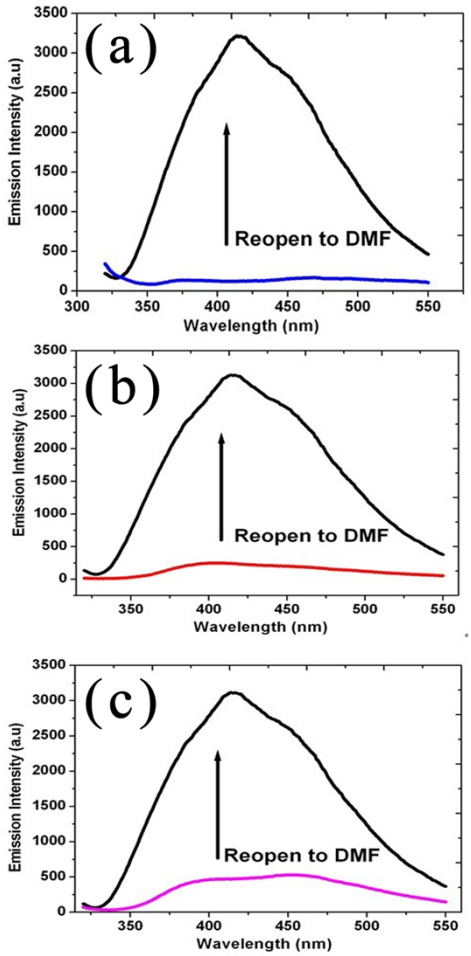


Figure S9. A recovery of fluorescence after removal from NB molecules (a), NM molecules (b) and NE molecules (c) reopen to DMF.

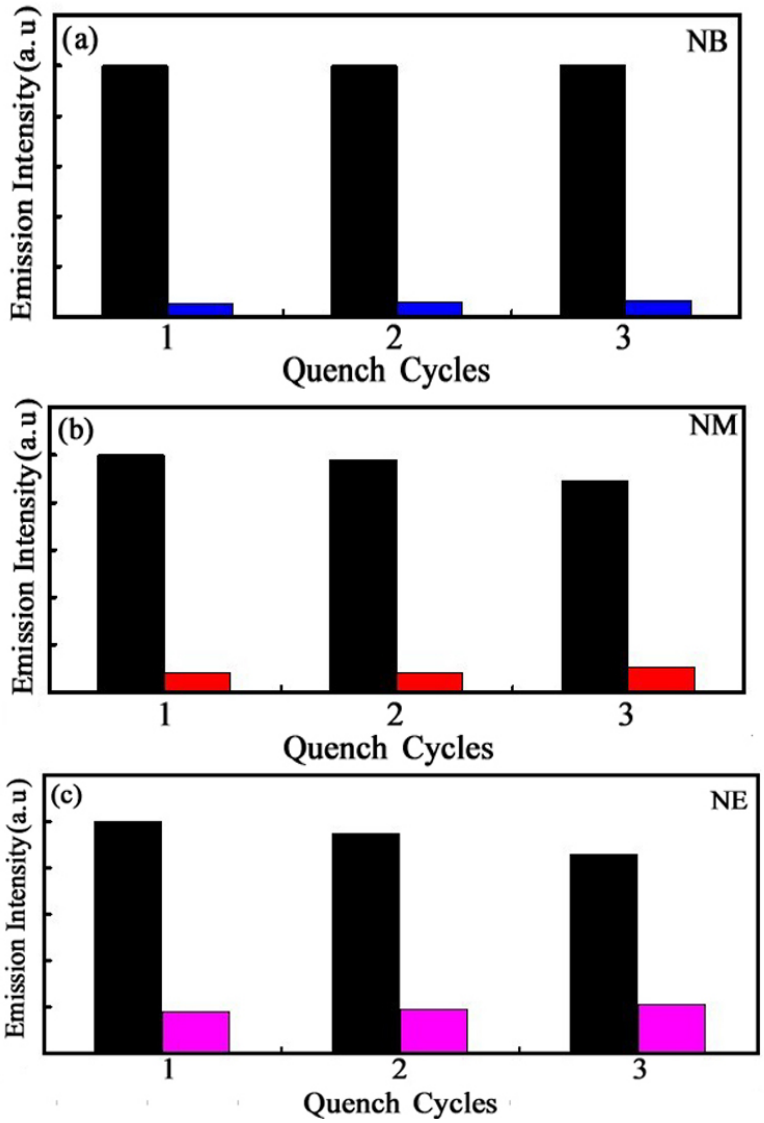


Figure S10. Three continuous cycles of quenching-recovery test of the desolvated **1**. The quenching was performed by exposing of the desolvated **1** to a saturated vapor of NB molecules (a), NM molecules (b) and NE molecules (c) for 8 minutes. After each cycle of quenching, the fluorescence of the desolvated **1** was recovered by immersing it into DMF.