

Electronic Supplementary Information

Size-exclusive and coordination-induced selective dyes adsorption in a nanotubular metal-organic framework

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Table S1. Crystal Data and Structure Refinement Details of BUT-51.

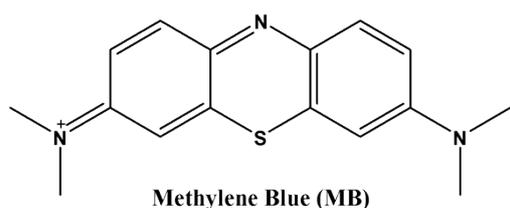
BUT-51	
Formula	C ₃₂ H ₁₈ Co ₂ N ₃ NaO ₁₂
Fw	777.34
temp/K	173(2)
cryst syst	tetragonal
space group	<i>P4</i> ₂ / <i>m</i>
<i>a</i> (Å)	14.8967(2)
<i>c</i> (Å)	10.0502(3)
<i>V</i> (Å ³)	2230.26(8)
<i>Z</i>	2
<i>D_c</i> (mg·m ⁻³)	1.158
<i>μ</i> /(mm ⁻¹)	6.367
<i>F</i> (000)	784
rflns collected	4616
unique rflns	2308
<i>R</i> _{int}	0.0275
GOF on <i>F</i> ²	1.060
<i>R</i> ₁ ^a (<i>I</i> >2σ(<i>I</i>))	0.0632
<i>wR</i> ₂ ^a	0.1874

$${}^a R_1 = \frac{\sum (|F_o| - |F_c|)}{\sum |F_o|} \quad wR_2 = [\sum w(|F_o|^2 - |F_c|^2)^2 / \sum w|F_o|^2]^{1/2}.$$

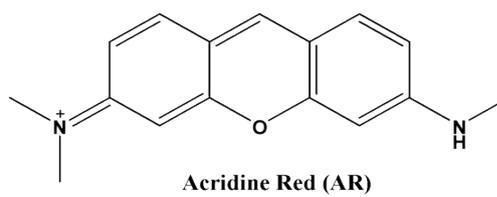
Table S2. Selected bond distances (Å) and angles (°) in BUT-51.

BUT-51			
Co(1)–O(4)	2.036(5)	Co(1)–N(1) ^{#2}	2.003(7)
Co(1)–O(1)	2.065(3)	Co(1)–O(3)	2.379(5)
Na(1)–O(1)	2.445(3)	Na(1)–O(1) ^{#1}	2.114(9)
Na(1)–O(3)	2.445(3)		
O(4)–Co(1)–O(1)	123.33(13)	O(1) ^{#1} –Co(1)–O(1)	89.50(17)
O(4)–Co(1)–N(1) ^{#2}	112.3(2)	O(1)–Co(1)–N(1) ^{#2}	101.97(13)
O(4)–Co(1)–O(3)	59.3(2)	O(1)–Co(1)–O(3)	83.89(13)
N(1) ^{#2} –Co(1)–O(3)	171.65(19)	O(1) ^{#3} –Na(1)–O(1)	180.0(2)
O(1) ^{#3} –Na(1)–O(1) ^{#1}	107.04(15)	O(1)–Na(1)–O(1) ^{#1}	72.96(15)
O(1)–Na(1)–O(3)	74.55(12)	O(1) ^{#3} –Na(1)–O(3)	105.45(12)

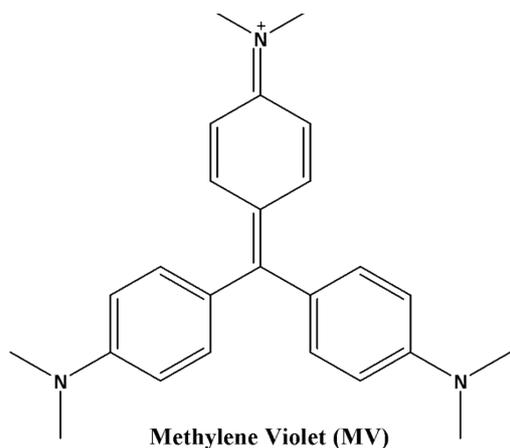
Symmetry codes #1: x, y, -z; #2: -y, x, z - 1/2; #3, -x + 1, -y, -z



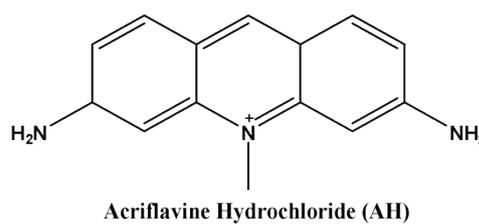
14.3×6.1×4.0 Å



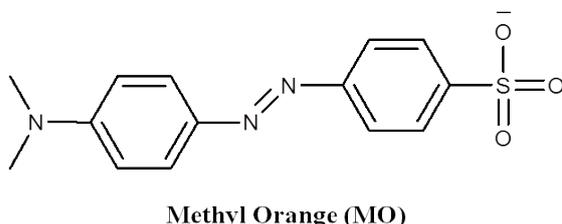
14.2×8.3×3.7 Å



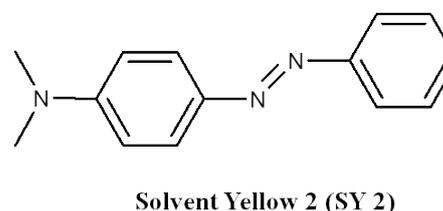
14.8×14.8×5.5 Å



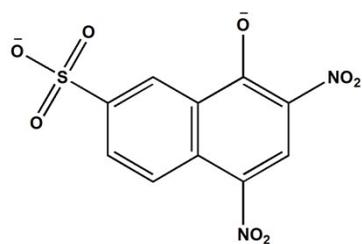
13.5×7.5×3.4 Å



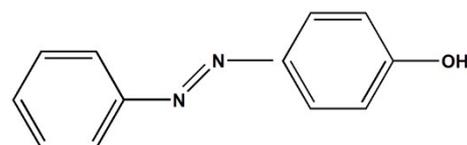
15.8×6.0×4.5 Å



15.1×6.0×4.5 Å



11.4×8.8×4.5 Å



13.1×5.8×4.5 Å

Fig. S1. The structures of dye molecules used in this work and their sizes evaluated from Materials Studio.

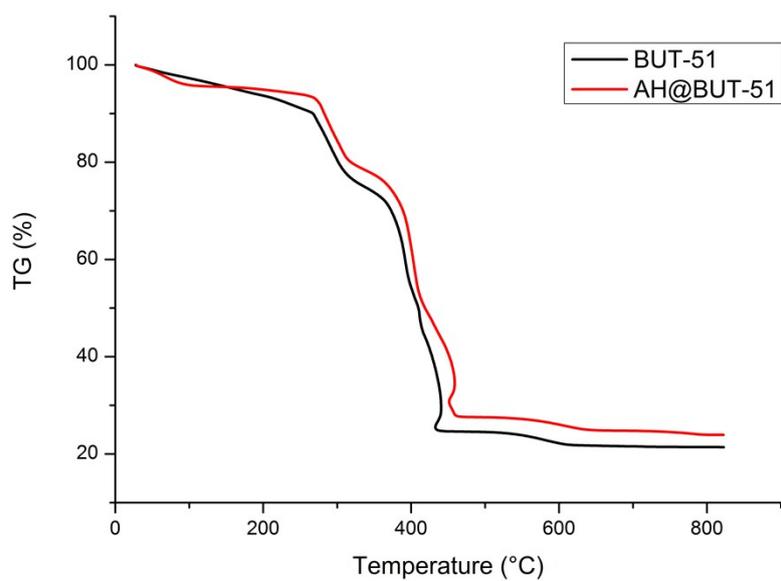


Fig. S2. TGA curves of as-synthesized BUT-51 and AH@BUT-51.

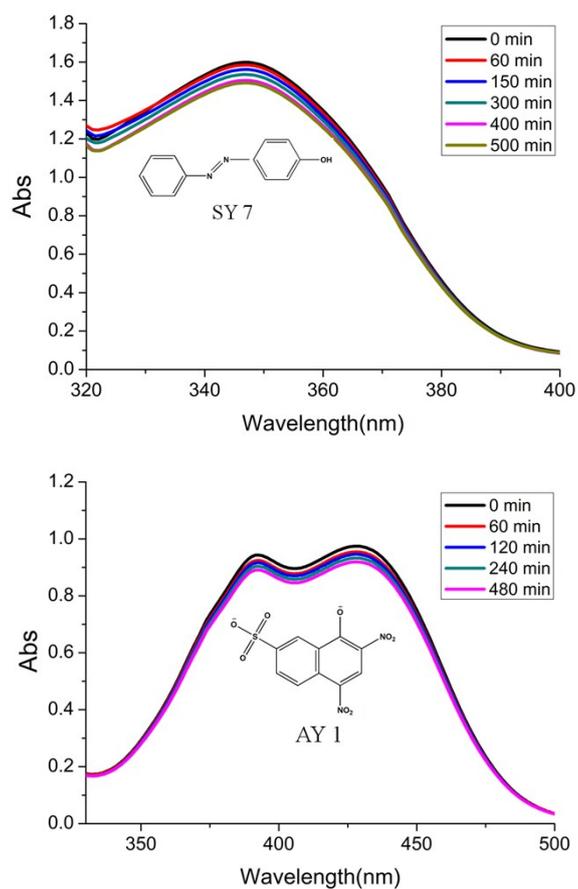


Fig. S3. UV-vis spectra of acetone solutions of SY7 and AY1 in the presence of BUT-51 monitored with time.

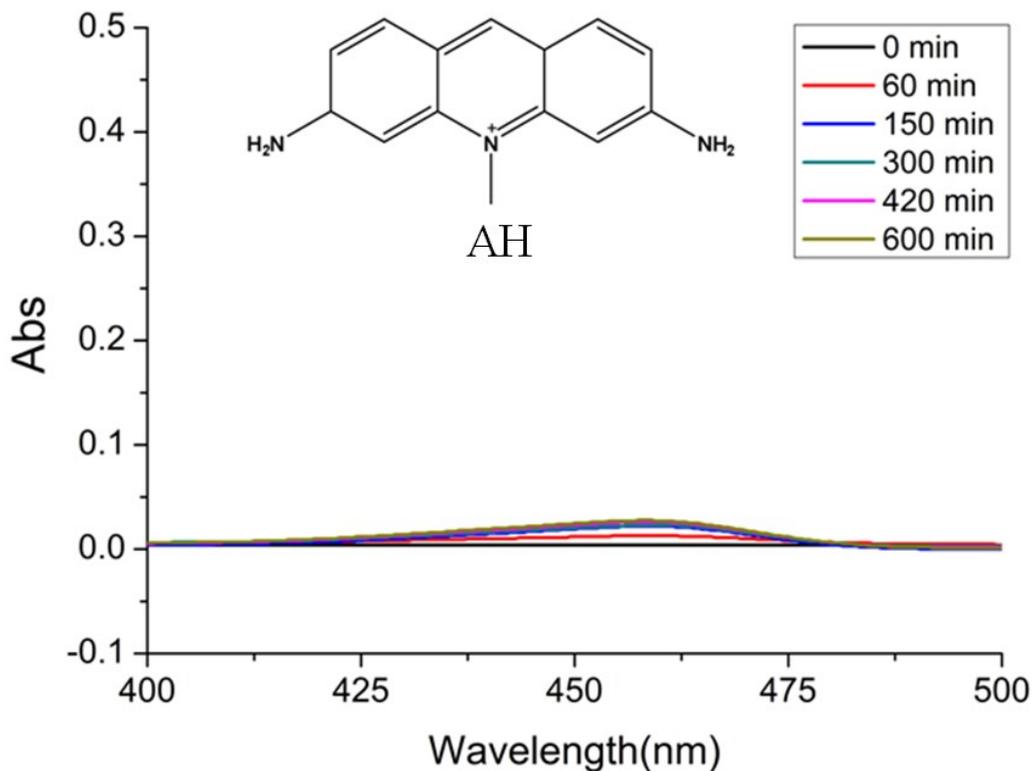


Fig. S4. The dyes release of AH@BUT-51 in the saturated acetone solution of NH_4Cl .

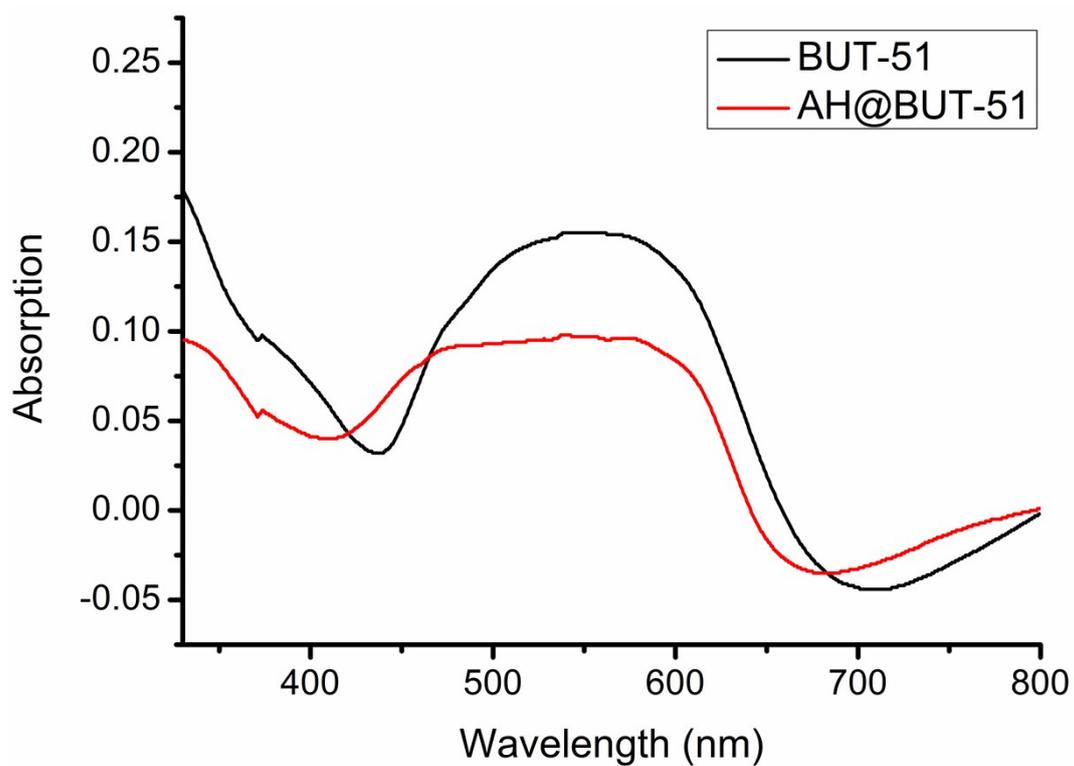


Fig. S5. Solid-state UV-Vis spectra of BUT-51 and AH@BUT-51.