

Supplementary Information

Selective Sacrificial Metal-Organic Framework; Highly Quantitative Colorimetric Naked-Eye Detector for Aluminum Ion in Aqueous Solutions

Farzaneh Rouhani, Fatemeh Rafizadeh-Masuleh and Ali Morsali*

Department of Chemistry, Faculty of Sciences, Tarbiat Modares University, P.O. Box 14115-175, Tehran, Iran

Materials and methods

All ingredients were purchased from companies of chemicals such as Aldrich and Merck and used without further purification. Melting point measurement of the ligands were performed on an Electrothermal 9100 apparatus. The IR spectra (KBr tablet) have been recorded in the range of 4000-400 cm^{-1} by Nicolet Fourier Transform IR, Nicolet 100 spectrometer. Thermogravimetric analysis (TGA) of the structure was recorded by computer-controlled PL-STA 1500 apparatus from 25 to 600 $^{\circ}\text{C}$ with the gradient of 10 $^{\circ}\text{C}/\text{min}$ under neutral N_2 atmosphere into alumina pans. The crystallographic measurements of TMU-60 was performed by the Bruker APEX area-detector diffractometer. Collection of the intensity data were done using graphite monochromated $\text{Mo-K}\alpha$ radiation ($\lambda=0.71073 \text{ \AA}$) at 298 K. The X- XRD measurements were done by a Philips X'pert diffractometer with monochromated $\text{Cu-K}\alpha$ radiation ($\lambda=1.54056 \text{ \AA}$). The adsorption/desorption isotherm of nitrogen gas was measured at liquid N_2 temperature (77 K) using a Micromeritics ASAP 2020 analyzer. The specific surface area was calculated by the Brunauer-Emmett-Teller (BET) method.

Table S.1. Crystal data and structure refinements of TMU-60.

Identification code	TMU-60
Chemical formula	C ₂₁ H ₁₅ N ₂ O ₅ Zn
computing_structure_refinement	SHELXL-2016/6
Chemical formula weight	420.38
T(K)	293.2
Crystal syst	Orthorhombic
Space group	I _{bca}
a (°A)	17.6350(15)
b (°A)	22.345(2)
c (°A)	22.944(2)
α (deg)	90
β (deg)	90
γ (deg)	90
V (Å ³)	9041.18
Z	16
F(000)	3600
R(int)	0.0448
Goodness-of-fit on F^2	1.103
wR factor	0.1080
CCDC number	1862166

Table S.2. Selected bond lengths (Å) and angles (°) for TMU-60.

Bond		Angle	
Zn ₁ -O ₃	2.046(2)	C ₁₇ -C ₁₉ -C ₂₀	122.34
Zn ₁ -N ₁	2.026(2)	C ₁₉ -C ₂₀ -C ₂₀	124.80
C ₂₀ -C ₂₀	1.371(3)	C ₂₀ -C ₂₀ -N ₂	120.65
C ₂₀ -N ₂	1.391(3)	C ₂₀ -N ₂ -C ₂₁	116.34
C ₂₁ -N ₂	1.438(4)	N ₂ -C ₂₁ -C ₂₁	110.70
C ₂₁ -C ₂₁	1.496(8)	C ₇ -O ₅ -C ₈	118.50
N ₂ -H ₂	0.820(3)	C ₆ -C ₇ -O ₅	122.95

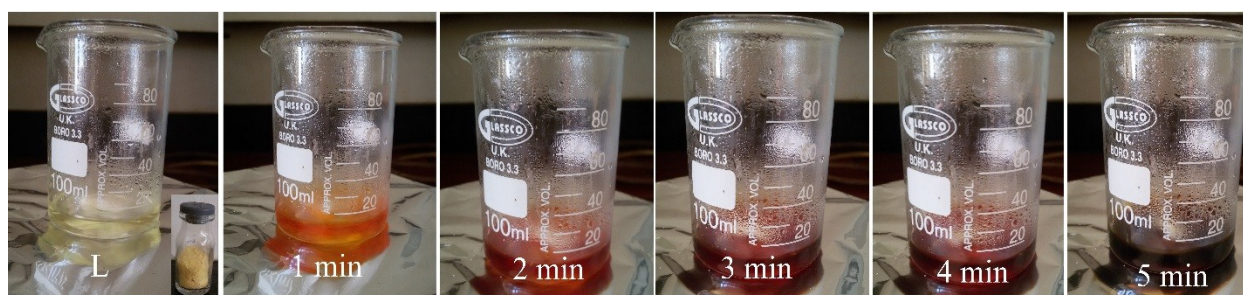


Figure S.1. Steps of convert L to L* in the presence of NaCN and heat in DMF.

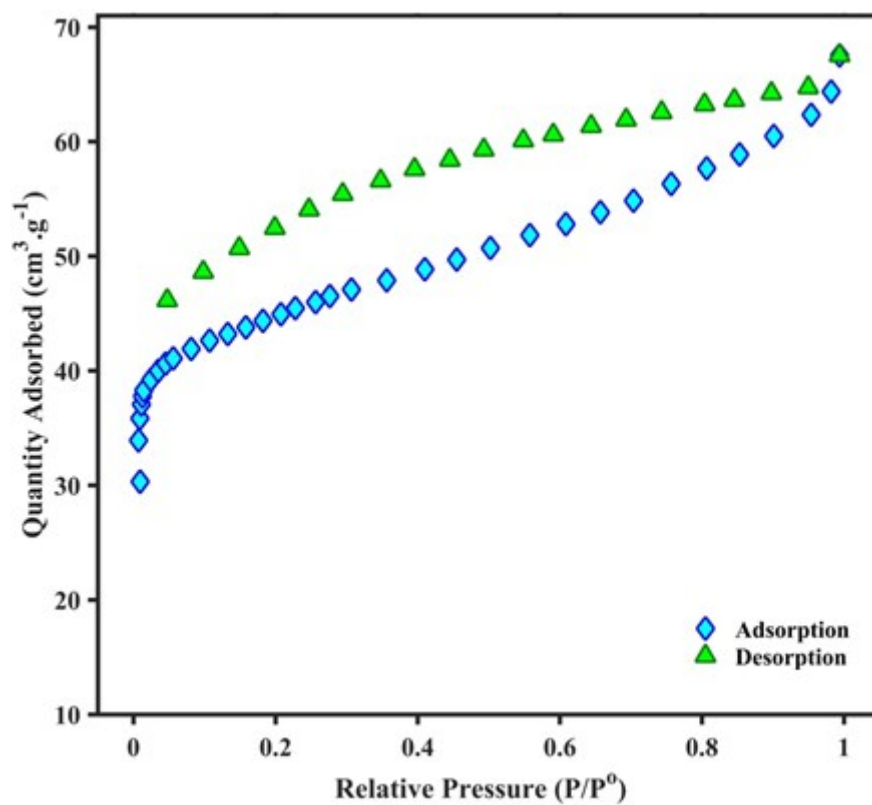


Figure S.2. N₂ adsorption-desorption isotherms of TMU-60 after activation.

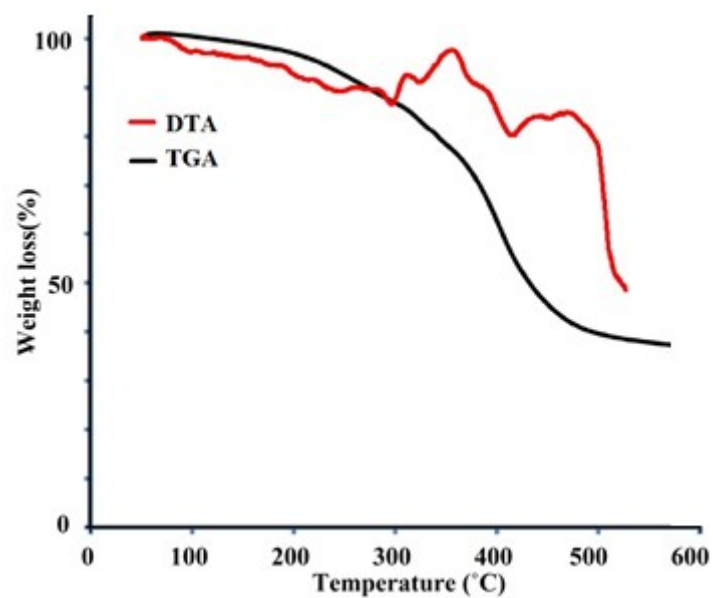


Figure S.3. The TGA and DTA curves of TMU-60.

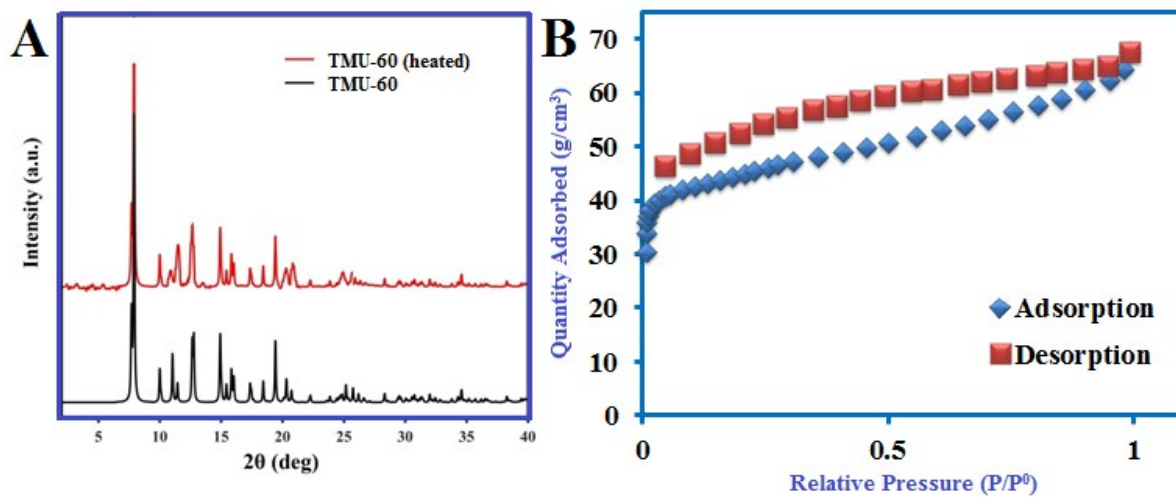


Figure S.4. The XRD pattern and BET of TMU-60 placed at 250°C for 12 hours.

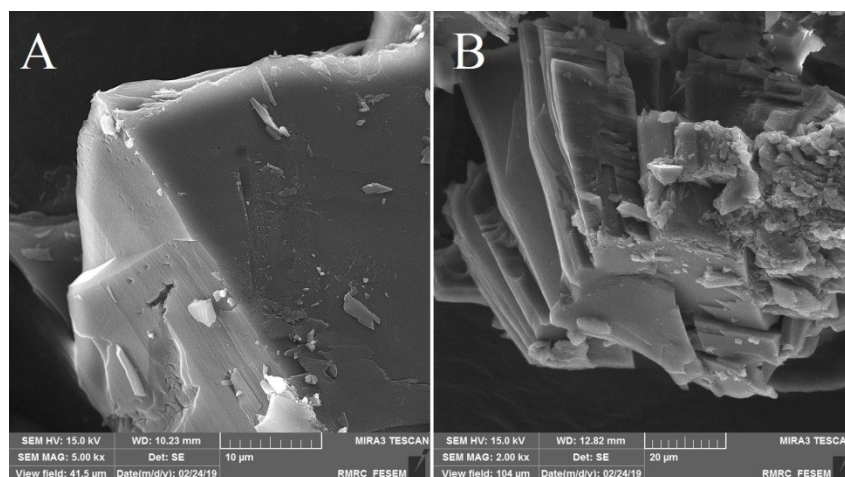


Figure S5. SEM images of TMU-60 power before (A) and after (B) of immersion in Al(III) aqueous solution.

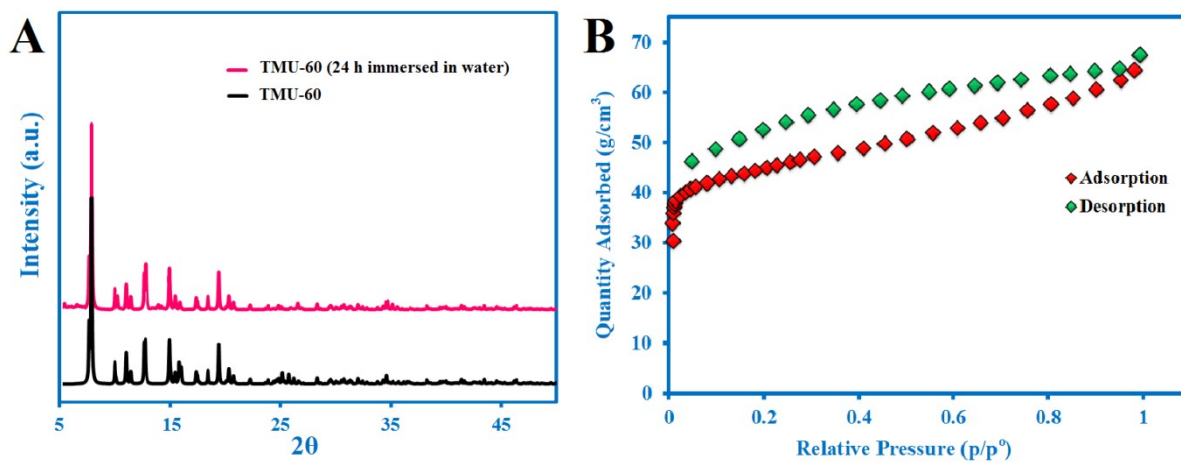


Figure S.6. The XRD pattern and BET of TMU-60 after 24 h immersion in water.

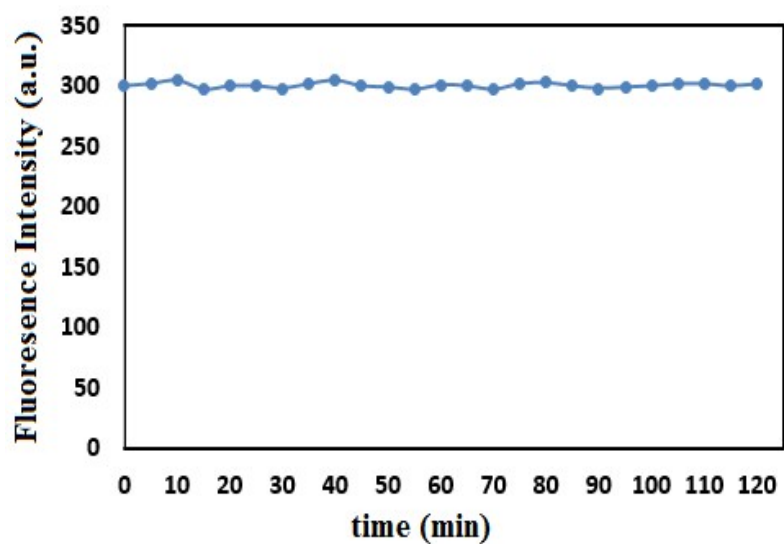


Figure S.7. Photostability of TMU-60 after 2 hours irradiation with 330 nm light for with 5 min duration for each time.

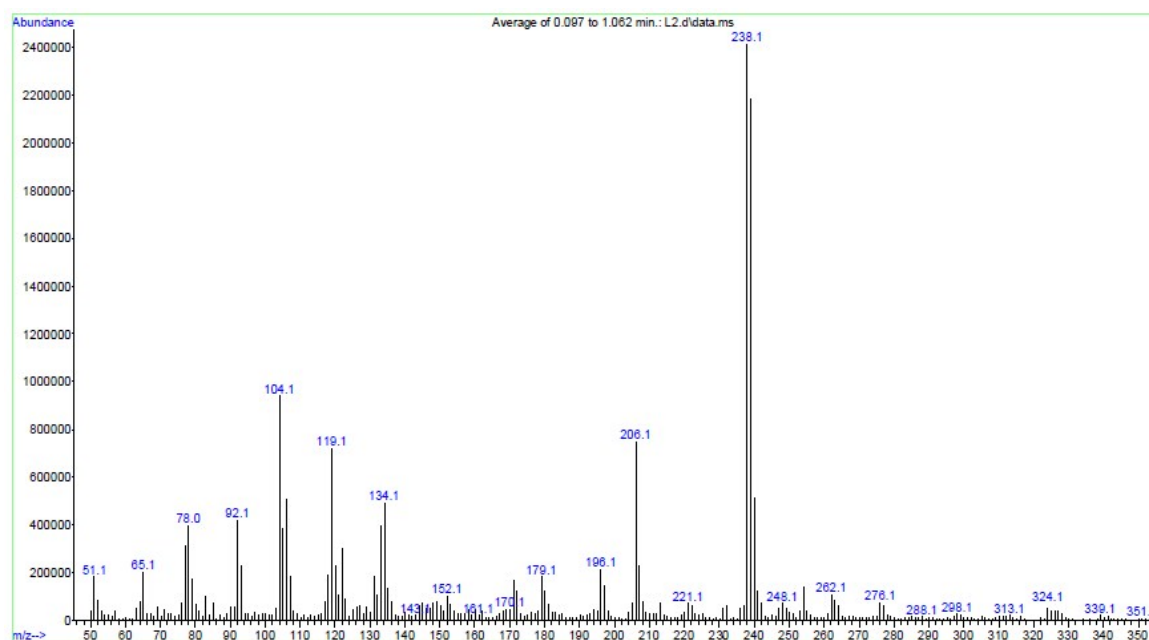


Fig S.8. The Mass Spectrum of L*.



Fig S.9. ¹H NMR spectrum of L* in DMSO as solvent.