Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.
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Electronic Supplementary Information

Experimental

Methods and instrumentation

ESI mass spectrometry was performed with Thermo Electron Corporation Finnigan LTQ. ^{1}H-NMR and ^{19}F-NMR spectra were recorded on a JOEL JNM-ECA600 NMR spectrometer. Single-crystal X-ray characterization was performed on a Bruker SMART APEX charge-coupled device (CCD) diffractometer equipped with graphite monochromatized Mo K_α radiation. The absorption and photoluminescence (PL) spectra were performed with a UV-vis spectrophotometer (Agilent 8453) and a fluorospectrophotometer (Jobin Yvon, FluoroMax-3), respectively. The excited state lifetimes were measured on a transient spectrofluorimeter (Edinburgh Instruments, FLSP920) with time-correlated single-photon counting technique at the peak emitting wavelength. Photoluminescent quantum yields (PLQYs) in degassed acetonitrile solution (1×10^{-5} M) were calculated with $[Ru(bpy)_3]Cl_2$ (φ = 4.0 % in non-degassed water) as the reference. PLQYs in neat film were measured at the excitation wavelength of 400 nm, using a Quantaurus-QY C11347-11. Cyclic voltammetry was performed on a Princeton Applied Research potentiostat/ galvanostat model 283 voltammetric analyzer in degassed N,N-dimethyl formamide (DMF) solution (1×10^{-3} M) at a scan rate of 100 mV s^{-1} with a platinum plate as the working electrode, a silver wire as the pseudo-reference electrode and a platinum wire as the counter electrode. The supporting electrolyte was tetrabutylammonium perchlorate (0.04 g mL^{-1}) and ferrocene was selected as the internal standard.

Device fabrication and characterization

OLEDs were fabricated on cleaned and ultraviolet-ozone-treated glass substrates precoated with an indium tin oxide (ITO) anode with a sheet resistance of ca. 20 Ω per sq. Then all the layers were fabricated in the vacuum chamber under a low pressure of about 1×10^{-4} Pa. The current density-voltage-luminance (*J*-*V*-*L*) characteristics of the devices were measured with Keithley 4200 semiconductor system, and EL spectra were collected with a Photo Research PR705 spectrophotometer in ambient atmosphere without further encapsulations.

Supplementary Scheme and Figures.

Scheme S1. Synthetic routes of the pop ligand, **1** and **2**.

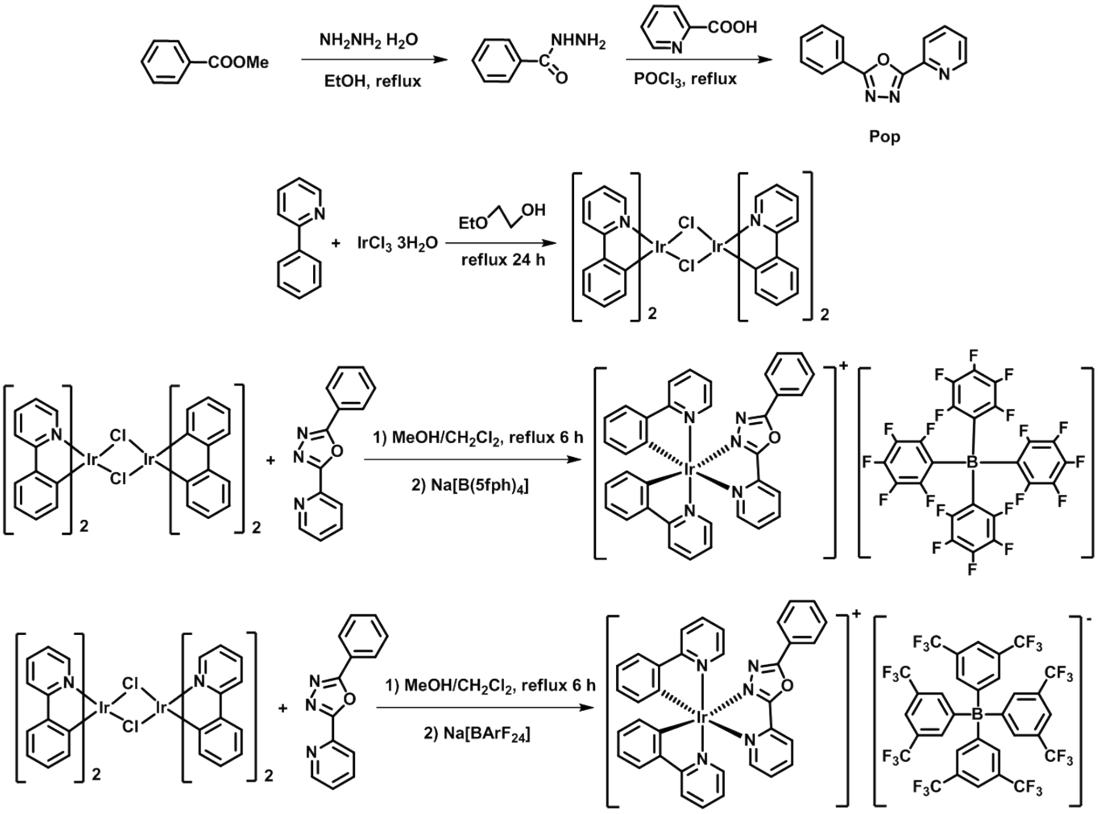
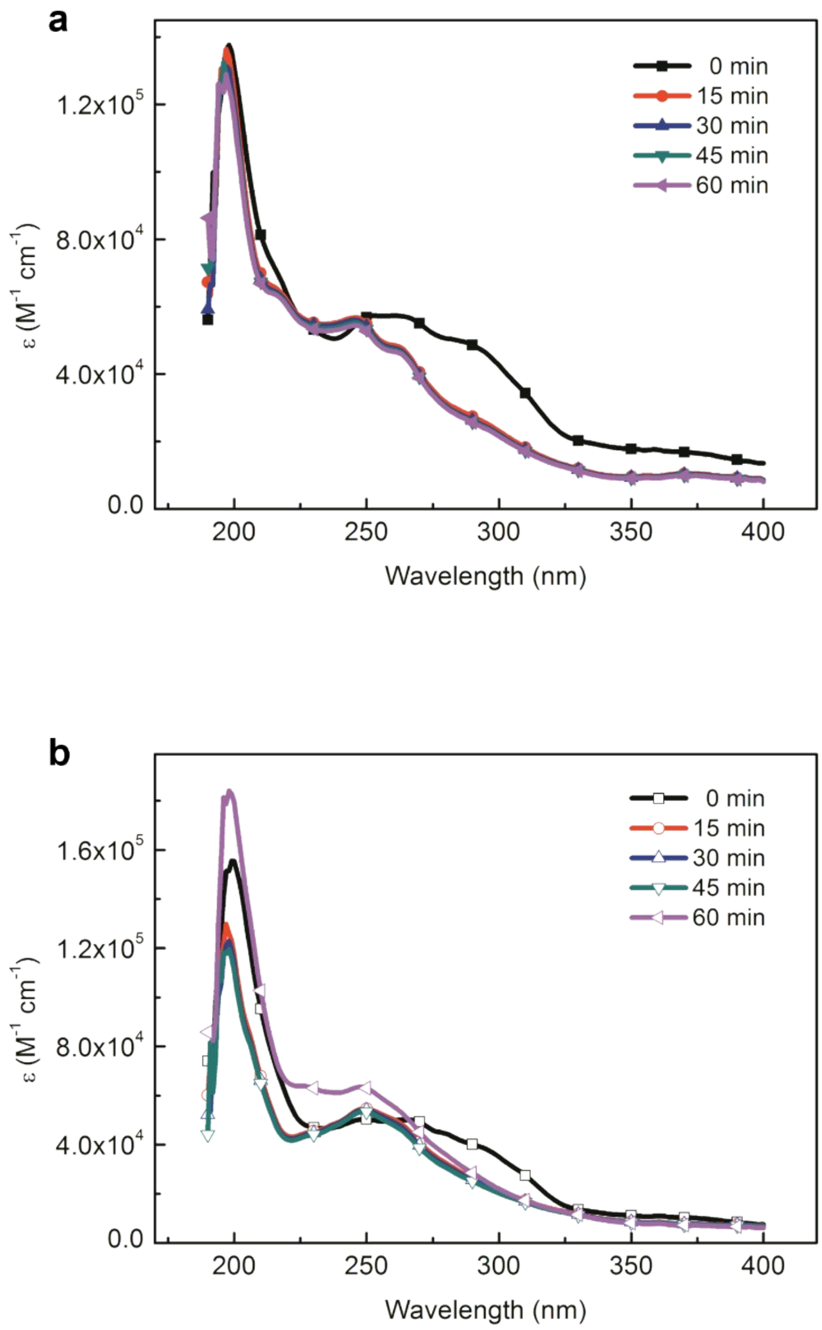
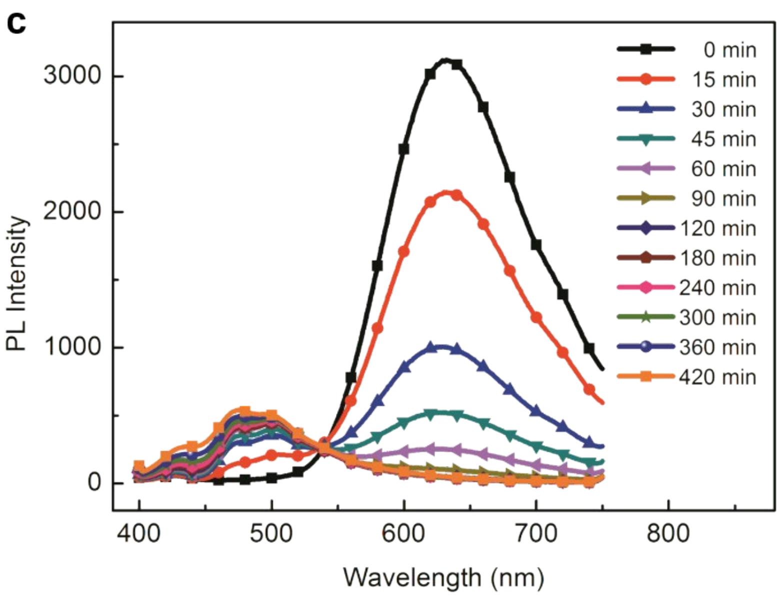


Figure S1. (a-b) Absorption and (c-d) photoluminescence spectra of **1** and **2** in acetonitrile solution (10^{-5} M) under UV irradiation (p_e = 500 W, λ = 365 nm).




c
PL Intensity
0
1000
2000
3000
400
500
600
700
800
Wavelength (nm)
0 min
15 min
30 min
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180 min
240 min
300 min
360 min
420 min

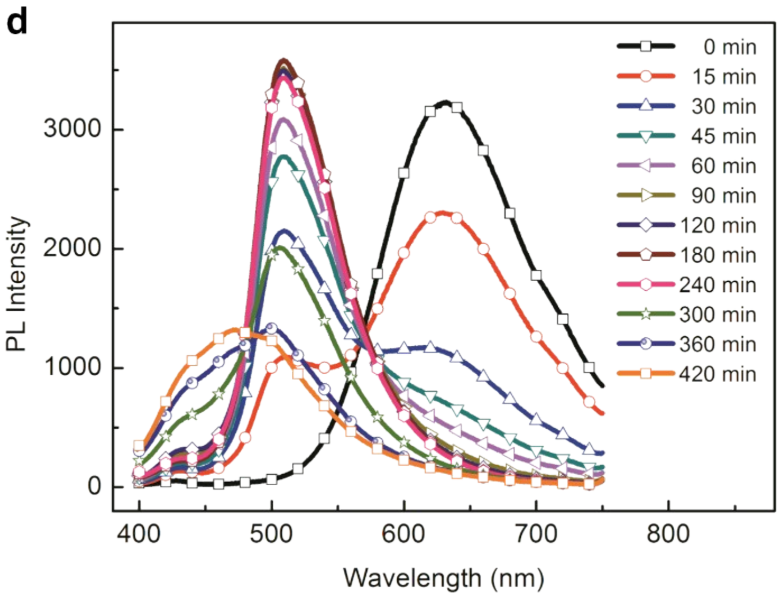

d
PL Intensity
0
1000
2000
3000
400
500
600
700
800
Wavelength (nm)
0 min
15 min
30 min
45 min
60 min
90 min
120 min
180 min
240 min
300 min
360 min
420 min

Figure S2. Photoluminescence spectra of (a) **1** and (b) **2** in solid states under UV irradiation (p_e = 500 W, λ = 365 nm).

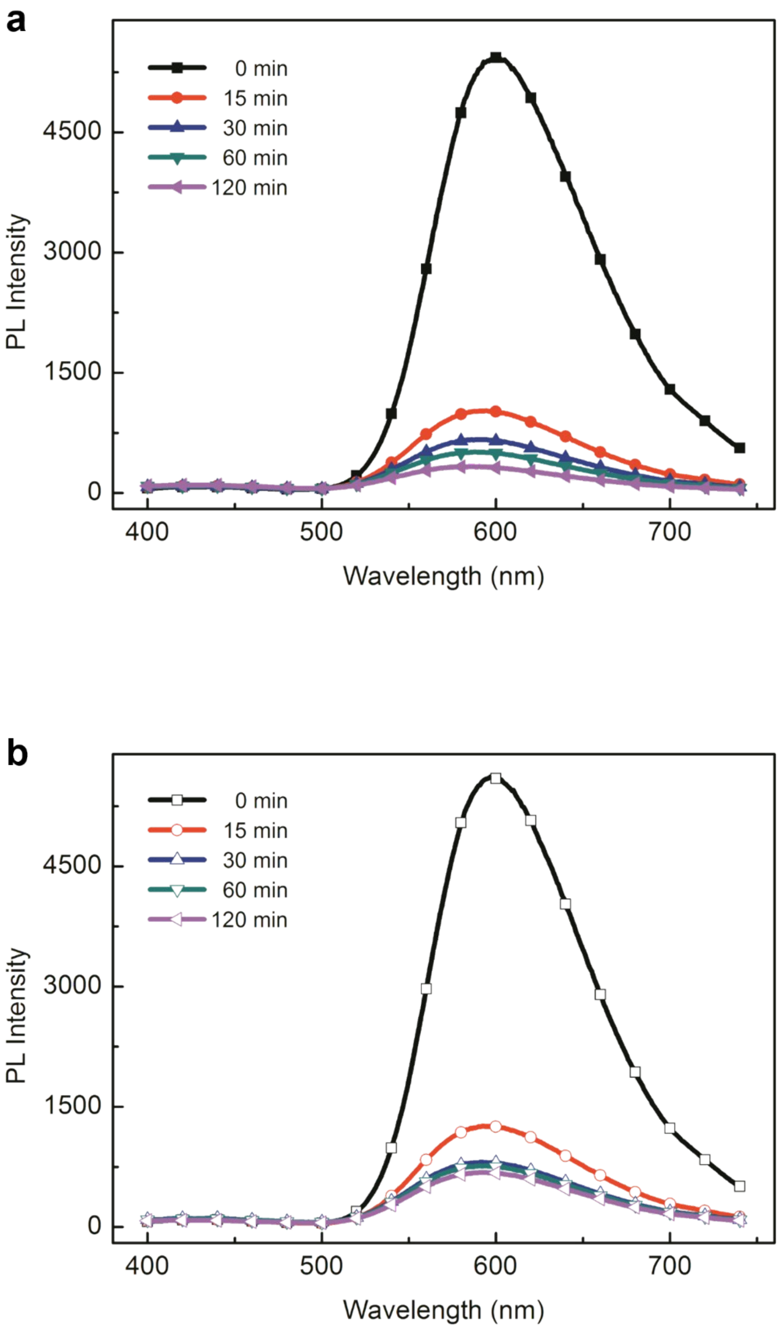
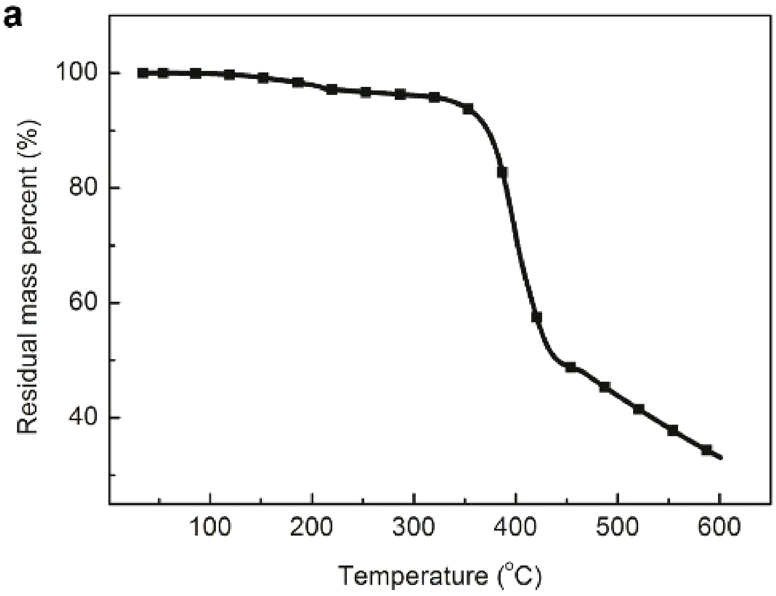
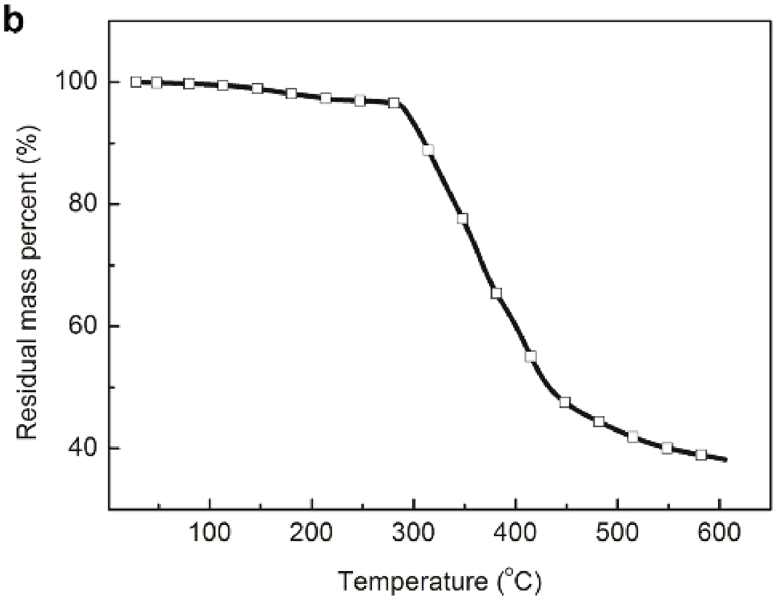
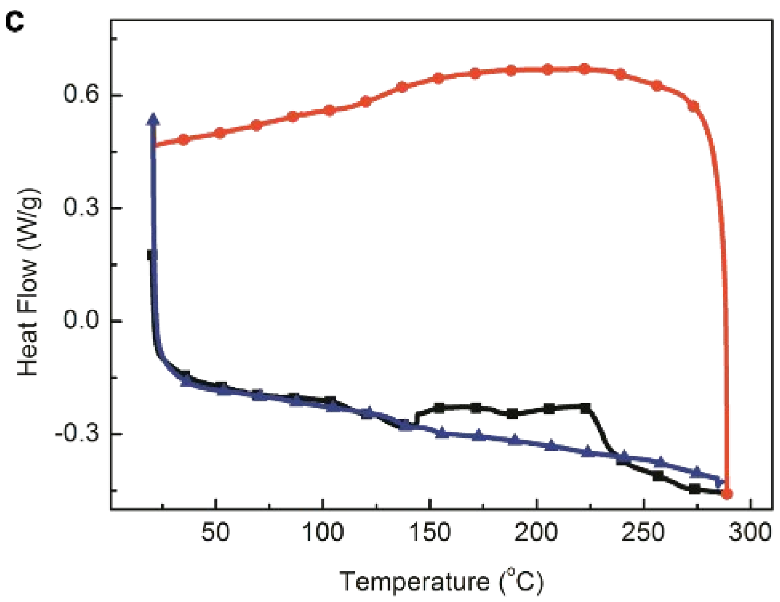


Figure S3. (a-b) Thermal gravimetric analysis (TGA) and (c-d) differential scanning calorimetry (DSC) curves of **1** and **2** under a dry nitrogen gas flow at a heating rate of 10 ^{o}C min^{-1}. First time heat the materials up to 290 ^{o}C (black square), then cool to room temperature (red circle), and second time heat up to 290 ^{o}C (blue triangle).






c
Heat Flow (W/g)
0.6
0.3
0.0
-0.3
50
100
150
200
250
300
Temperature (°C)

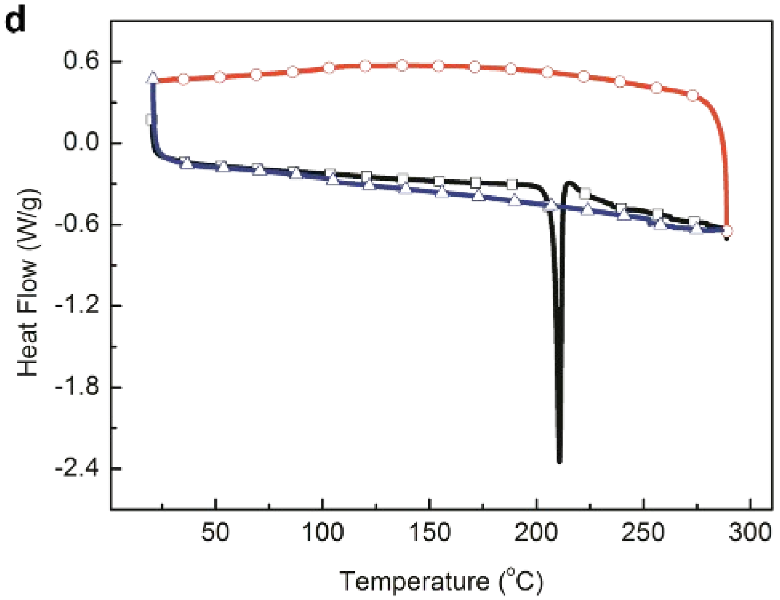

d
Heat Flow (W/g)
0.6
0.0
-0.6
-1.2
-1.8
-2.4
50
100
150
200
250
300
Temperature (°C)

Figure S4. Cyclic voltammogram of (a) **1** and (b) **2** in degassed N, N-dimethyl formamide (DMF) solution (1×10^{-3} M). Potentials were recorded *versus* the ferrocenium/ ferrocence (Fc^+/ Fc) couple.

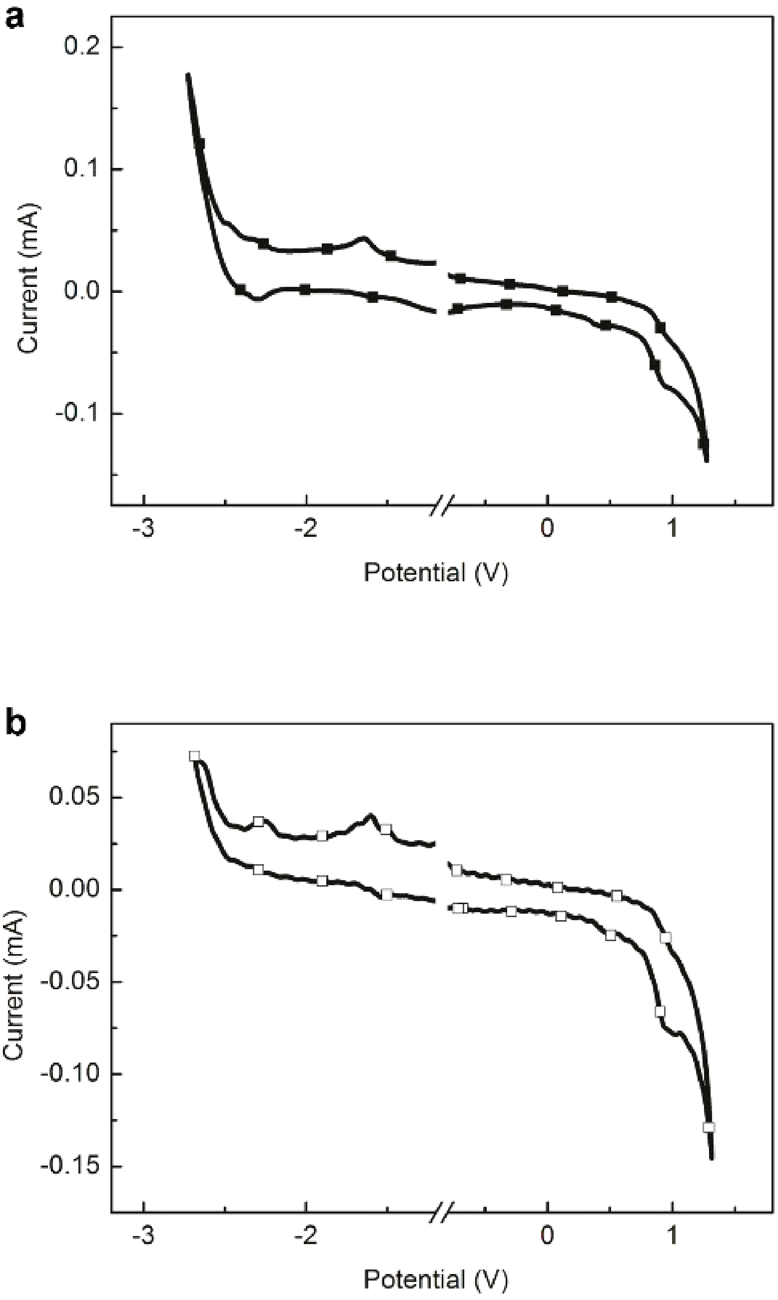
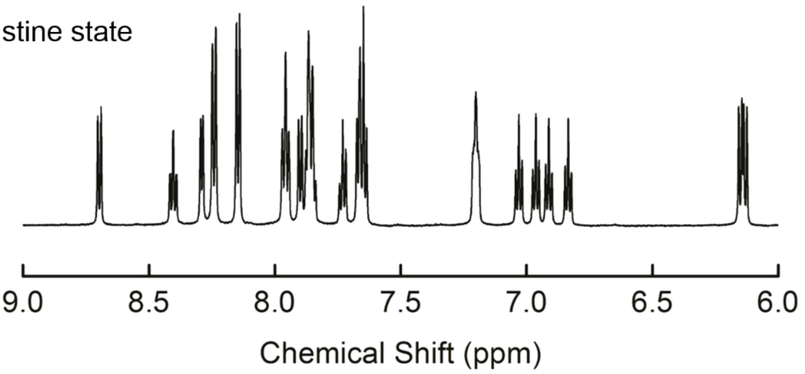


Figure S5. ^1H NMR spectra of **1** in the pristine state and after sublimation.

In the pristine state



After sublimation

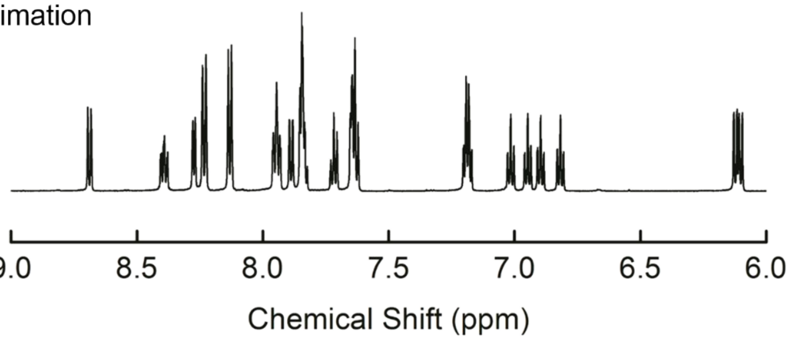
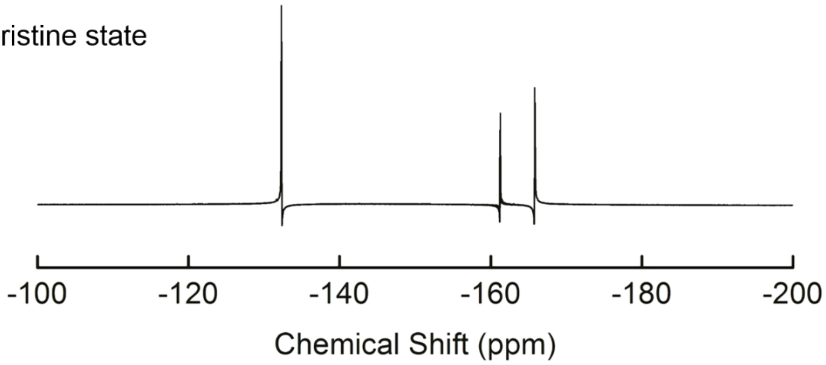


Figure S6. ^{19}F NMR spectra of **1** in the pristine state and after sublimation.

In the pristine state



After sublimation

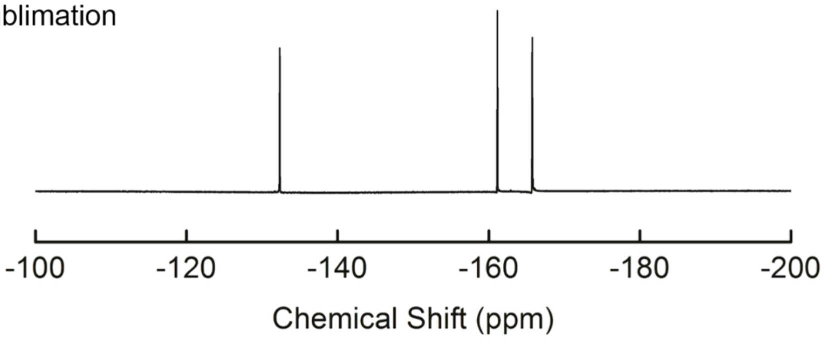


Figure S7. ^{1}H NMR spectra of **2** in the pristine state and after sublimation.

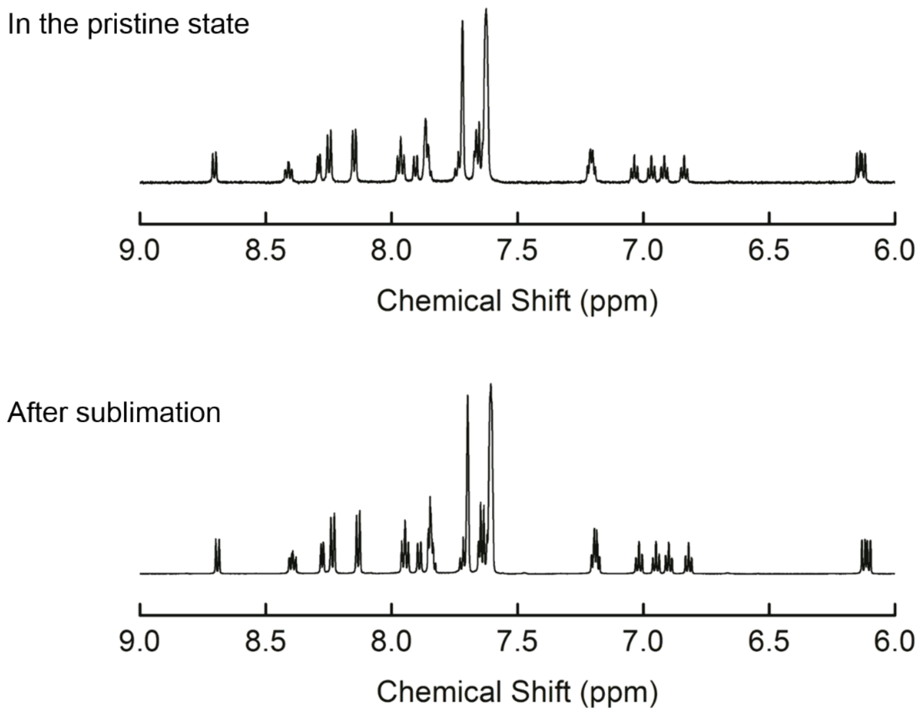


Figure S8. ^{19}F NMR spectra of **2** in the pristine state and after sublimation.