Multi-Functional Bis(alkynyl)gold(III) N^C Complexes with Distinct Mechanochromic Luminescence and Electroluminescence Properties

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Supporting Information

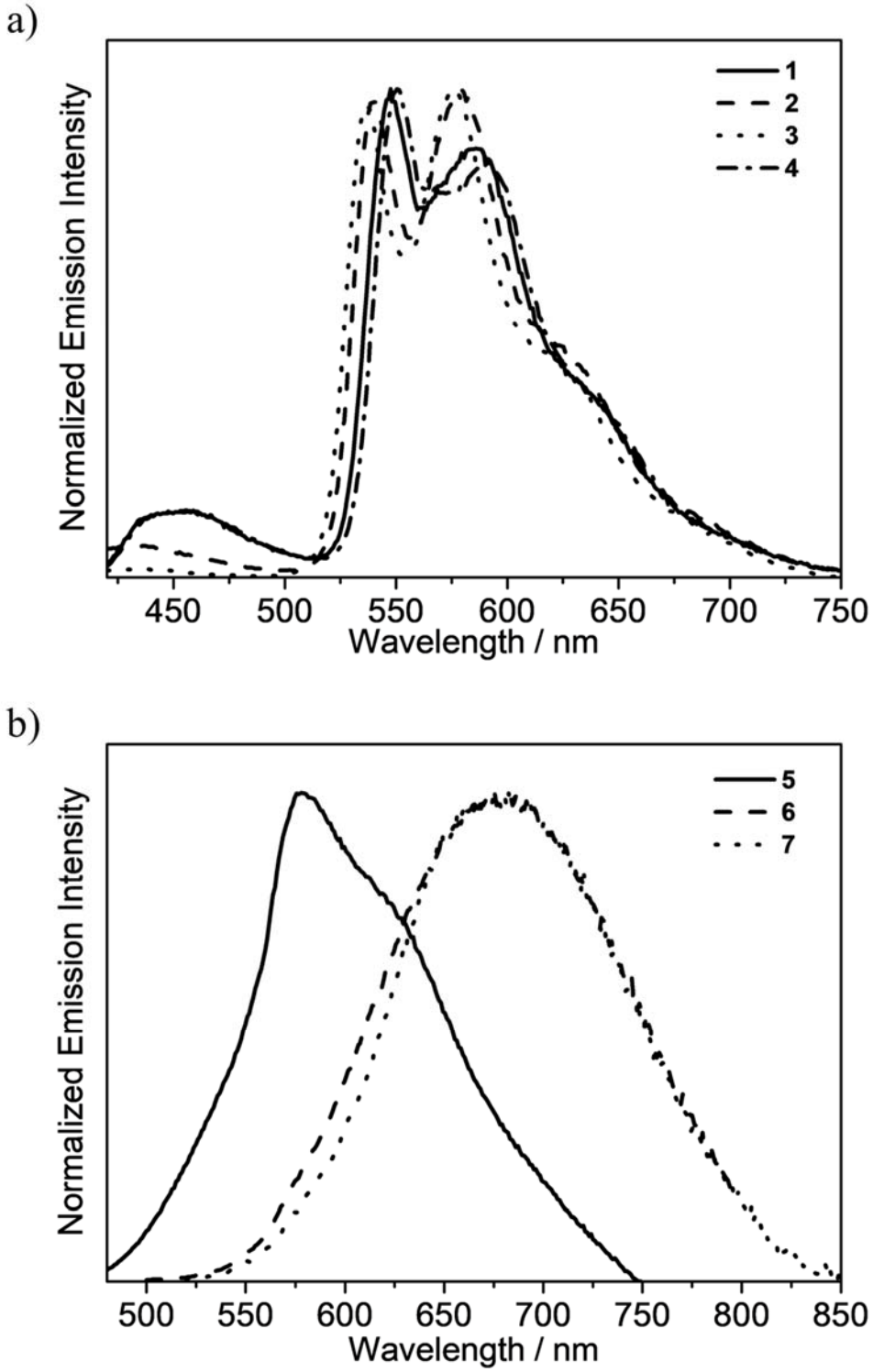


Figure S1 Emission spectra of a) **1**–**4** and b) **5**–**7** in dichloromethane at 298 K.

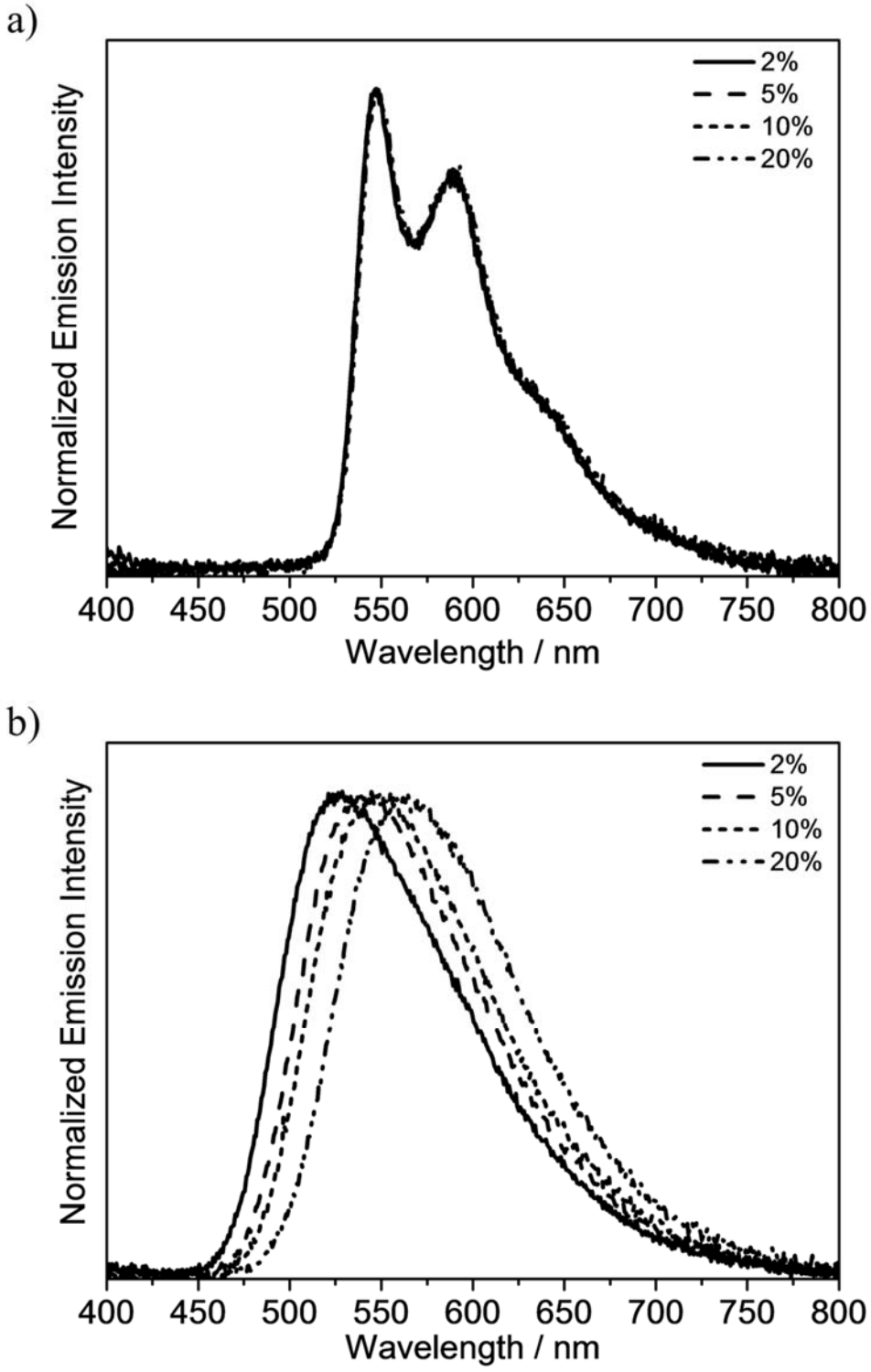
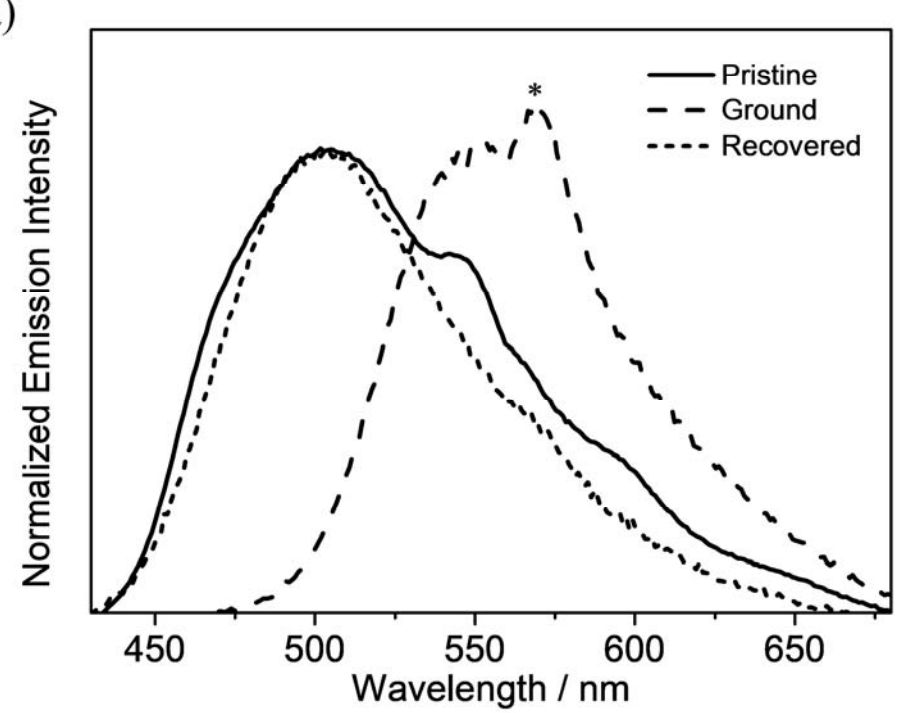
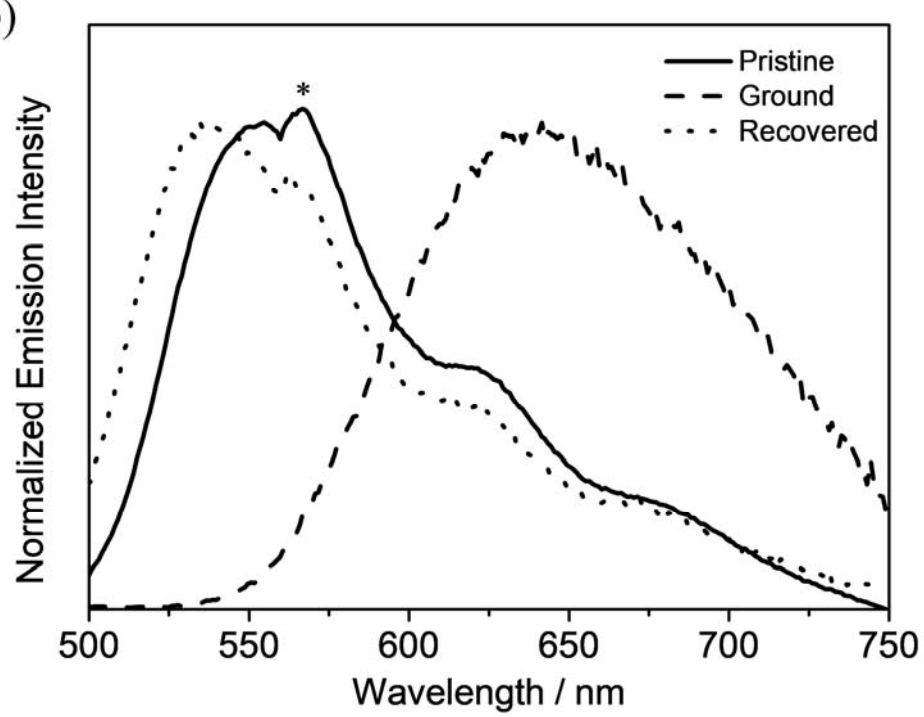


Figure S2 Normalized emission spectra of a) **4** and b) **6** doped in MCP thin films at different concentrations at 298 K.

a)


Pristine
Ground
Recovered
*
Normalized Emission Intensity
450
500
550
600
650
Wavelength / nm

b)


Pristine
Ground
Recovered
*
Normalized Emission Intensity
500
550
600
650
700
750
Wavelength / nm

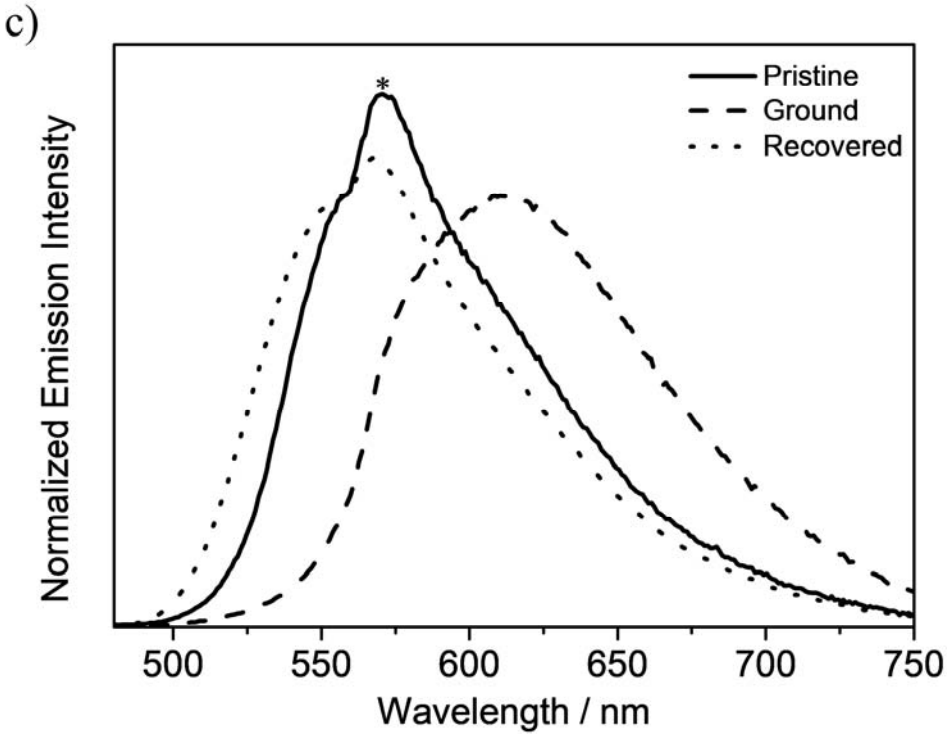


Figure S3 Normalized emission spectra of a) **5**, a) **7** and c) **8** in pristine, ground and recovered forms (asterisk indicates an instrumental artifact).

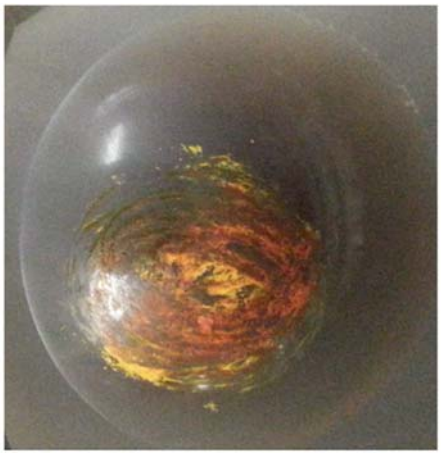
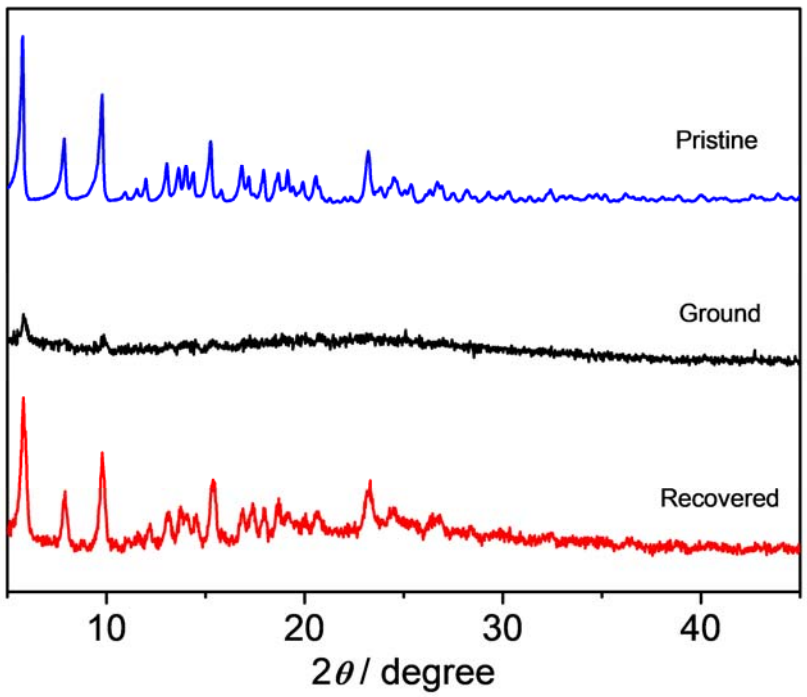
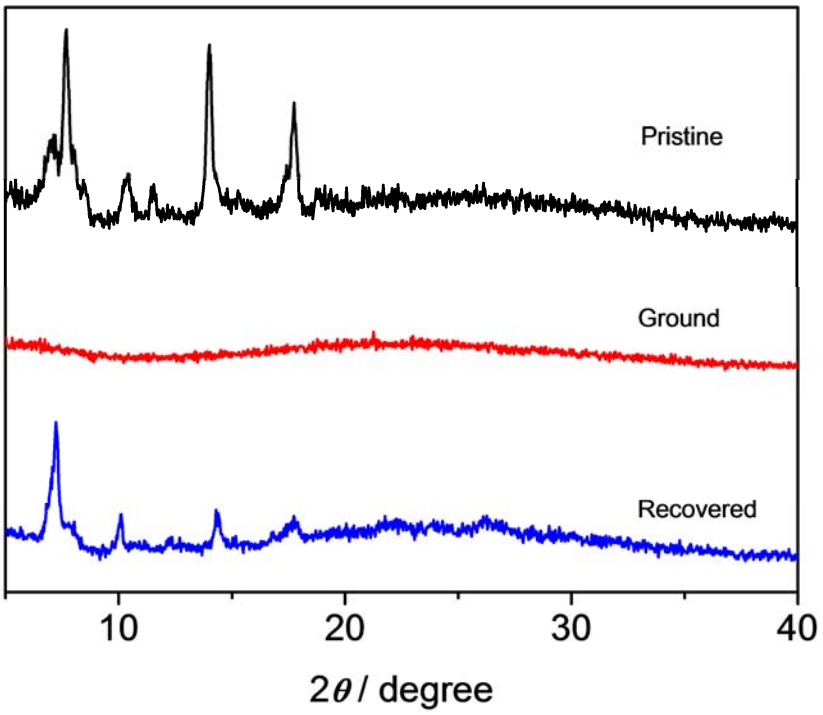


Figure S4 Photographic image of **6** in response to mechanical grinding (red solid) under ambient light.

a)


Pristine
Ground
Recovered
10
20
30
40
2θ / degree

b)


Pristine
Ground
Recovered
10
20
30
40
2θ / degree

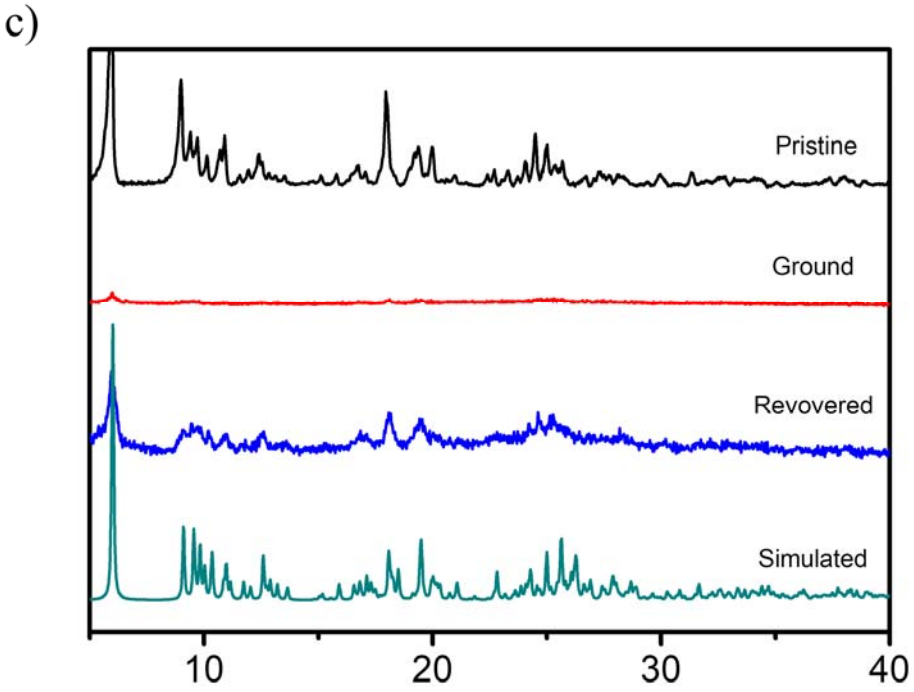


Figure S5 XRD patterns of a) **5**, b) **7** and c) **8** in different forms.

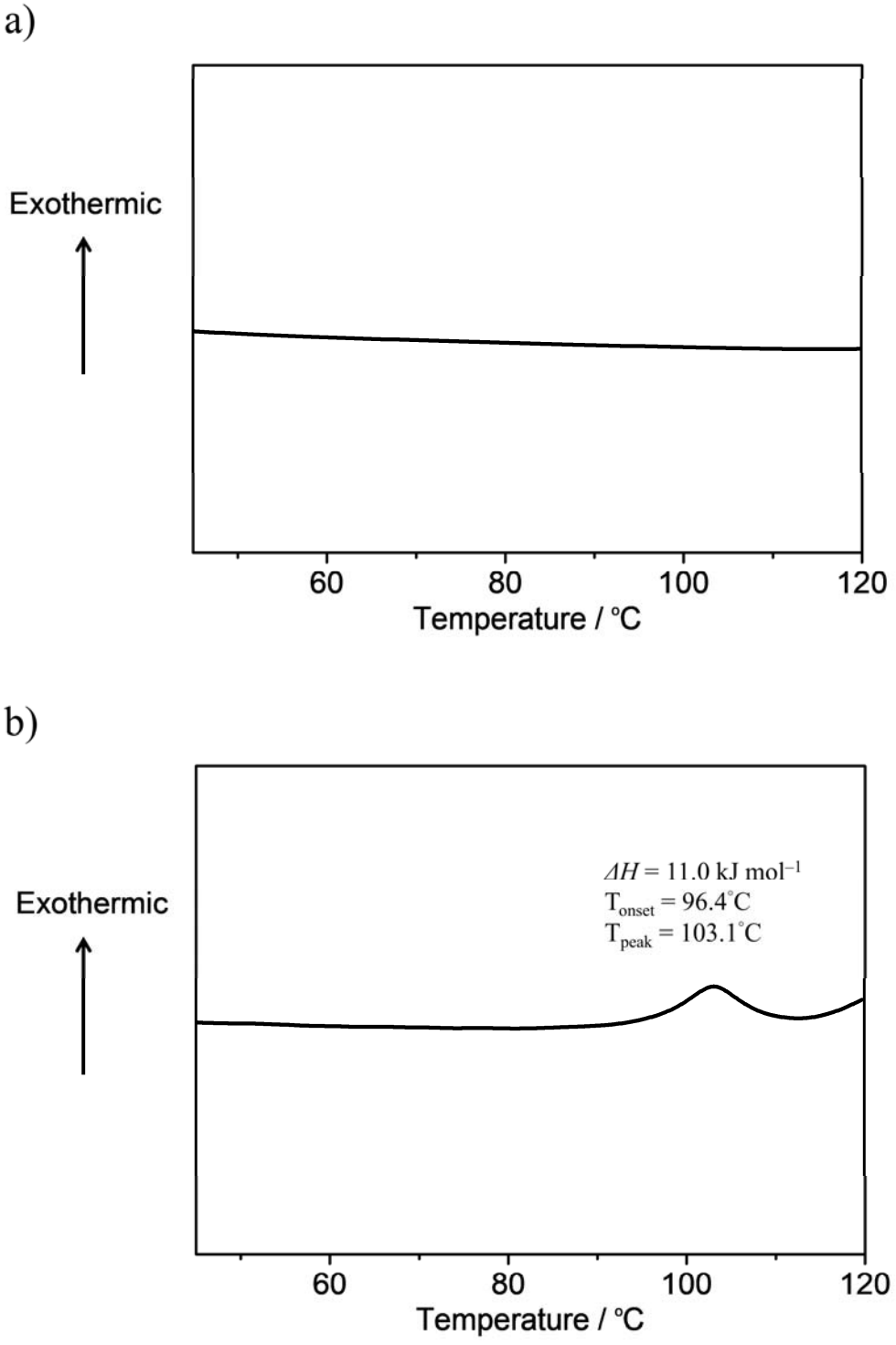


Figure S6 Differential scanning calorimetry (DSC) trace of a) pristine solid sample of **8** at a heating rate of 2.5 °C min^{-1} and b) ground solid sample of **8** at a heating rate of 2.5 °C min^{-1}.

Table S1 Crystal and structure determination data of **8**

Empirical formula	$C_{40}H_{26}AuF_3N_2$
Formula weight	788.59
Temperature, K	100
Wavelength, Å	0.71
Crystal system	Triclinic
Space group	$P\bar{1}$
a, Å	10.6675(4)
b, Å	10.7859(4)
c, Å	29.4456(13)
α, deg	87.957(1)
β, deg	86.644(1)
γ, deg	64.109(1)
Volume, Å^3	3042.5(2)
Z	4
Density (calcd), g cm^{-3}	1.722
F_{000}	1544
θ range for data collection, deg	3.4 to 29.9
Index ranges	$-12 \le h \le 12$
	$-12 \le k \le 12$
	$-35 \le l \le 35$
Reflections collected (unique)	75889/10772
Goodness-of-fit on F^2	1.04
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.041$, $wR_2 = 0.057^a$
Largest diff. peak and hole e Å^{-3}	1.10 and –1.05

Table S2 Selected bond distances (Å) and bond angles (°) of **8** with estimated standard deviations (esds) in parentheses

Bond distances (Å)	
Au(1)–C(8)	2.046(5)
Au(1)–C(25)	1.949(6)
Au(1)–C(33)	2.042(6)
Au(1)–N(1)	2.060(4)
C(25)–C(26)	1.195(8)
C(33)–C(34)	1.191(8)

Bond angles (°)	
C(8)–Au(1)–C(25)	92.1(2)
C(8)–Au(1)–C(33)	174.9(2)
C(8)–Au(1)–N(1)	80.8(2)
C(25)–Au(1)–C(33)	93.0(2)
C(25)–Au(1)–N(1)	172.8(2)
C(33)–Au(1)–N(1)	94.2(2)
Au(1)–C(25)–C(26)	174.1(5)
Au(1)–C(33)–C(34)	171.9(5)

Table S3 Photophysical data of **6** in different solvents

Compound	Medium	Absorption λ_{max} / nm	Emission λ_{max} / nm	Stokes shift $\nu_{abs}-\nu_{em}$ / cm^{-1}
6	Cyclohexane	446	505	2620
	Toluene	436	548	4690
	Ethyl acetate	425	655	8260
	THF	428	670	8440
	Dichloromethane	436	680	8230