Electronic Supplementary Information

Single-component gold(I)-containing highly white-emissive crystals based on a polymorph doping strategy

Yubao Dong,[a] Fei Zhu,[a] Zhao Chen,*[a,b] Jun Yin[a] and Sheng Hua Liu*[a,c]

[a] *Key Laboratory of Pesticide and Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, PR China. E-mail: chshliu@mail.ccnu.edu.cn; Fax: +86-27-67867725; Tel: +86-27-67867725.*

[b] *Jiangxi Key Laboratory of Organic Chemistry, Jiangxi Science and Technology Normal University, Nanchang 330013, PR China. E-mail: chenzhao666@126.com; Fax: +86-791-83831996; Tel: +86-791-83831996.*

[c] *State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, PR China*

Contents

1. Tables S1-S7

Table S1. Optical properties of three polymorphs **1W**, **1B** and **1G**.

Sample	λ_{em}[a] (nm)	Φ[b](%)	τ[c] (μs)	
1W	455, 500	88.2	15.29 (455 nm)	253.12 (500 nm)
1B	455	52.4	15.86 (455 nm)	
1G	455, 520	87.6	21.55 (455 nm)	192.59 (520 nm)

[a]Emission maximum, [b]Absolute photoluminescence quantum yields, [c]Average lifetime.

Table S2. Structure determination summary of **1B**.

Empirical formula	$C_{18}H_{15}AuF_5NO$
Formula weight	553.28
Temperature (K)	100(2)
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	7.3042(9)
b (Å)	19.814(3)
c (Å)	11.9572(15)
α (deg)	90
β (deg)	95.327(2)
γ (deg)	90
V (Å^3)	1723.0(4)
Z	4
$Density_{calcd}$ (Mg/m^3)	2.133
Absorption coefficient (mm^{-1})	8.596
F(000)	1048
Crystal size (mm$^{3)}$	0.20 x 0.20 x 0.10
Theta range for data collection (deg)	2.00 to 26.00
Index ranges	-8<=h<=9, -24<=k<=23, -14<=l<=14
Reflections collected	12639
Independent reflections	3377 [R(int) = 0.2015]
Data / restraints / parameters	3377 / 0 / 236
Final R indices [I>2sigma(I)]	R1 = 0.0604, wR2 = 0.1386
R indices (all data)	R1 = 0.0638, wR2 = 0.1421
Goodness of fit on F^2	1.042
Largest diff. peak and hole (e Å^{-3})	4.074 and -6.162

Table S3. Selective bond lengths [Å] and angles [o] of **1B**.

Au(1)-C(7)	1.984(8)	F(4)-C(5)-C(4)	119.0(5)
Au(1)-C(1)	2.027(6)	C(6)-C(5)-C(4)	119.3(5)
C(1)-C(6)	1.384(8)	F(5)-C(6)-C(5)	116.1(5)
C(1)-C(2)	1.403(8)	F(5)-C(6)-C(1)	118.9(5)
C(2)-C(3)	1.353(9)	C(5)-C(6)-C(1)	125.0(5)
C(2)-F(1)	1.357(6)	N(1)-C(7)-Au(1)	178.8(6)
C(3)-F(2)	1.347(7)	C(9)-C(8)-N(1)	119.8(5)
C(3)-C(4)	1.395(8)	C(9)-C(8)-C(13)	120.4(6)
C(4)-F(3)	1.312(7)	N(1)-C(8)-C(13)	119.7(5)
C(4)-C(5)	1.391(8)	C(10)-C(9)-C(8)	119.8(5)
C(5)-F(4)	1.333(7)	C(10)-C(9)-H(9)	120.1
C(5)-C(6)	1.372(9)	C(8)-C(9)-H(9)	120.1
C(6)-F(5)	1.362(7)	C(9)-C(10)-C(11)	120.8(5)
C(7)-N(1)	1.127(9)	C(9)-C(10)-H(10)	119.6
C(8)-C(9)	1.387(8)	C(11)-C(10)-H(10)	119.6
C(8)-N(1)	1.391(8)	O(1)-C(11)-C(10)	126.1(5)
C(8)-C(13)	1.423(8)	O(1)-C(11)-C(12)	115.6(5)
C(9)-C(10)	1.377(8)	C(10)-C(11)-C(12)	118.2(5)
C(9)-H(9)	0.93	C(13)-C(12)-C(11)	121.7(5)
C(10)-C(11)	1.394(8)	C(13)-C(12)-H(12)	119.1
C(10)-H(10)	0.93	C(11)-C(12)-H(12)	119.1
C(11)-O(1)	1.344(7)	C(12)-C(13)-C(8)	119.0(5)
C(11)-C(12)	1.425(8)	C(12)-C(13)-H(13)	120.5
C(12)-C(13)	1.340(8)	C(8)-C(13)-H(13)	120.5
C(12)-H(12)	0.93	O(1)-C(14)-C(15)	106.8(5)
C(13)-H(13)	0.93	O(1)-C(14)-H(14A)	110.4
C(14)-O(1)	1.451(7)	C(15)-C(14)-H(14A)	110.4
C(14)-C(15)	1.505(9)	O(1)-C(14)-H(14B)	110.4
C(14)-H(14A)	0.97	C(15)-C(14)-H(14B)	110.4
C(14)-H(14B)	0.97	H(14A)-C(14)-H(14B)	108.6
C(15)-C(16)	1.519(9)	C(14)-C(15)-C(16)	112.9(6)
C(15)-H(15A)	0.97	C(14)-C(15)-H(15A)	109
C(15)-H(15B)	0.97	C(16)-C(15)-H(15A)	109
C(16)-C(17)	1.530(9)	C(14)-C(15)-H(15B)	109
C(16)-H(16A)	0.97	C(16)-C(15)-H(15B)	109
C(16)-H(16B)	0.97	H(15A)-C(15)-H(15B)	107.8
C(17)-C(18)	1.535(12)	C(15)-C(16)-C(17)	113.7(6)
C(17)-H(17A)	0.97	C(15)-C(16)-H(16A)	108.8
C(17)-H(17B)	0.97	C(17)-C(16)-H(16A)	108.8

C(18)-H(18A)	0.96	C(15)-C(16)-H(16B)	108.8
C(18)-H(18B)	0.96	C(17)-C(16)-H(16B)	108.8
C(18)-H(18C)	0.96	H(16A)-C(16)-H(16B)	107.7
C(7)-Au(1)-C(1)	177.3(2)	C(16)-C(17)-C(18)	112.5(6)
C(6)-C(1)-C(2)	113.3(6)	C(16)-C(17)-H(17A)	109.1
C(6)-C(1)-Au(1)	123.5(4)	C(18)-C(17)-H(17A)	109.1
C(2)-C(1)-Au(1)	123.2(4)	C(16)-C(17)-H(17B)	109.1
C(3)-C(2)-F(1)	117.3(5)	C(18)-C(17)-H(17B)	109.1
C(3)-C(2)-C(1)	124.3(5)	H(17A)-C(17)-H(17B)	107.8
F(1)-C(2)-C(1)	118.4(5)	C(17)-C(18)-H(18A)	109.5
F(2)-C(3)-C(2)	121.5(5)	C(17)-C(18)-H(18B)	109.5
F(2)-C(3)-C(4)	118.2(6)	H(18A)-C(18)-H(18B)	109.5
C(2)-C(3)-C(4)	120.2(5)	C(17)-C(18)-H(18C)	109.5
F(3)-C(4)-C(5)	121.1(5)	H(18A)-C(18)-H(18C)	109.5
F(3)-C(4)-C(3)	120.9(5)	H(18B)-C(18)-H(18C)	109.5
C(5)-C(4)-C(3)	118.0(6)	C(7)-N(1)-C(8)	174.4(7)
F(4)-C(5)-C(6)	121.7(5)	C(11)-O(1)-C(14)	117.1(4)

Table S4. Structure determination summary of **1W**.

Empirical formula	$C_{18}H_{15}AuF_5NO$
Formula weight	553.28
Temperature (K)	100(2)
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	7.402(2)
b (Å)	19.562(5)
c (Å)	12.283(3)
α (deg)	90
β (deg)	97.320(4)
γ (deg)	90
V (Å^3)	1764.0(8)
Z	4
$Density_{calcd}$ (Mg/m^3)	2.083
Absorption coefficient (mm^{-1})	8.396
F(000)	1048
Crystal size (mm$^{3)}$	0.120 x 0.100 x 0.100
Theta range for data collection (deg)	1.969 to 25.499
Index ranges	-8<=h<=8, -23<=k<=22, -12<=l<=14

Reflections collected	12438
Independent reflections	3271 [R(int) = 0.0478]
Data / restraints / parameters	3271 / 0 / 236
Final R indices [I>2sigma(I)]	R_1 = 0.0334, wR_2 = 0.0902
R indices (all data)	R_1 = 0.0470, wR_2 = 0.0964
Goodness of fit on F^2	1.047
Largest diff. peak and hole (e $Å^{-3}$)	1.255 and -1.068

Table S5. Selective bond lengths [Å] and angles [o] of **1W**.

Au(1)-C(7)	1.974(9)	C(7)-Au(1)-C(1)	177.5(3)
Au(1)-C(1)	2.025(7)	C(6)-C(1)-C(2)	114.2(6)
C(1)-C(6)	1.372(8)	C(6)-C(1)-Au(1)	122.8(5)
C(1)-C(2)	1.378(8)	C(2)-C(1)-Au(1)	122.9(5)
F(6)-C(6)	1.348(7)	C(11)-O(1)-C(14)	119.7(5)
O(1)-C(11)	1.336(7)	C(5)-C(6)-F(6)	116.4(6)
O(1)-C(14)	1.422(8)	C(5)-C(6)-C(1)	123.8(6)
F(1)-C(2)	1.362(7)	F(6)-C(6)-C(1)	119.8(6)
F(3)-C(4)	1.330(7)	C(8)-C(13)-C(12)	118.9(6)
C(6)-C(5)	1.348(9)	C(8)-C(13)-H(13)	120.6
C(13)-C(8)	1.362(8)	C(12)-C(13)-H(13)	120.6
C(13)-C(12)	1.377(9)	O(1)-C(11)-C(12)	124.8(6)
C(13)-H(13)	0.93	O(1)-C(11)-C(10)	116.4(6)
F(5)-C(5)	1.340(7)	C(12)-C(11)-C(10)	118.7(6)
C(11)-C(12)	1.371(9)	F(3)-C(4)-C(3)	120.7(6)
C(11)-C(10)	1.391(9)	F(3)-C(4)-C(5)	120.0(6)
C(4)-C(3)	1.356(9)	C(3)-C(4)-C(5)	119.3(6)
C(4)-C(5)	1.384(9)	N(1)-C(7)-Au(1)	176.8(7)
F(2)-C(3)	1.333(7)	F(1)-C(2)-C(3)	116.2(6)
C(7)-N(1)	1.128(9)	F(1)-C(2)-C(1)	119.5(6)
C(2)-C(3)	1.365(9)	C(3)-C(2)-C(1)	124.3(6)
C(8)-C(9)	1.394(9)	C(13)-C(8)-C(9)	121.6(6)
C(8)-N(1)	1.396(9)	C(13)-C(8)-N(1)	118.6(5)
C(12)-H(12)	0.93	C(9)-C(8)-N(1)	119.9(6)
C(9)-C(10)	1.338(9)	F(2)-C(3)-C(4)	120.0(6)
C(9)-H(9)	0.93	F(2)-C(3)-C(2)	121.1(6)
C(10)-H(10)	0.93	C(4)-C(3)-C(2)	118.8(6)
C(14)-C(15)	1.493(11)	C(11)-C(12)-C(13)	120.7(6)
C(14)-H(14A)	0.97	C(11)-C(12)-H(12)	119.7
C(14)-H(14B)	0.97	C(13)-C(12)-H(12)	119.7

C(15)-C(16)	1.536(14)	F(5)-C(5)-C(6)	122.0(6)
C(15)-H(15A)	0.97	F(5)-C(5)-C(4)	118.4(6)
C(15)-H(15B)	0.97	C(6)-C(5)-C(4)	119.6(6)
C(16)-C(17)	1.409(13)	C(10)-C(9)-C(8)	118.4(6)
C(16)-H(16A)	0.97	C(10)-C(9)-H(9)	120.8
C(16)-H(16B)	0.97	C(8)-C(9)-H(9)	120.8
C(17)-C(18)	1.462(17)	C(9)-C(10)-C(11)	121.8(6)
C(17)-H(17A)	0.97	C(9)-C(10)-H(10)	119.1
C(17)-H(17B)	0.97	C(11)-C(10)-H(10)	119.1
C(18)-H(18A)	0.96	C(7)-N(1)-C(8)	176.2(6)
C(18)-H(18B)	0.96	O(1)-C(14)-C(15)	108.5(6)
C(18)-H(18C)	0.96	O(1)-C(14)-H(14A)	110
C(15)-C(14)-H(14A)	110	C(15)-C(16)-H(16B)	108.2
O(1)-C(14)-H(14B)	110	H(16A)-C(16)-H(16B)	107.4
C(15)-C(14)-H(14B)	110	C(16)-C(17)-C(18)	114.0(10)
H(14A)-C(14)-H(14B)	108.4	C(16)-C(17)-H(17A)	108.8
C(14)-C(15)-C(16)	111.5(8)	C(18)-C(17)-H(17A)	108.8
C(14)-C(15)-H(15A)	109.3	C(16)-C(17)-H(17B)	108.8
C(16)-C(15)-H(15A)	109.3	C(18)-C(17)-H(17B)	108.8
C(14)-C(15)-H(15B)	109.3	H(17A)-C(17)-H(17B)	107.6
C(16)-C(15)-H(15B)	109.3	C(17)-C(18)-H(18A)	109.5
H(15A)-C(15)-H(15B)	108	C(17)-C(18)-H(18B)	109.5
C(17)-C(16)-C(15)	116.3(9)	H(18A)-C(18)-H(18B)	109.5
C(17)-C(16)-H(16A)	108.2	C(17)-C(18)-H(18C)	109.5
C(15)-C(16)-H(16A)	108.2	H(18A)-C(18)-H(18C)	109.5
C(17)-C(16)-H(16B)	108.2	H(18B)-C(18)-H(18C)	109.5

Table S6. Structure determination summary of **1G**.

Empirical formula	$C_{18}H_{15}AuF_5NO$
Formula weight	553.28
Temperature (K)	100(2)
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	7.2889(4)
b (Å)	19.8254(10)
c (Å)	11.9641(6)
α (deg)	90
β (deg)	95.3060(10)
γ (deg)	90

V (Å^3)	1764.0(8)
Z	4
Density$_{calcd}$ (Mg/m^3)	2.135
Absorption coefficient (mm^{-1})	8.603
F(000)	1048
Crystal size (mm$^{3)}$	0.100 x 0.100 x 0.080
Theta range for data collection (deg)	1.994 to 30.496
Index ranges	-10<=h<=9, -28<=k<=28, -17<=l<=14
Reflections collected	18008
Independent reflections	5219 [R(int) = 0.0316]
Data / restraints / parameters	5219 / 0 / 236
Final R indices [I>2sigma(I)]	R1 = 0.0209, wR2 = 0.0489
R indices (all data)	R1 = 0.0296, wR2 = 0.0647
Goodness of fit on F^2	1.109
Largest diff. peak and hole (e Å^{-3})	0.739 and -0.691

Table S7. Selective bond lengths [Å] and angles [^{o}] of **1G**.

Au(1)-C(7)	1.966(4)	F(4)-C(5)-C(6)	121.1(3)
Au(1)-C(1)	2.028(3)	C(4)-C(5)-C(6)	119.7(3)
C(1)-C(2)	1.380(4)	F(5)-C(6)-C(5)	116.6(3)
C(1)-C(6)	1.386(4)	F(5)-C(6)-C(1)	119.4(3)
C(2)-F(1)	1.361(4)	C(5)-C(6)-C(1)	123.9(3)
C(2)-C(3)	1.381(4)	N(1)-C(7)-Au(1)	177.6(3)
C(3)-F(2)	1.350(4)	C(9)-C(8)-C(13)	121.7(3)
C(3)-C(4)	1.377(5)	C(9)-C(8)-N(1)	118.8(3)
C(4)-F(3)	1.334(4)	C(13)-C(8)-N(1)	119.5(3)
C(4)-C(5)	1.378(5)	C(10)-C(9)-C(8)	119.6(3)
C(5)-F(4)	1.347(4)	C(10)-C(9)-H(9)	120.2
C(5)-C(6)	1.379(4)	C(8)-C(9)-H(9)	120.2
C(6)-F(5)	1.359(4)	C(9)-C(10)-C(11)	119.7(3)
C(7)-N(1)	1.152(4)	C(9)-C(10)-H(10)	120.1
C(8)-C(9)	1.384(5)	C(11)-C(10)-H(10)	120.1
C(8)-C(13)	1.393(5)	O(1)-C(11)-C(12)	115.5(3)
C(8)-N(1)	1.399(4)	O(1)-C(11)-C(10)	124.7(3)
C(9)-C(10)	1.381(4)	C(12)-C(11)-C(10)	119.7(3)
C(9)-H(9)	0.95	C(13)-C(12)-C(11)	120.8(3)
C(10)-C(11)	1.399(4)	C(13)-C(12)-H(12)	119.6
C(10)-H(10)	0.95	C(11)-C(12)-H(12)	119.6

C(11)-O(1)	1.351(4)	C(12)-C(13)-C(8)	118.4(3)
C(11)-C(12)	1.396(5)	C(12)-C(13)-H(13)	120.8
C(12)-C(13)	1.381(4)	C(8)-C(13)-H(13)	120.8
C(12)-H(12)	0.95	O(1)-C(14)-C(15)	107.4(3)
C(13)-H(13)	0.95	O(1)-C(14)-H(14A)	110.2
C(14)-O(1)	1.439(4)	C(15)-C(14)-H(14A)	110.2
C(14)-C(15)	1.518(5)	O(1)-C(14)-H(14B)	110.2
C(14)-H(14A)	0.99	C(15)-C(14)-H(14B)	110.2
C(14)-H(14B)	0.99	H(14A)-C(14)-H(14B)	108.5
C(15)-C(16)	1.517(5)	C(16)-C(15)-C(14)	112.9(3)
C(15)-H(15A)	0.99	C(16)-C(15)-H(15A)	109
C(15)-H(15B)	0.99	C(14)-C(15)-H(15A)	109
C(16)-C(17)	1.518(5)	C(16)-C(15)-H(15B)	109
C(16)-H(16A)	0.99	C(14)-C(15)-H(15B)	109
C(16)-H(16B)	0.99	H(15A)-C(15)-H(15B)	107.8
C(17)-C(18)	1.522(6)	C(15)-C(16)-C(17)	113.2(3)
C(17)-H(17A)	0.99	C(15)-C(16)-H(16A)	108.9
C(17)-H(17B)	0.99	C(17)-C(16)-H(16A)	108.9
C(18)-H(18A)	0.98	C(15)-C(16)-H(16B)	108.9
C(18)-H(18B)	0.98	C(17)-C(16)-H(16B)	108.9
C(18)-H(18C)	0.98	H(16A)-C(16)-H(16B)	107.7
C(7)-Au(1)-C(1)	177.76(13)	C(16)-C(17)-C(18)	112.4(3)
C(2)-C(1)-C(6)	114.1(3)	C(16)-C(17)-H(17A)	109.1
C(2)-C(1)-Au(1)	123.3(2)	C(18)-C(17)-H(17A)	109.1
C(6)-C(1)-Au(1)	122.6(2)	C(16)-C(17)-H(17B)	109.1
F(1)-C(2)-C(1)	119.5(3)	C(18)-C(17)-H(17B)	109.1
F(1)-C(2)-C(3)	116.5(3)	H(17A)-C(17)-H(17B)	107.8
C(1)-C(2)-C(3)	123.9(3)	C(17)-C(18)-H(18A)	109.5
F(2)-C(3)-C(4)	119.0(3)	C(17)-C(18)-H(18B)	109.5
F(2)-C(3)-C(2)	121.2(3)	H(18A)-C(18)-H(18B)	109.5
C(4)-C(3)-C(2)	119.8(3)	C(17)-C(18)-H(18C)	109.5
F(3)-C(4)-C(3)	120.8(3)	H(18A)-C(18)-H(18C)	109.5
F(3)-C(4)-C(5)	120.6(3)	H(18B)-C(18)-H(18C)	109.5
C(3)-C(4)-C(5)	118.6(3)	C(7)-N(1)-C(8)	175.8(3)
F(4)-C(5)-C(4)	119.2(3)	C(11)-O(1)-C(14)	118.0(2)

2. Figs. S1-S8

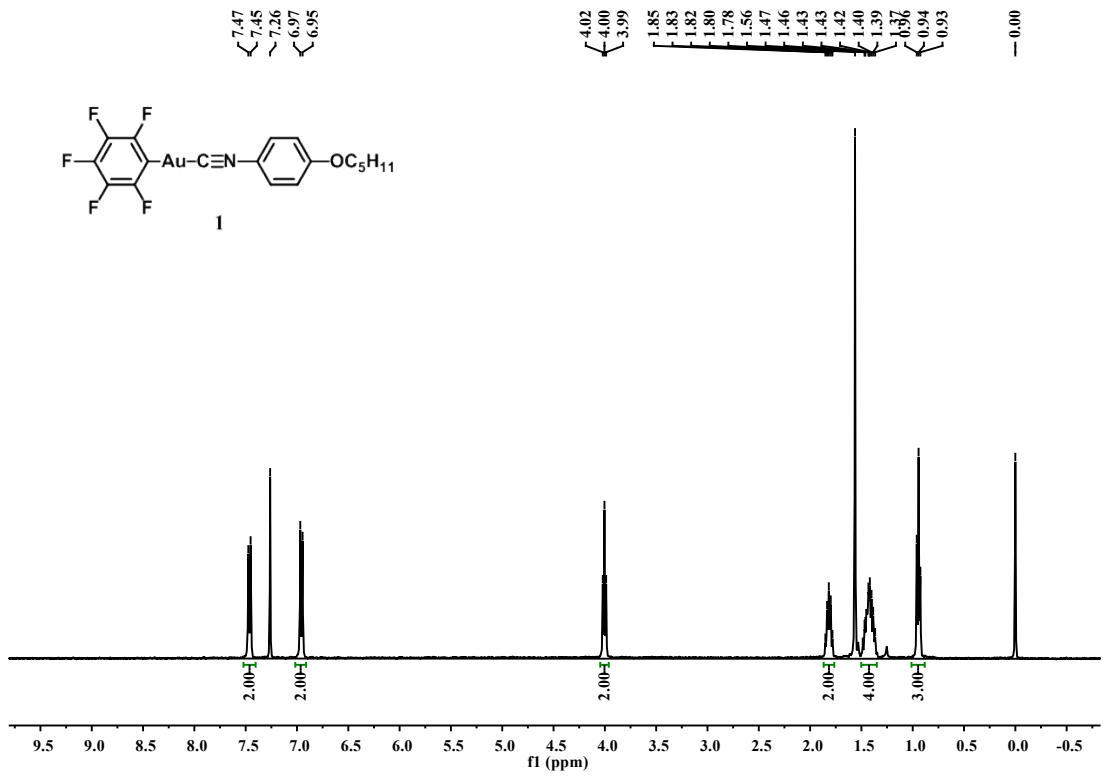

Fig. S1. ^{1}H NMR spectrum of complex **1** in $CDCl_3$ at room temperature.

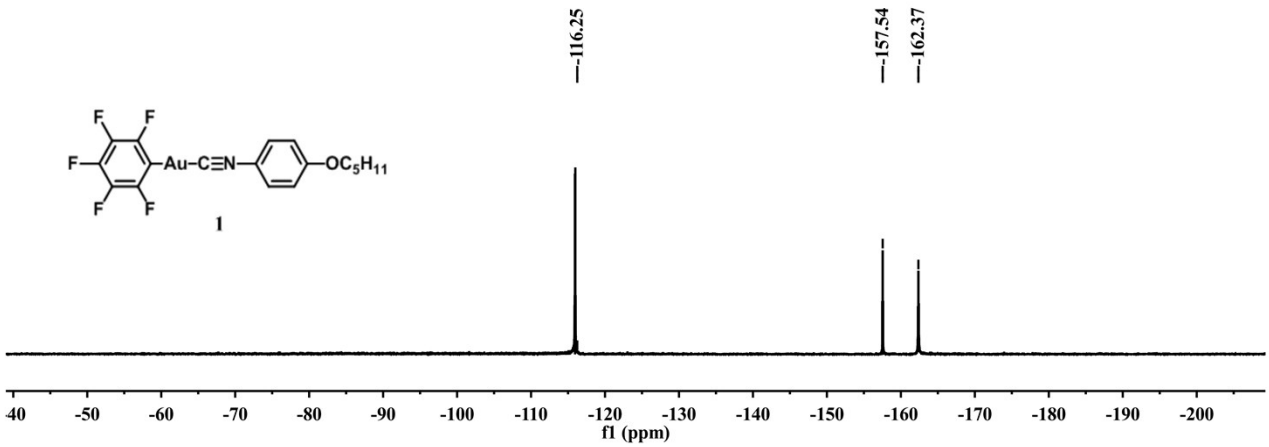

Fig. S2. ^{19}F NMR spectrum of complex **1** in $CDCl_3$ at room temperature.

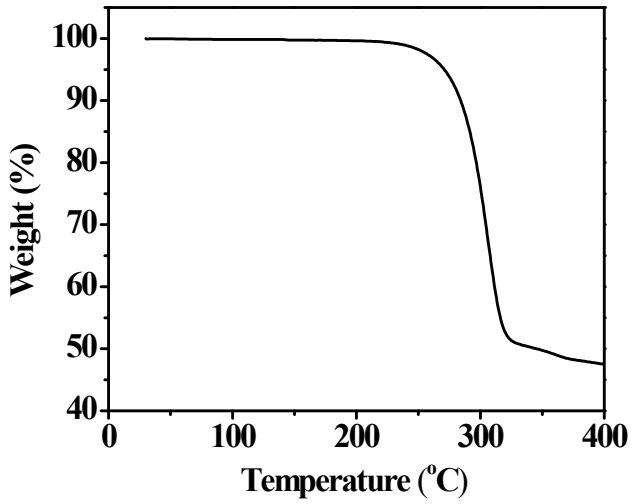

Fig. S3. Thermal gravimetric analysis (TGA) thermogram of complex **1** at a heating rate of 10 ˚C min^{-1}.

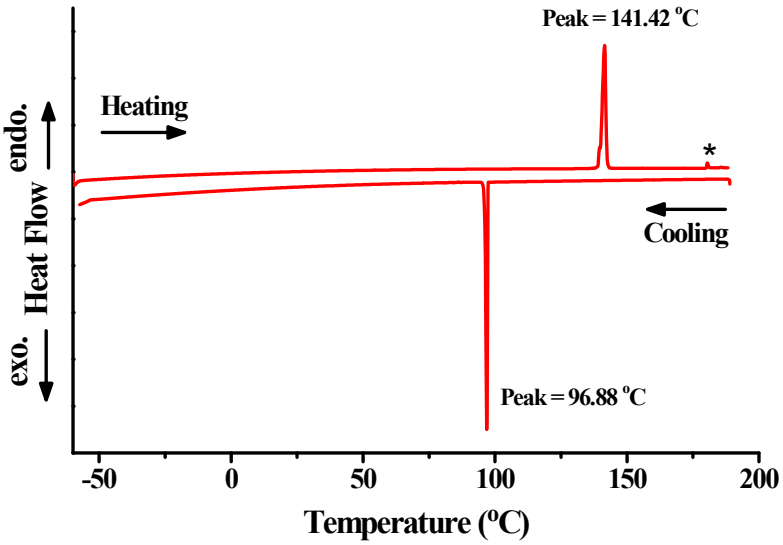

Fig. S4. Differential scanning calorimetry (DSC) curves of complex **1** at a heating/cooling rate of 10 °C min^{-1}.

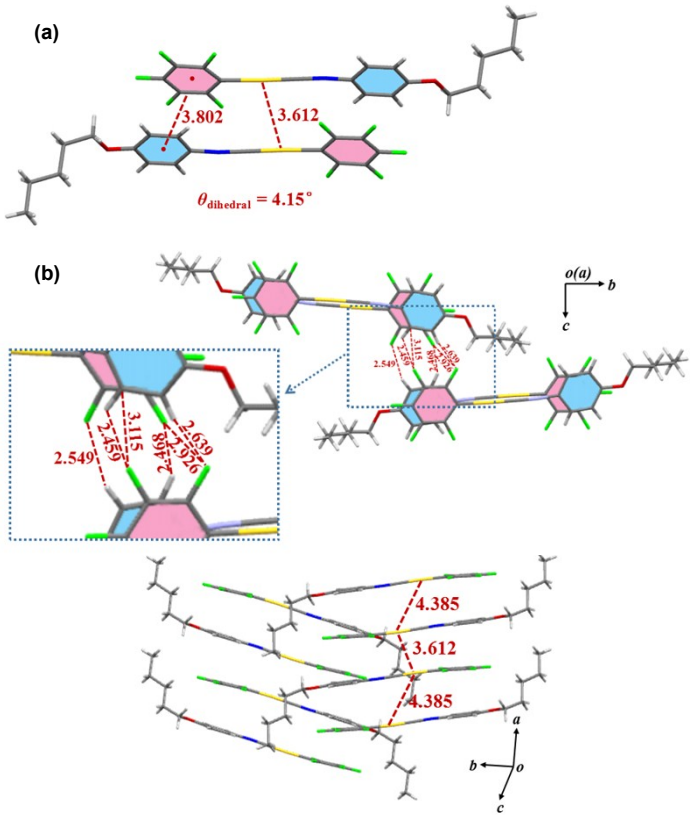

Fig. S5. (a) Stacked pair structure of polymorph **1B**. (b) molecular packing patterns of polymorph **1B**.

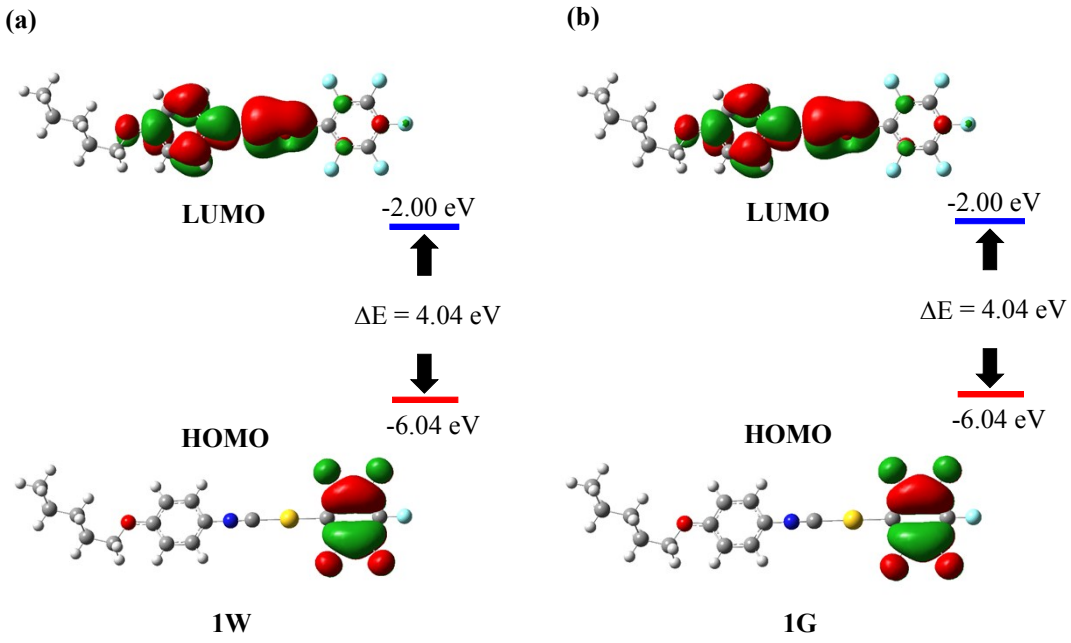

Fig. S6. HOMO and LUMO frontier molecular orbitals of **1W** (left) and **1G** (right) obtained at the

density functional theory (DFT) calculations level. using a B3LYP/6-31G* basis set.

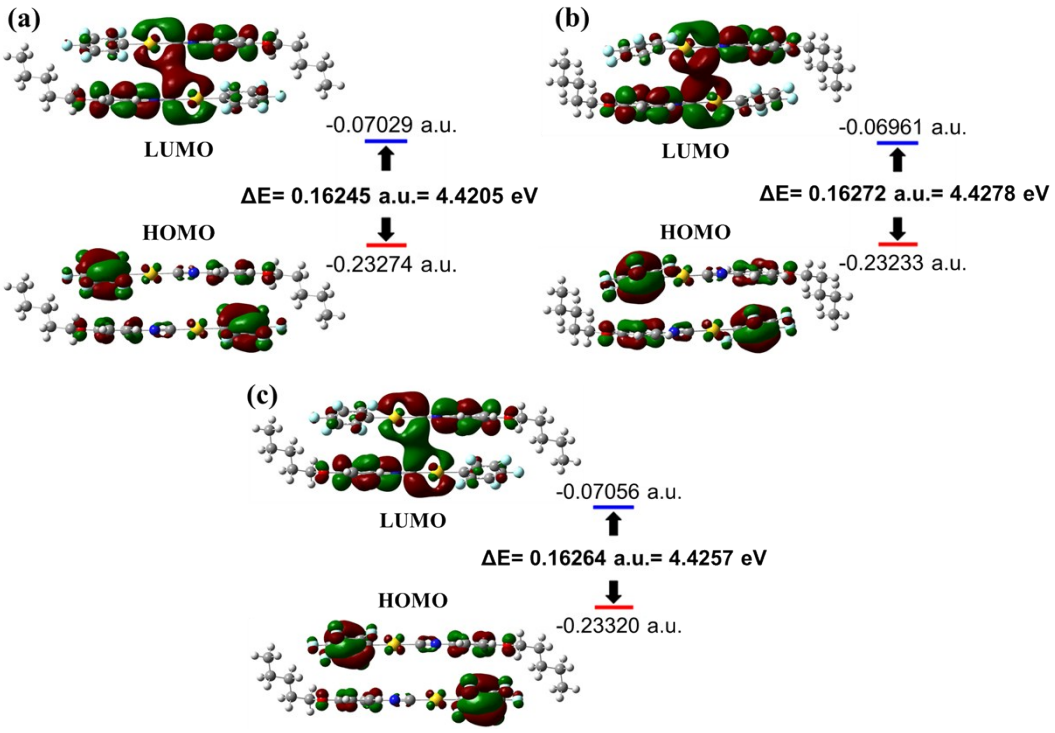

Fig. S7. (a) HOMO and LUMO frontier molecular orbitals of **1W** in aggregation state calculated using B3LYP/6-31G* basis set. (b) HOMO and LUMO frontier molecular orbitals of **1B** in aggregation state calculated using B3LYP/6-31G* basis set. (c) HOMO and LUMO frontier molecular orbitals of **1G** in aggregation state calculated using B3LYP/6-31G* basis set.

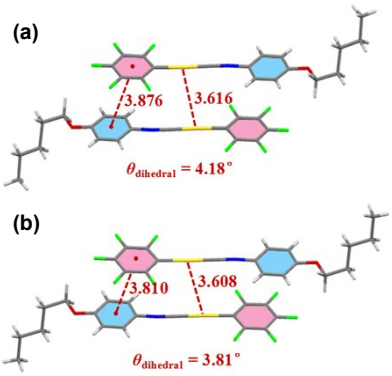

Fig. S8. Stacked pair structures of polymorphs (a) **1W** and (b) **1G**. Dihedral angles ($\theta_{dihedral}$) between isocyanide phenyl and pentafluorophenyl groups are shown.