Synthesis, crystal structure, photophysical properties and theoretical study of a new iridium(III) complex containing 2-phenylbenzothiazole ligand

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Supporting materials

Table S1 Crystallographic data and structure refinement details for **3**.

Empirical formula	$C_{40}H_{34}F_6IrN_6PS_2$
M_r	1000.02
Crystal system	Triclinic
Space group	$P\bar{1}$
Wavelength / Å	0.71073
X-radiation (graphite monochromator)	Mo-Kα
T / K	293(2)
a (Å)	10.5274(3)
b (Å)	15.7581(6)
c (Å)	23.8577(7)
α (°)	88.861(3)
β (°)	85.958(3)
γ (°)	82.435(3)
V (Å^3)	3913.4(2)
Z	4
D_{calcd} (Mg/m^3)	1.697
F(000)	1976
μ(Mo-Kα)/ mm^{-1}	3.627
index ranges	$-13 \le h \le 13$
	$-19 \le k \le 19$
	$-27 \le l \le 29$
R_{int}	0.0881
GOF (F^2)	0.890
$R_1{}^a$, $wR_2{}^b$ ($I > 2\sigma(I)$)	0.0616, 0.0781
$R_1{}^a$, $wR_2{}^b$ (all data)	0.1507, 0.1041

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

Table S2 Selected bond distances (Å) and angles (◦) for complex **3**.

Ir(1)-N(1)	2.114(9)	C(5)-C(6)	1.477(14)
Ir(1)-N(2)	2.133(8)	C(17)-C(18)	1.413(11)
Ir(1)-N(3)	2.056(8)	N(4)-C(21)	1.341(11)
Ir(1)-N(5)	2.044(7)	N(4)-C(24)	1.451(12)
Ir(1)-C(19)	2.022(8)	S(1)-C(16)	1.720(11)
Ir(1)-C(38)	1.996(10)	S(1)-C(17)	1.715(8)
N(3)-Ir(1)-N(5)	170.2(3)	N(5)-Ir(1)-C(19)	91.0(3)
C(19)-Ir(1)-N(2)	174.6(4)	N(5)-Ir(1)-C(38)	80.1(3)
C(38)-Ir(1)-N(1)	173.7(3)	C(19)-Ir(1)-C(38)	88.0(3)
N(5)-Ir(1)-N(2)	91.1(3)	N(1)-Ir(1)-N(2)	76.5(3)
N(5)-Ir(1)-N(1)	101.4(3)	N(3)-Ir(1)-N(2)	97.9(3)

Table S3 Frontier orbital energy and electron density distribution for **3**.

Orbital	Energy (eV)	Composition (%)			
		Ir	Ph-R	benzothiazole	2,2'-bipyridine
LUMO+3	-1.724	5.11	6.43	13.04	75.46
LUMO+2	-1.835	3.12	28.04	50.40	19.23
LUMO+1	-1.842	2.77	34.59	59.50	4.24
LUMO	-2.703	4.70	4.31	0.27	90.78
HOMO	-5.351	0.21	91.62	21.72	1.06
HOMO-1	-5.371	4.25	87.40	22.17	1.06
HOMO-2	-6.247	45.69	51.27	5.12	4.87
HOMO-5	-6.523	31.09	6.12	56.55	8.12
HOMO-12	-7.630	17.85	11.50	3.39	69.78

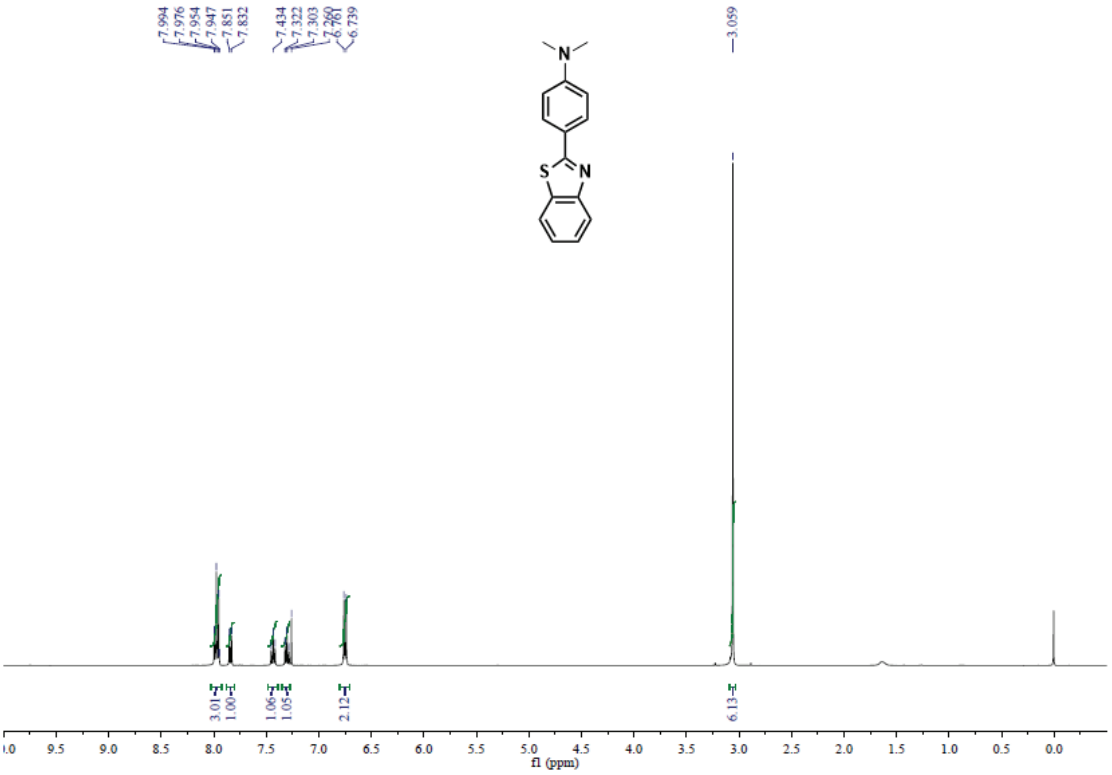

Fig. S1. ^{1}H NMR of **dmabt** (**1**) in $CDCl_3$.

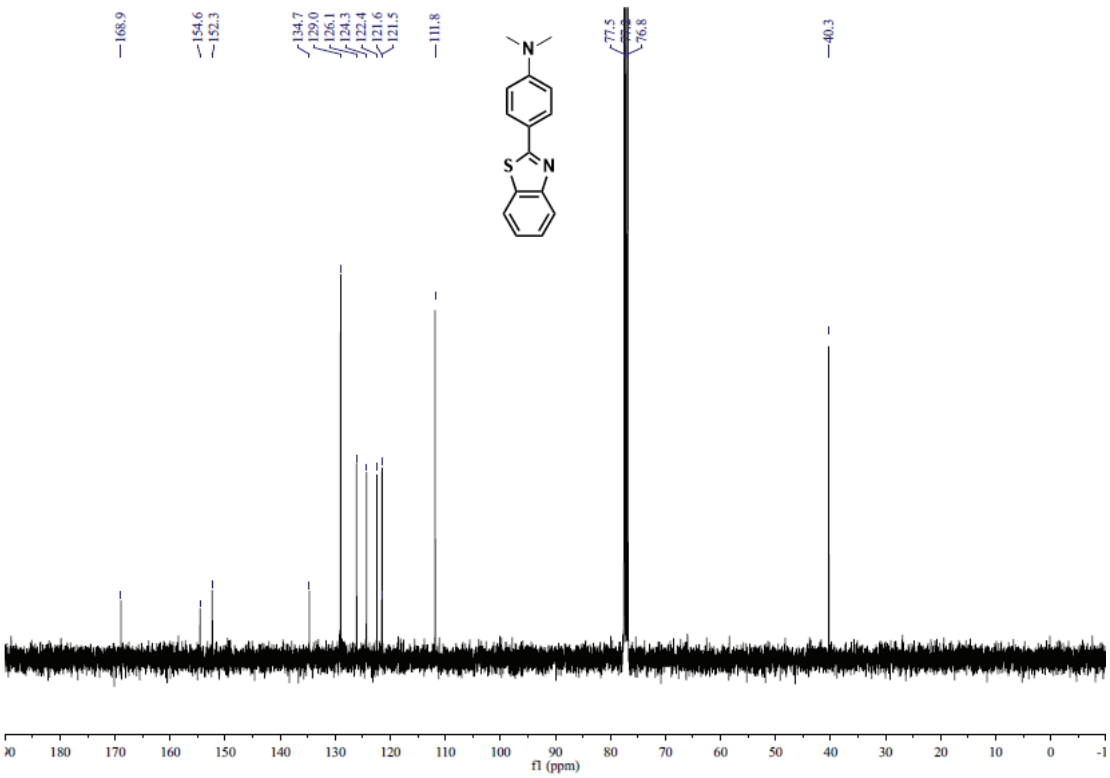

Fig. S2. ^{13}C NMR of **dmabt** (**1**) in $CDCl_3$.

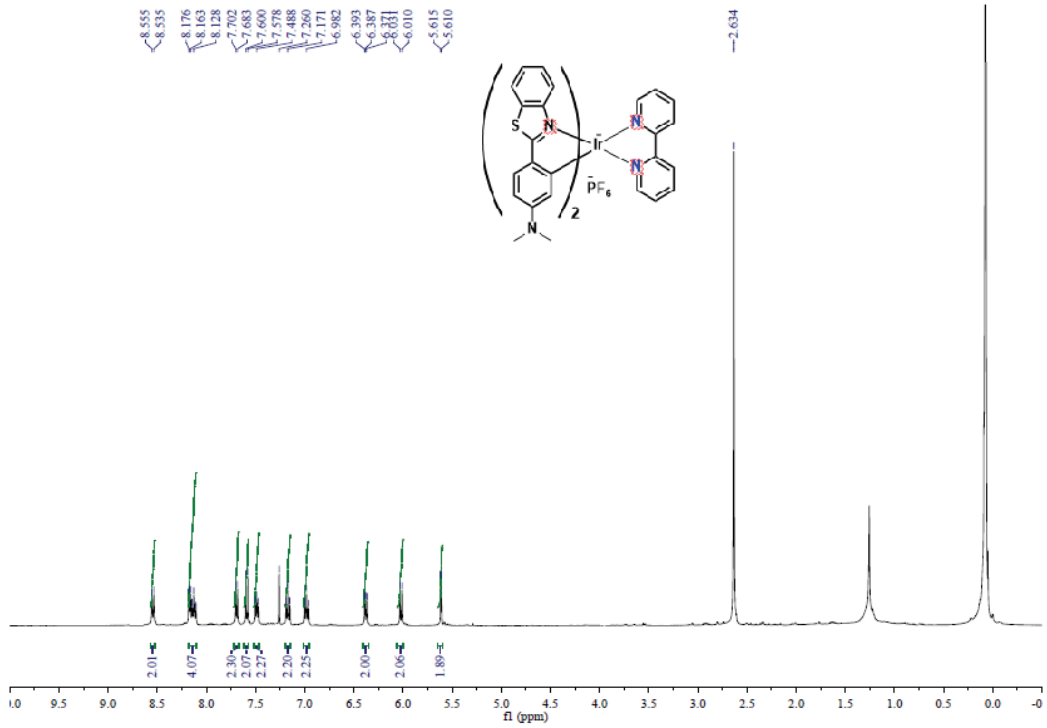

Fig. S3. ^{1}H NMR of **[Ir(dmabt)$_2$(bipy)][PF$_6$]** (**3**) in $CDCl_3$.

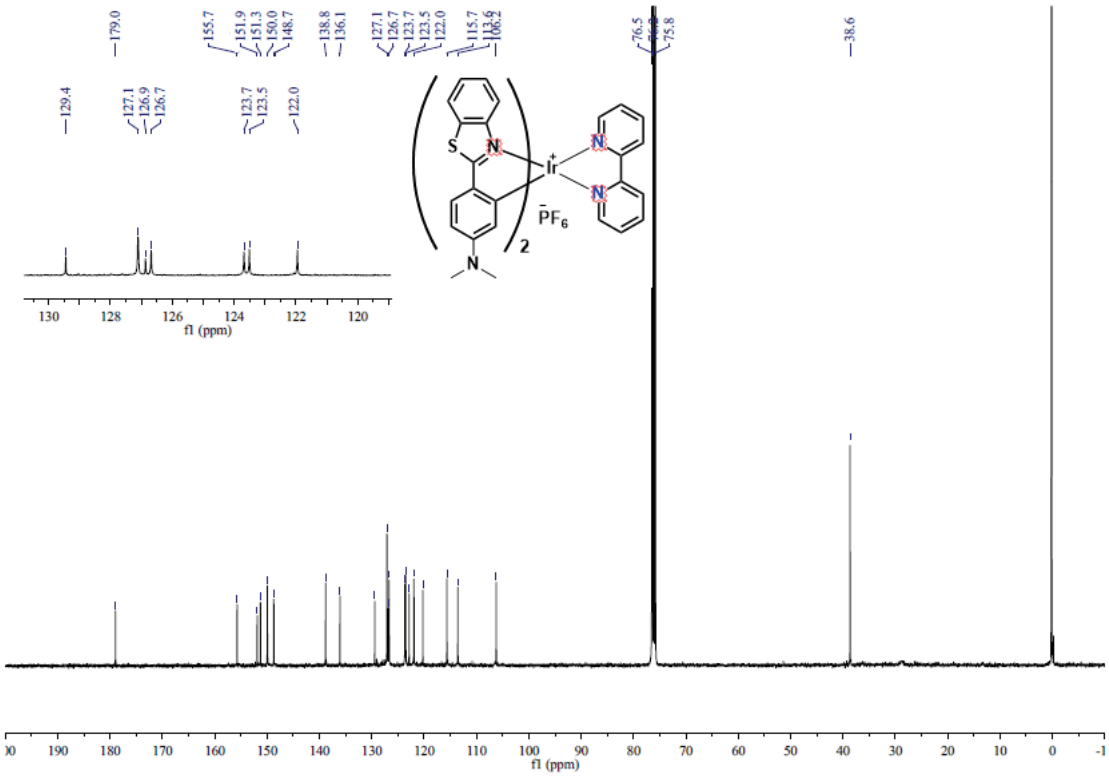

Fig. S4. ^{13}C NMR of **[Ir(dmabt)$_2$(bipy)][PF$_6$]** (**3**) in $CDCl_3$.