Electronic Supplementary Material (ESI) for RSC Advances

Supporting information for

BF_2-Bound Chromophore-containing *N^N* Pt(II) Bisacetylide Complex and Its Applications As Sensitizer for Triplet-triplet annihilation Based Upconversion

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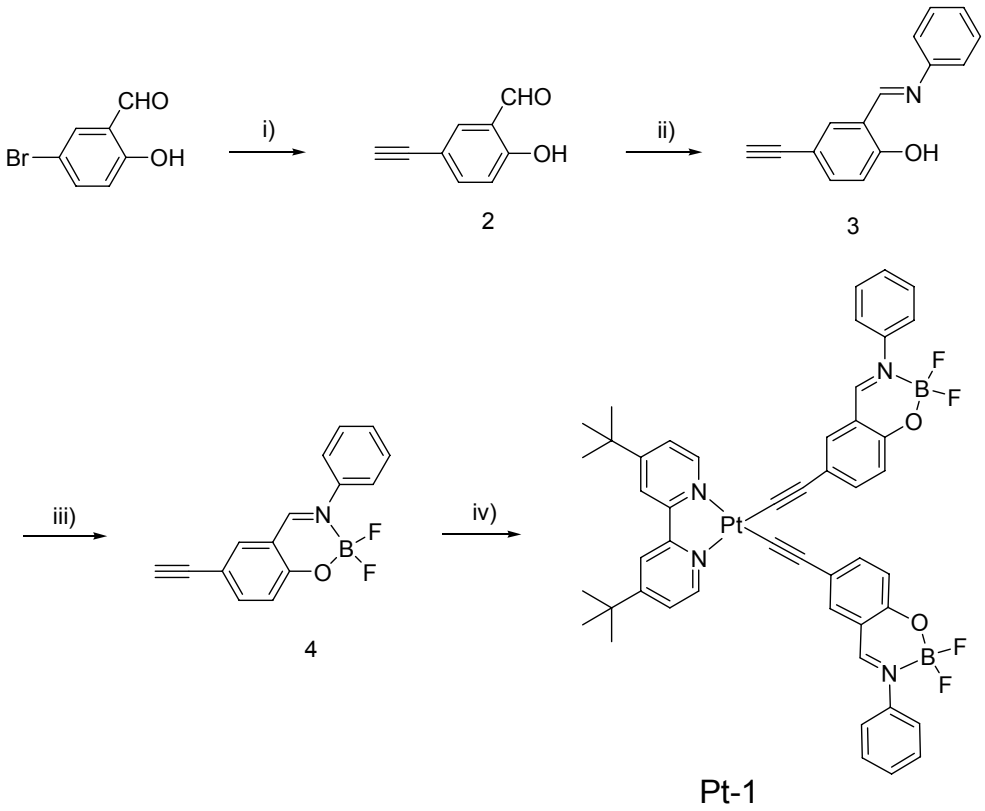
Experimental Section

Synthesis:



Scheme 1. Synthesis route of target donors **Pt-1**. i) $Pd(PPh_3)_4$, CuI, NEt_3,ethynyltrimethylsilane, argon atmosphere, 80 °C, 3 h, then THF, TBAF, room temperature, 30 min, 36.8 %; ii) aniline, ethanol, 50 °C, 4 h, 95 % iii) CH_2Cl_2, NEt_3, BF_3-Et_2O, room temperature, 20 min, 71%. iv) CH2Cl2, i-Pr_2NH, room temperature,24 h.

Synthesis Procedures

5-ethynyl-2-hydroxybenzaldehyde (2)

5-ethynyl-2-hydroxybenzaldehyde was synthesized according to a literature procedure.[1]

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[1]. Christoph Beyer and Hans-Achim Wagenknecht. *J. Org. Chem*., 2010, **75**, 2752–2755.

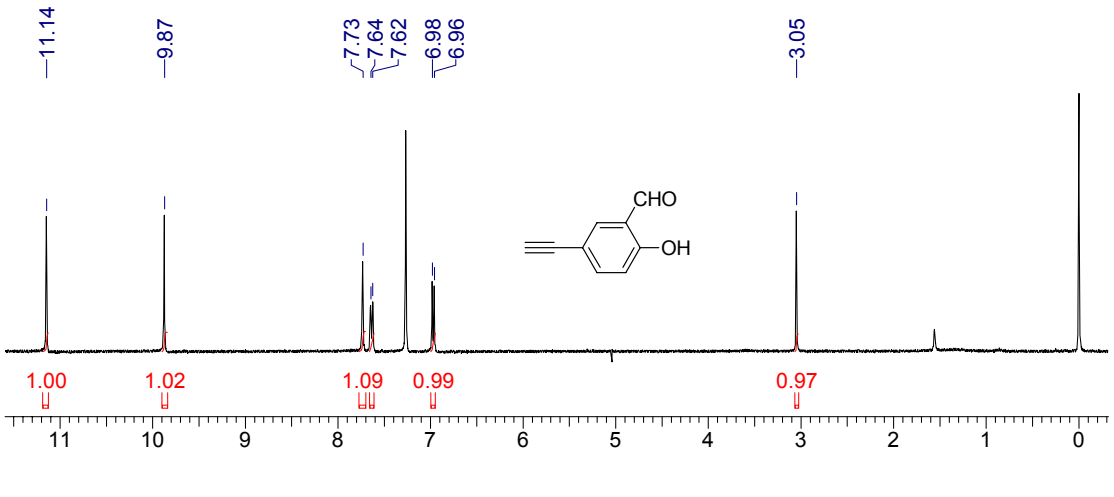

Figure S1. ^{1}H NMR of **2** ($CDCl_3$, 400 MHz).

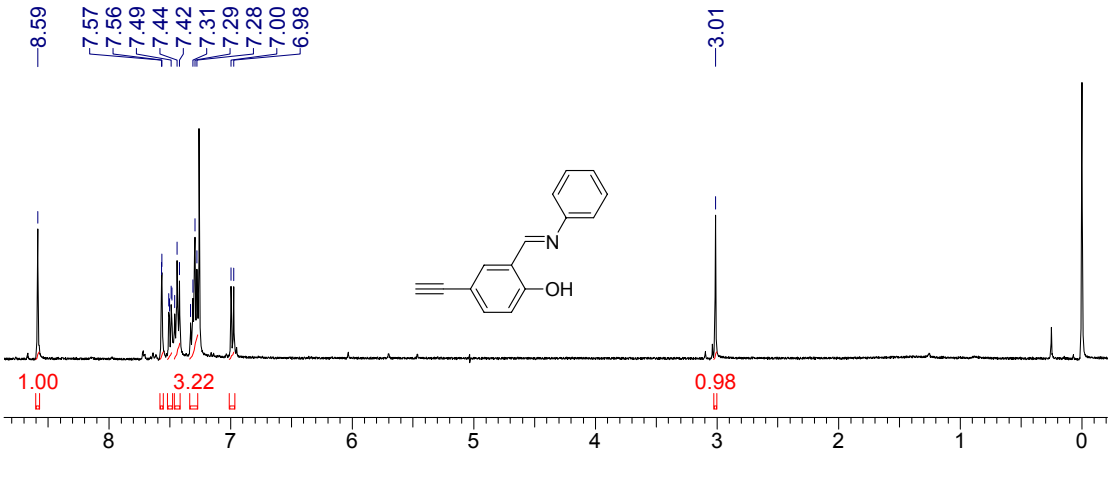

Figure S2. ^{1}H NMR of **3** ($CDCl_3$, 400 MHz).

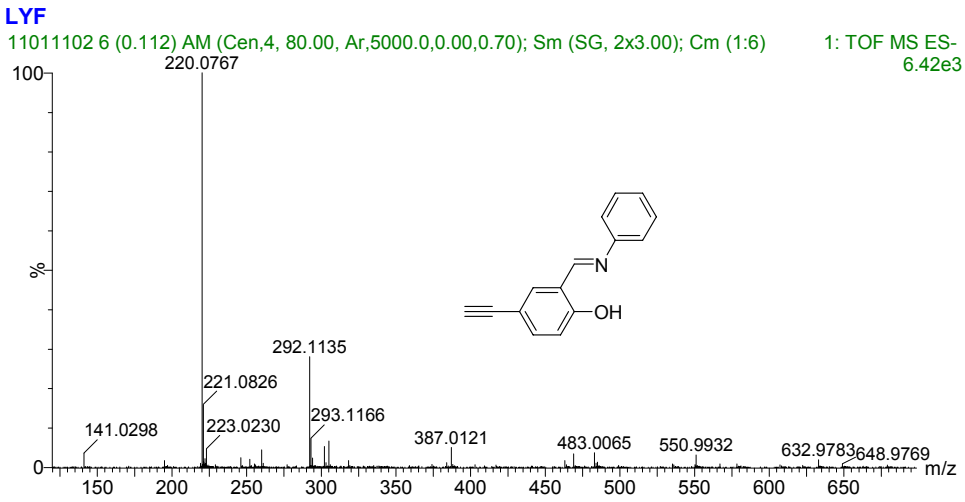

Figure S3. TOF HRMS ESI of **3**.

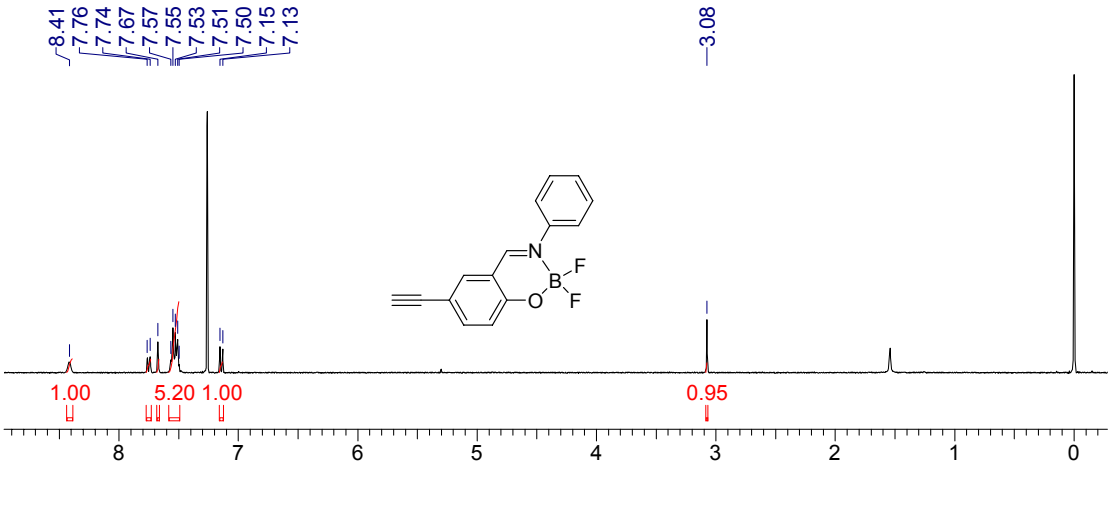

Figure S4. ^{1}H NMR of **4** ($CDCl_3$, 400 MHz).

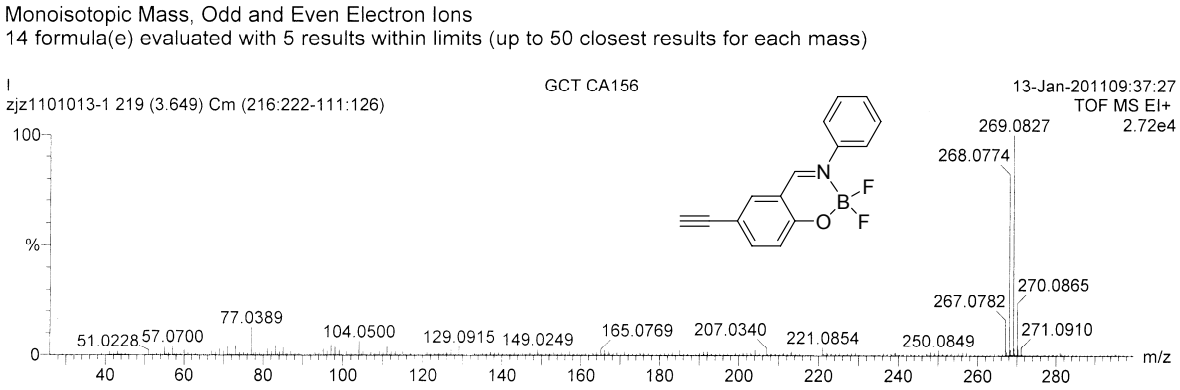

Figure S5. TOF HRMS ESI of **4**.

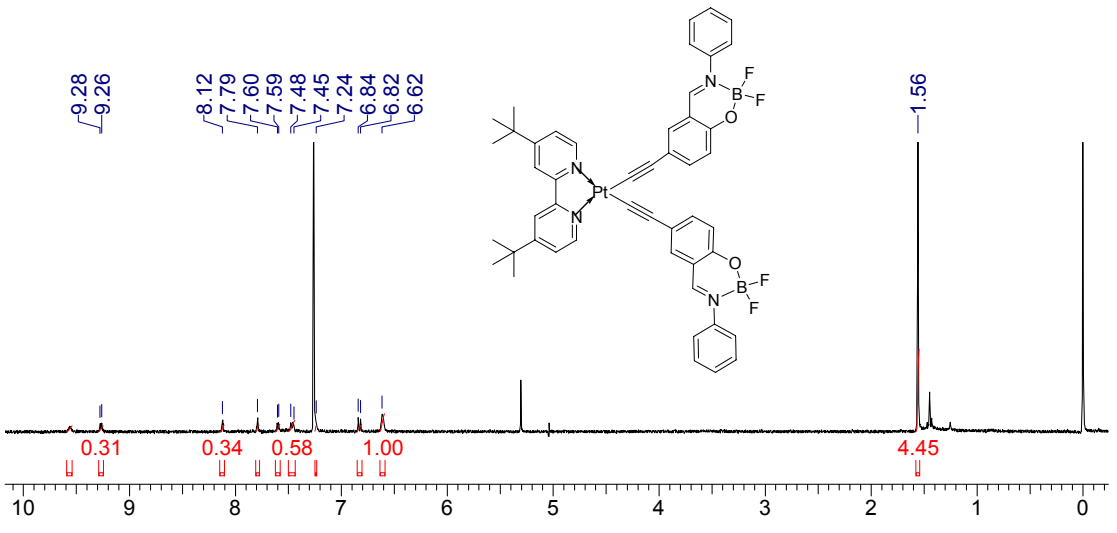

Figure S6. ^{1}H NMR of **Pt-1** ($CDCl_3$, 400 MHz).

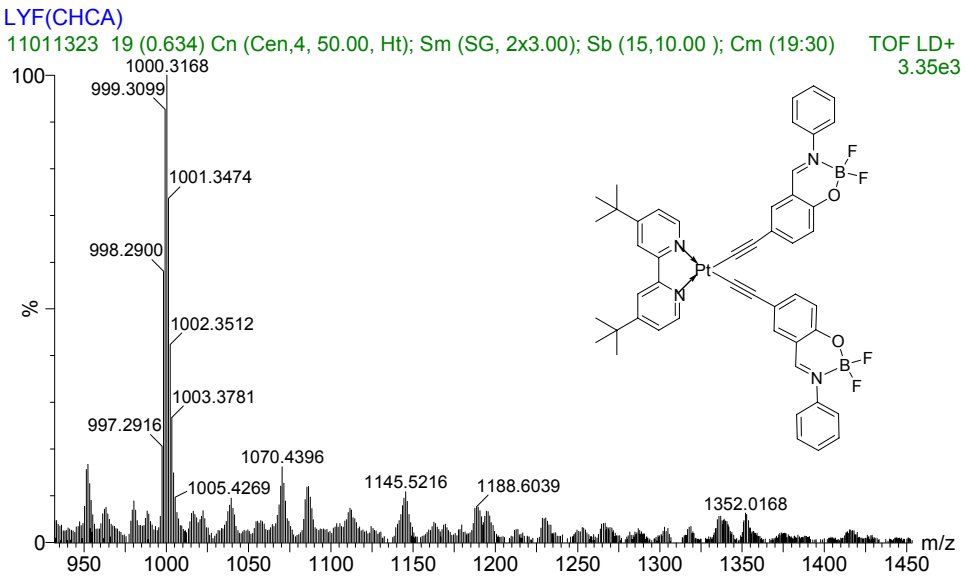

Figure S7. TOF HRMS ESI of **Pt-1**.

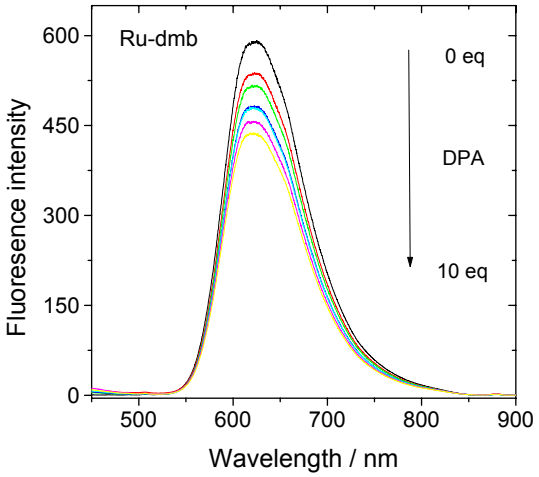

Figure S8. Phosphorescence emission spectra of **Ru(dmb)$_3$[PF$_6$]$_2$** (λ_{ex} = 440 nm) with increasing the DPA concentration in deaerated toluene. The concentration of all complexes is 1.0 × 10^{-5} mol L^{-1}, 25 °C.

Symbolic Z-matrix for Complex Pt-1 (DFT//B3LYP/6-31G(d) / LanL2DZ)

Charge = 0 Multiplicity = 3

0 3

C	-3.45221085	-2.31530735	-2.16484355
C	-4.48456667	-3.18249014	-2.46667471
C	-5.61287470	-3.26102850	-1.62649584
C	-5.64714565	-2.44650455	-0.46110271
C	-4.58078628	-1.56765053	-0.17179887
C	-3.47263384	-1.47758744	-1.01150007
H	-2.58992407	-2.25876304	-2.82190169
H	-4.45487957	-3.81264588	-3.34889108
H	-4.62450794	-0.95759560	0.72616758
O	-6.59036637	-4.09779687	-1.91455187
C	-6.75254427	-2.58385841	0.42436435
H	-6.74961480	-2.02897490	1.36227270
N	-7.77723013	-3.35393356	0.16527134
C	-8.81297088	-3.51890874	1.13891452
C	-10.15003816	-3.51953344	0.72121663
C	-11.16135452	-3.66247978	1.66805369
C	-10.85329568	-3.80848920	3.02311436
C	-9.51910177	-3.82172301	3.43163434
C	-8.49682187	-3.68370599	2.49307387
H	-10.37458130	-3.39627833	-0.33105100
H	-12.19755607	-3.65757302	1.34335239
H	-11.64796856	-3.92303910	3.75414780
H	-9.26871076	-3.95756376	4.47951486
H	-7.45835829	-3.74252945	2.80485483
B	-7.90839841	-4.11334462	-1.26006718
F	-8.83061285	-3.39816884	-2.00761228
F	-8.29913320	-5.40279139	-1.01673847
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C	3.32505232	-4.47211021	0.39233618
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C	5.26324955	-2.93081546	0.11080733
C	4.35444750	-1.87192162	0.01896636
C	2.94809533	-2.08215874	0.10456888
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H	2.97834567	-5.48896965	0.54149573
H	4.72061509	-0.86165607	-0.13384602
O	5.52019603	-5.28559008	0.44158542
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