

Supporting information

Effective visible-light driving CO₂ photoreduction via a promising bifunctional iridium coordination polymer

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Table 1. Crystal Data and Structure Refinements for **Ir-Y**

formula	C ₆₈ H ₄₄ Ir ₂ N ₈ YO ₉
formula weight (g/mol)	1590.5
crystal system	triclinic
space group	<i>P</i> -1
<i>a</i> (Å)	9.059(4)
<i>b</i> (Å)	15.197(6)
<i>c</i> (Å)	23.751(10)
α (deg)	73.595(8)
β (deg)	88.406(14)
γ (deg)	81.684(12)
<i>V</i> (Å ³)	3014 (2)
<i>Z</i>	2
<i>T</i> (K)	173(2)
ρ_c (g/cm ³)	1.702
F000	3588
crystal size (mm ³)	0.3 × 0.05 × 0.05
data/restraints/parameters	14147/0/793
Goodness-of-fit on F ²	1.023
R(int)	0.0805
R1, wR2 ^a [I > 2sigma(I)]	0.0641, 0.1239
R1, wR2 (all data)	0.1059, 0.1503
^a R1 = $\Sigma F_o - F_c /\Sigma F_o $, wR2 = $\{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma w[(F_o^2)^2]\}^{1/2}$.	

Table 2. Selected Bond lengths [Å] and angles [deg] for **Ir-Y**.

Y(1)-O(7)#1	2.244(7)	Y(1)-O(2)	2.260(7)
Y(1)-O(13)#2	2.265(7)	Y(1)-O(6)	2.272(7)
Y(1)-O(9)	2.284(10)	Y(1)-O(5)#3	2.331(7)
O(7)#1-Y(1)-O(2)	97.4(3)	O(7)#1-Y(1)-O(3)#2	151.6(3)
O(2)-Y(1)-O(3)#2	89.6(3)	O(7)#1-Y(1)-O(6)	87.1(2)
O(2)-Y(1)-O(6)	169.9(3)	O(3)#2-Y(1)-O(6)	82.3(3)
O(7)#1-Y(1)-O(9)	132.5(4)	O(2)-Y(1)-O(9)	83.6(3)
O(3)#2-Y(1)-O(9)	75.5(4)	O(6)-Y(1)-O(9)	100.1(3)
O(7)#1-Y(1)-O(5)#3	76.0(3)	O(2)-Y(1)-O(5)#3	80.7(3)
O(9)-Y(1)-O(5)#3	149.2(4)	O(7)#1-Y(1)-O(9)#1	69.9(3)
O(2)-Y(1)-O(9)#1	89.6(3)	O(3)#2-Y(1)-O(9)#1	137.9(4)
O(6)-Y(1)-O(9)#1	100.5(3)		

^aSymmetry transformations used to generate equivalent atoms: #1 -x+2, -y, -z+1; #2 x-1, y, z; #3 -x+1, -y, -z+1; #4 x+1, y, z.

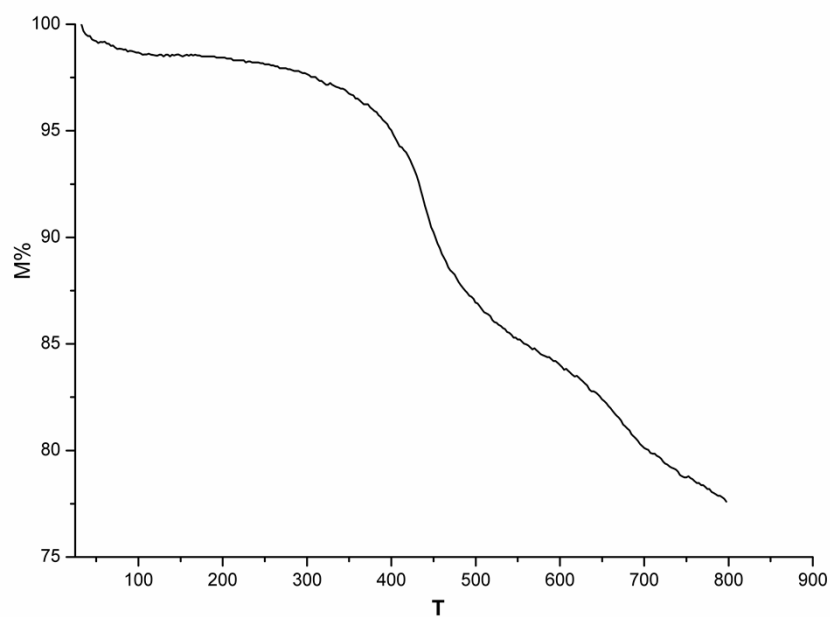


Figure S1. TGA curve of Ir-Y.

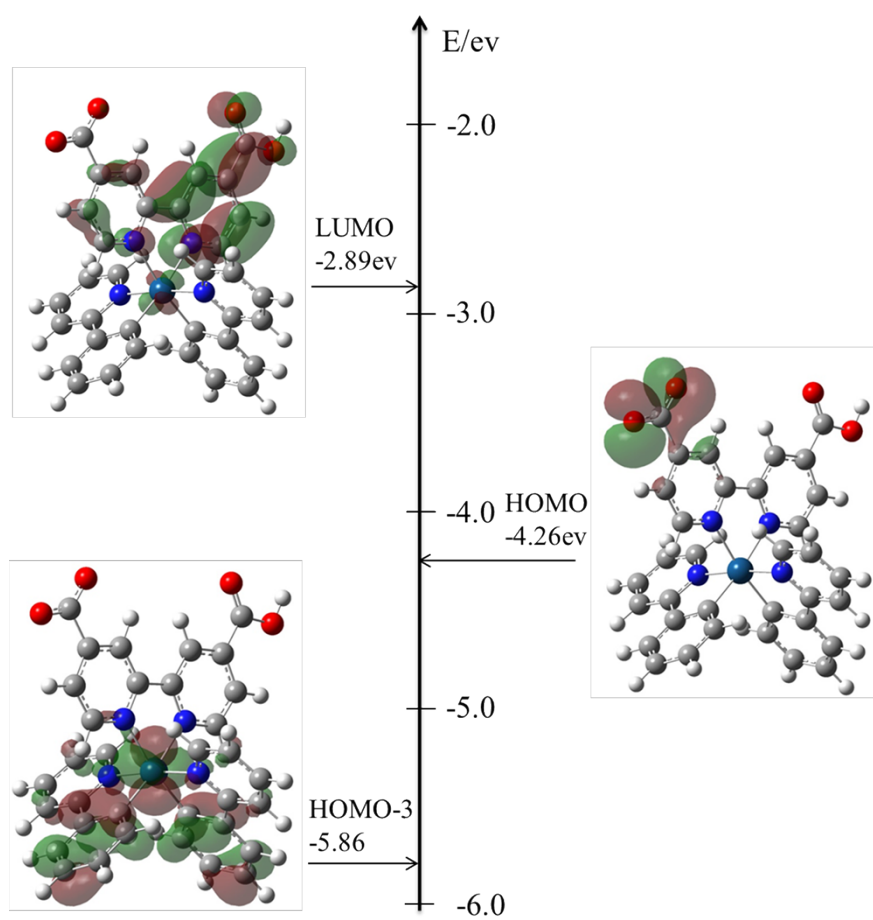


Figure S2. Schematic molecular orbital diagrams of Ir unit. The molecular orbital was calculated by DFT method at the PBE1PBE level.

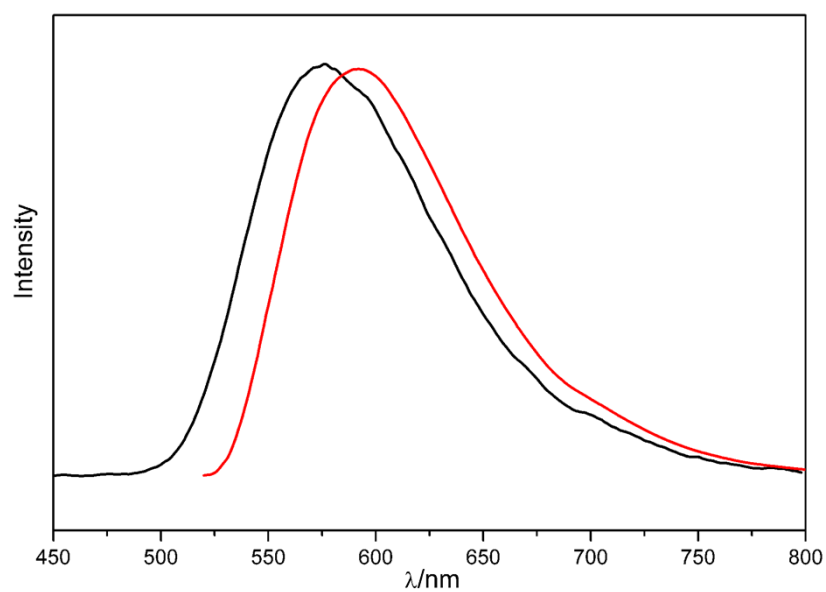
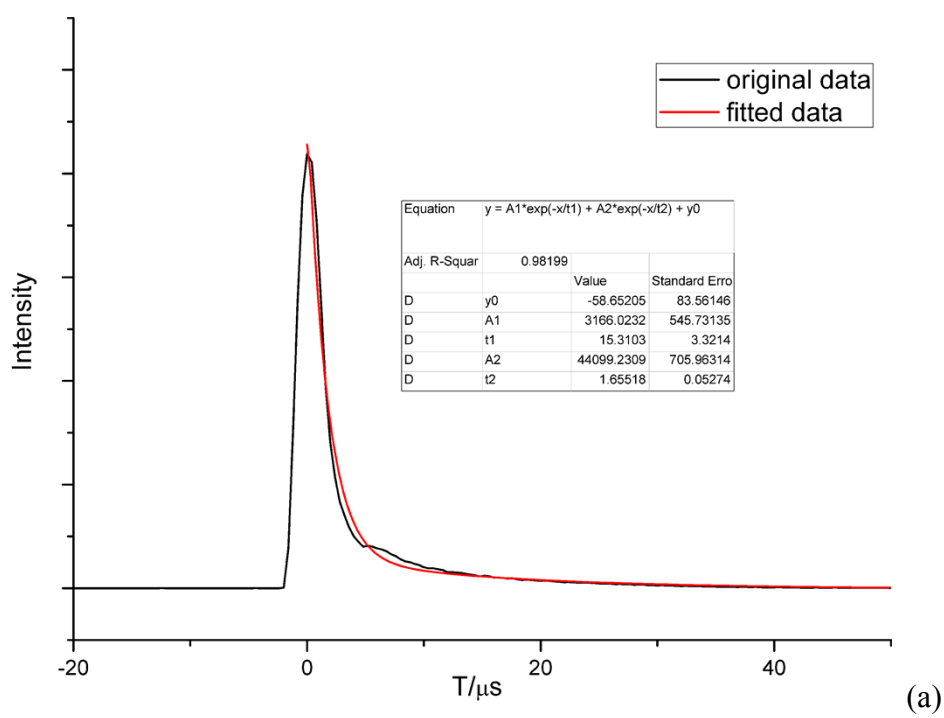


Figure S3. The emissions of the **L-H** ligand (black) and **Ir-Y**(red).



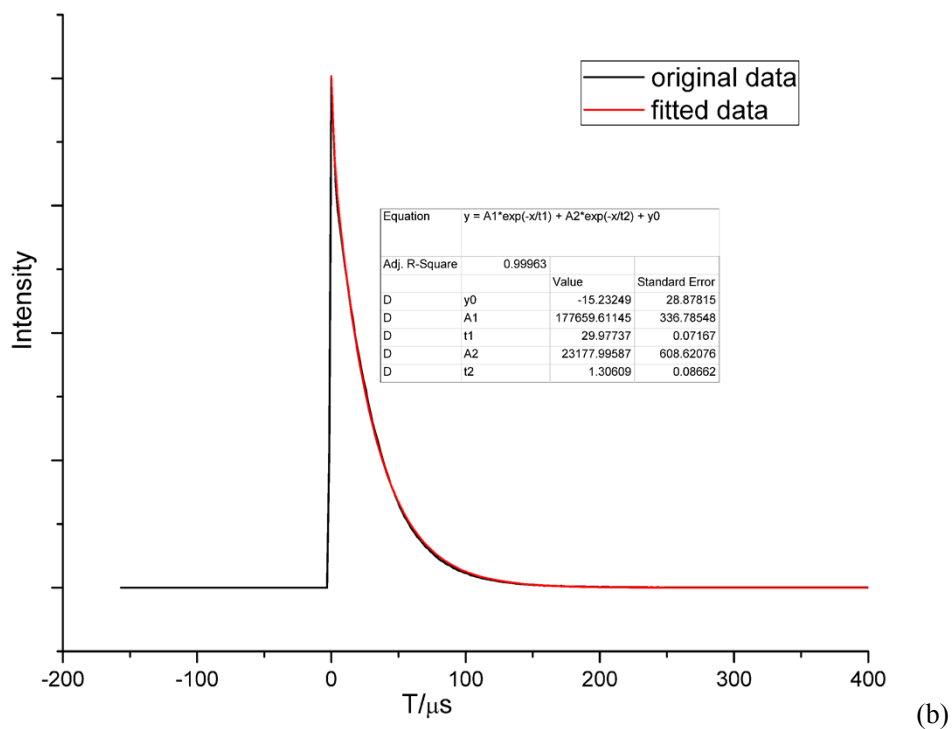


Figure S4. Transient emission decay profiles of **L-H** ligand (a) and **Ir-Y**(b).

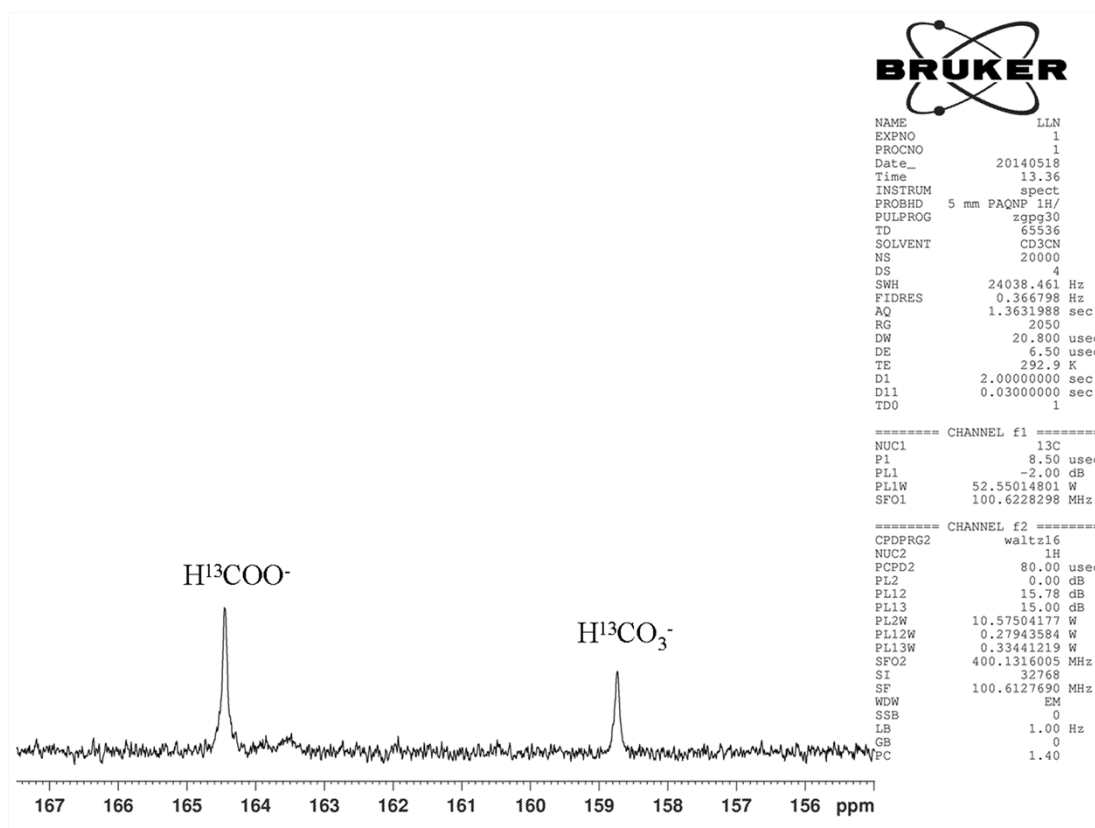


Figure S5. The ^{13}C NMR spectra for the product obtained under the following reaction conditions: 4 mg photocatalyst, 6ml $\text{CD}_3\text{CN}/\text{TEOA}$ (20:1 v/v), $^{13}\text{CO}_2$, 6h.

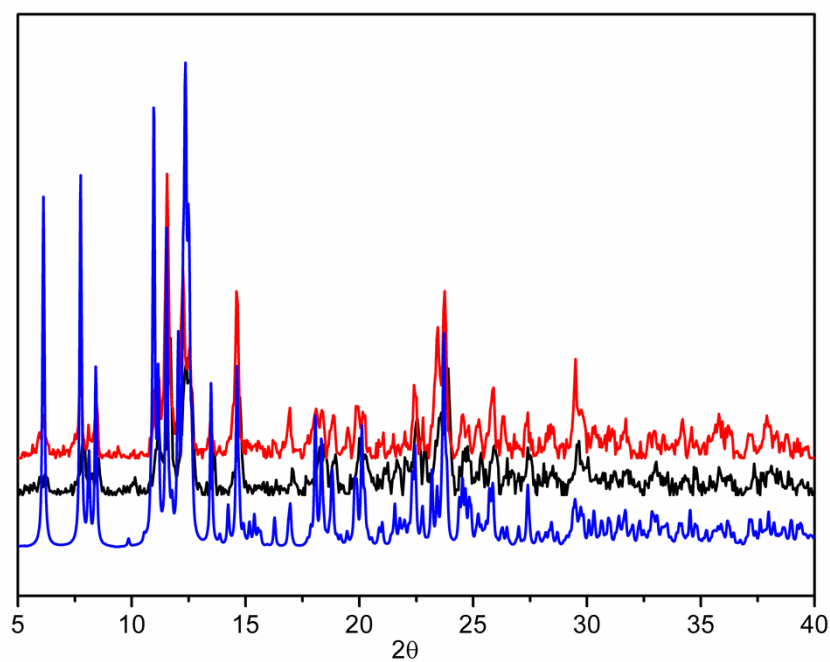


Figure S6. Powder X-ray diffraction (PXRD) patterns of simulated **Ir-Y** (blue), as-synthesized (black) and **Ir-Y** after the catalyst experiment (red).

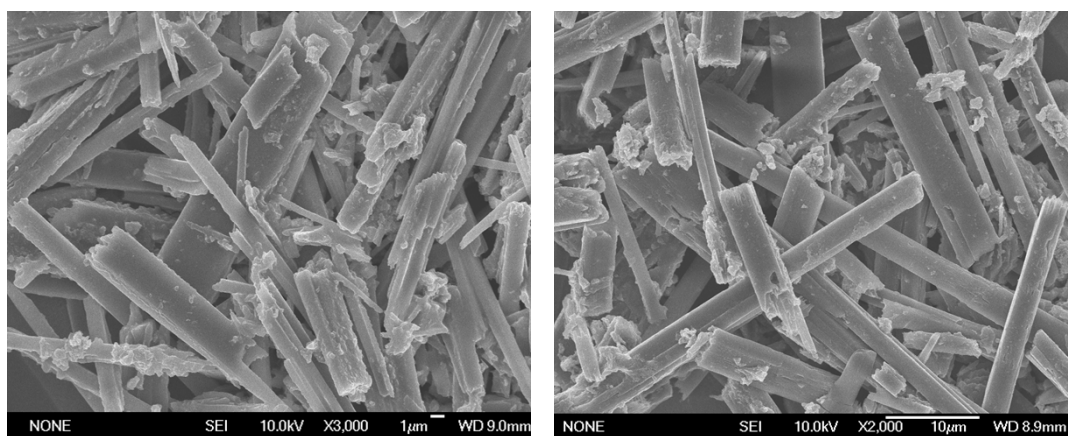


Figure S7. The SEM images of the as-synthesized **Ir-Y** (left) and after the catalyst experiment (right).

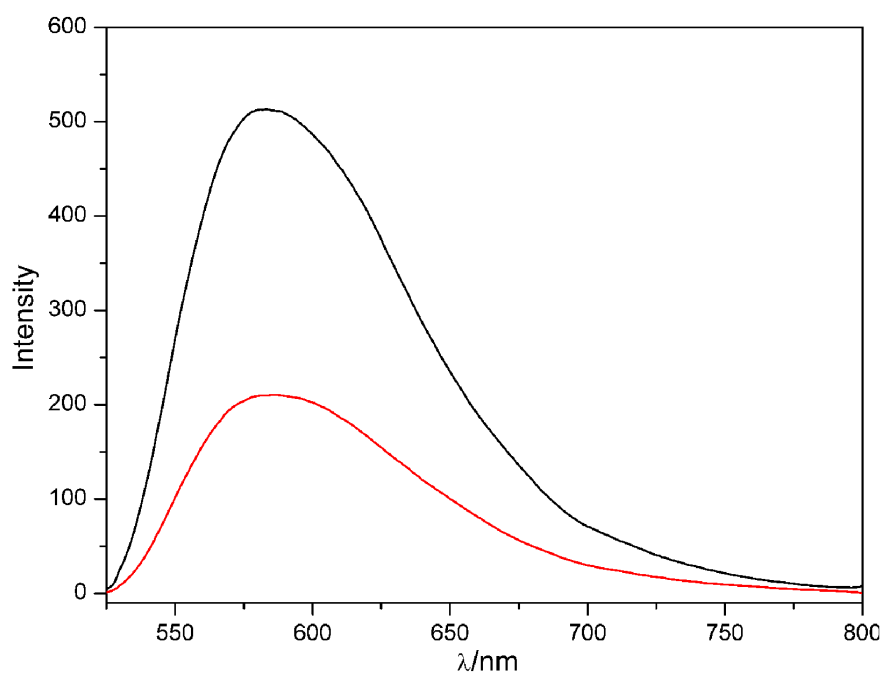


Figure S8. The luminescence quenching of **Ir-CP** by TEOA

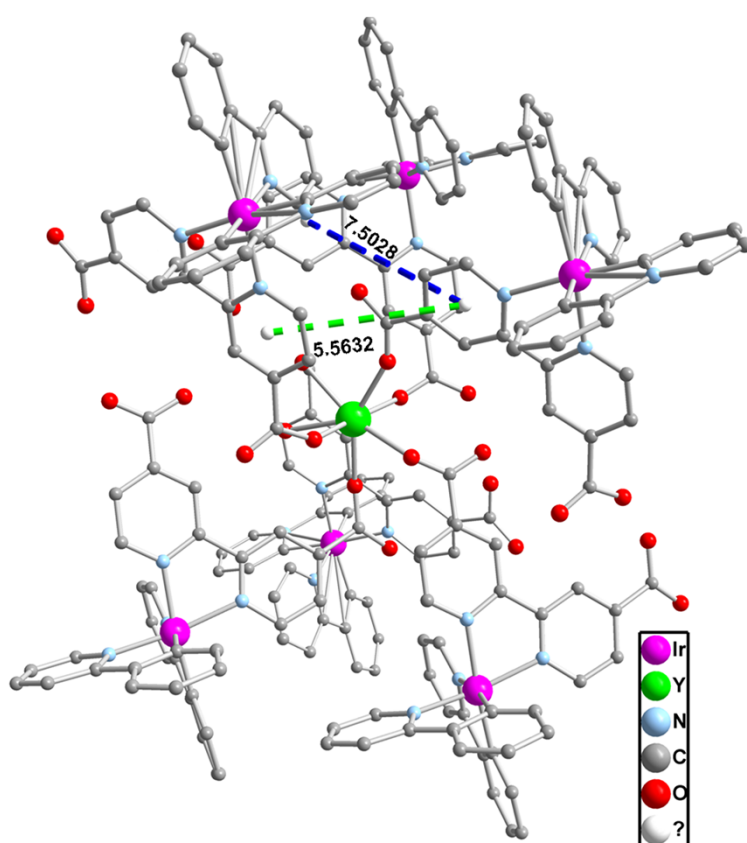


Figure S9. The centroid distances of the pyridine rings of adjacent dc bpy^{2-} in **Ir-CP** (range from 2.16 to 4.10 Å after considering the van der waals radius).