Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Supporting information

Highly Sensitized Near-Infrared Luminescence in Ir-Ln Heteronuclear Coordination Polymers via Light-Harvesting Antenna of Ir(III) Unit

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Table 1. Crystal Data and Structure Refinements of **Ir-Gd**, **Ir-Yb and Ir-Er**.

formula	$C_{68}H_{46}Ir_2N_8GdO_{10}$	$C_{68}H_{46}Ir_2N_8YbO_{10}$	$C_{68}H_{46}Ir_2N_8ErO_{10}$
formula weight (g/mol)	1676.8	1692.6	1686.8
crystal system	triclinic	triclinic	triclinic
space group	*P*-1	*P*-1	*P*-1
a (Å)	8.9631(3)	8.9717(3)	9.0025(2)
b (Å)	15.2186(5)	15.1215(4)	15.2262(3)
c (Å)	23.6351(8)	23.7174(6)	23.4324(5)
α (deg)	73.861(3)	73.467(2)	73.838 (2)
β (deg)	88.732(3)	88.039(3)	89.079(2)
γ (deg)	82.398(3)	81.392(3)	83.074 (2)
V (Å^3)	3069.32(17)	3049.73(16)	3061.99(11)
Z	2	2	2
T (K)	293(2)	293(2)	293(2)
ρ_c (g/cm^3)	1.791	1.841	1.827
F000	1620.0	1582.0	1620.0
crystal size (mm^3)	0.52 × 0.18 × 0.12	0.32 × 0.12 × 0.08	0.36 × 0.15 × 0.12
data/restraints/parameters	11925/0/802	11812/0/802	11877/0/802
R1, wR2*a* [I > 2sigma(I)]	0.0432, 0.1145	0.0755, 0.2307	0.0419, 0.1072
R1, wR2 (all data)	0.0498, 0.1145	0.0834, 0.2897	0.0482, 0.1136

[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-Nd**.

Nd(1)-O(5)	2.365(4)	Nd(1)-O(2)#1	2.369(4)
Nd(1)-O(8)#2	2.392(5)	Nd(1)-O(9)	2.406(5)
Nd(1)-O(9)#1	2.429(6)	Nd(1)-O(1)#3	2.443(4)
O(5)-Nd(1)-O(2)#1	80.07(18)	O(5)-Nd(1)-O(3)	146.43(17)
O(2)#1-Nd(1)-O(3)	88.02(15)	O(5)-Nd(1)-O(8)#2	101.01(17)
O(2)#1-Nd(1)-O(8)#2	168.83(17)	O(2)-Nd(1)-O(9)#2	95.55(18)
O(5)-Nd(1)-O(9)	136.35(19)	O(8)#2-Nd(1)-O(1)#3	79.87(17)
O(3)-Nd(1)-O(9)	75.66(19)	O(8)#2-Nd(1)-O(9)	93.07(19)
O(5)-Nd(1)-O(9)#1	72.63(18)	O(2)#1-Nd(1)-O(9)#1	96.86(17)
O(3)-Nd(1)-O(9)#1	140.41(18)	O(5)-Nd(1)-O(1)#3	75.83(16)
O(2)#1-Nd(1)-O(1)#3	96.47(16)	O(3)-Nd(1)-O(1)#3	74.48(17)

[a]Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z #2 x-1,y,z #3 x+1,y,z

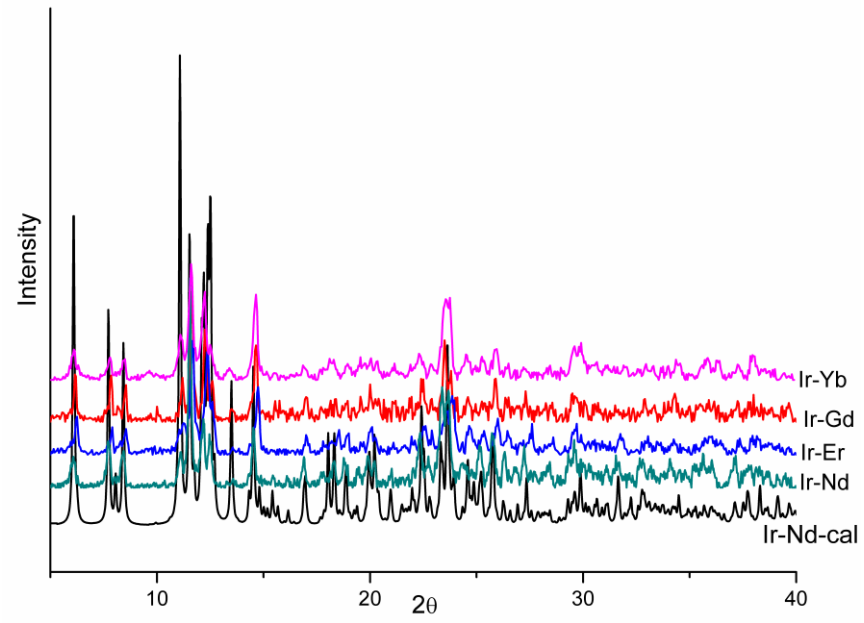


Figure S1. Powder X-ray diffraction (PXRD) patterns of the **Ir-Ln** complexes.

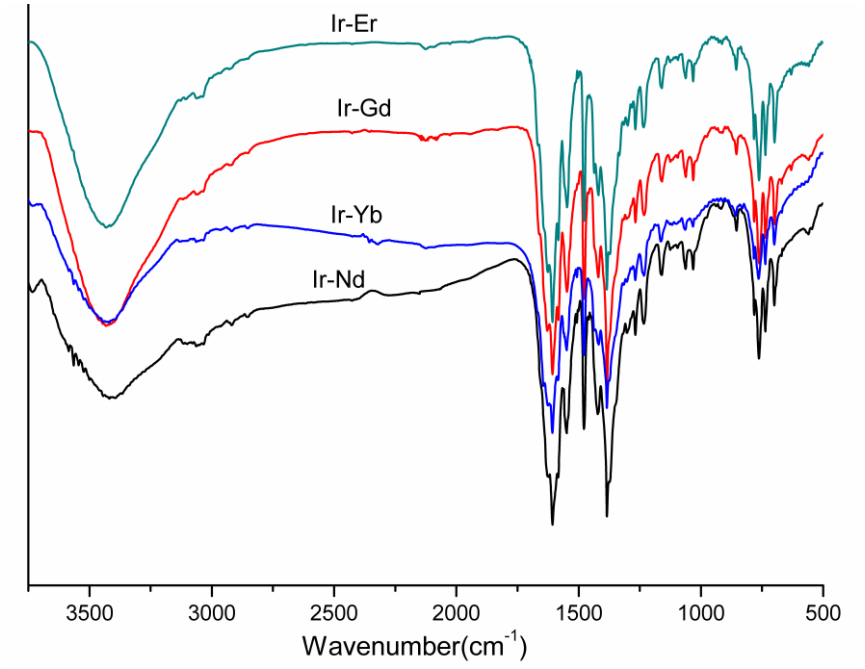


Figure S2. IR spectra of the four Ir-Ln complexes.

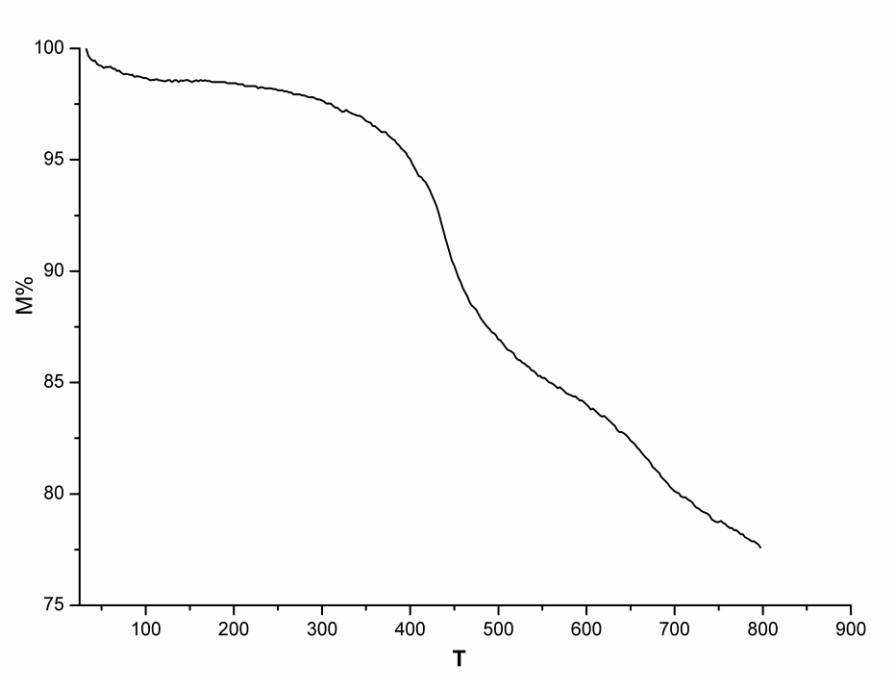


Figure S3. TGA curve of Ir-Nd.

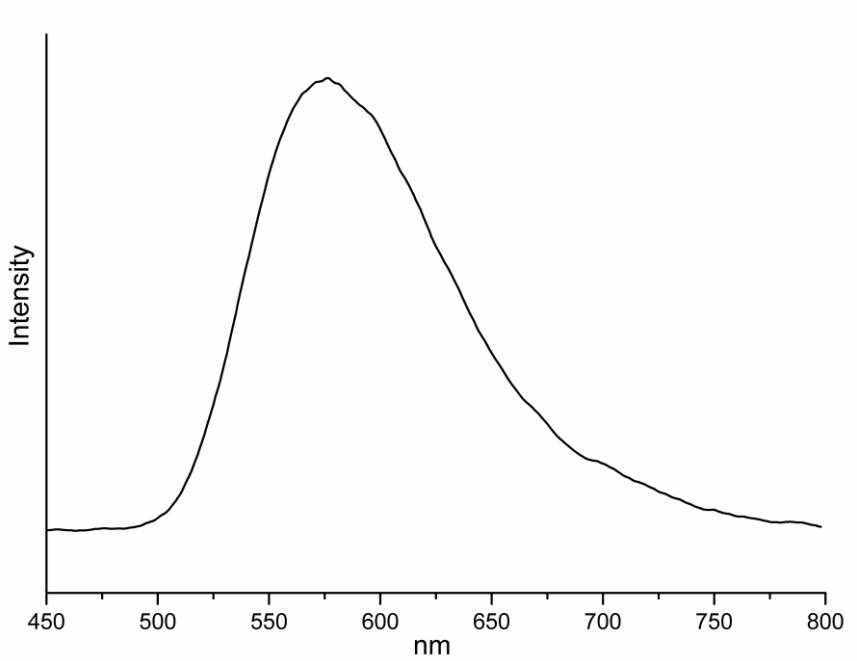
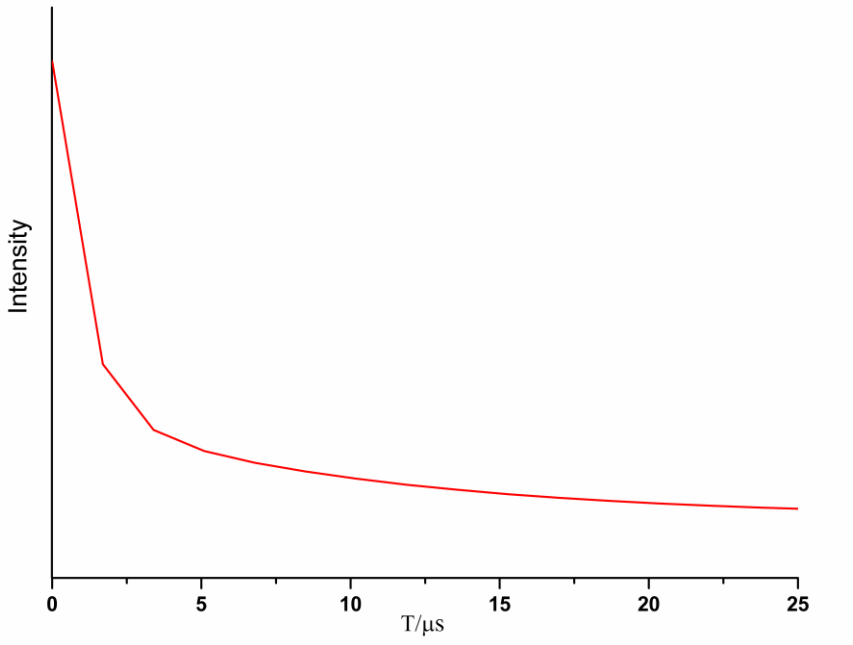
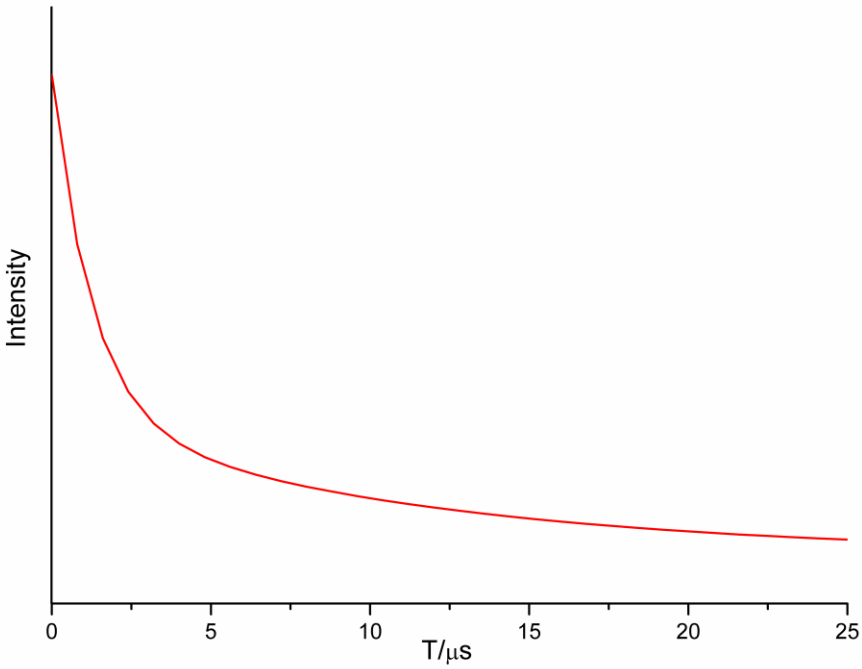


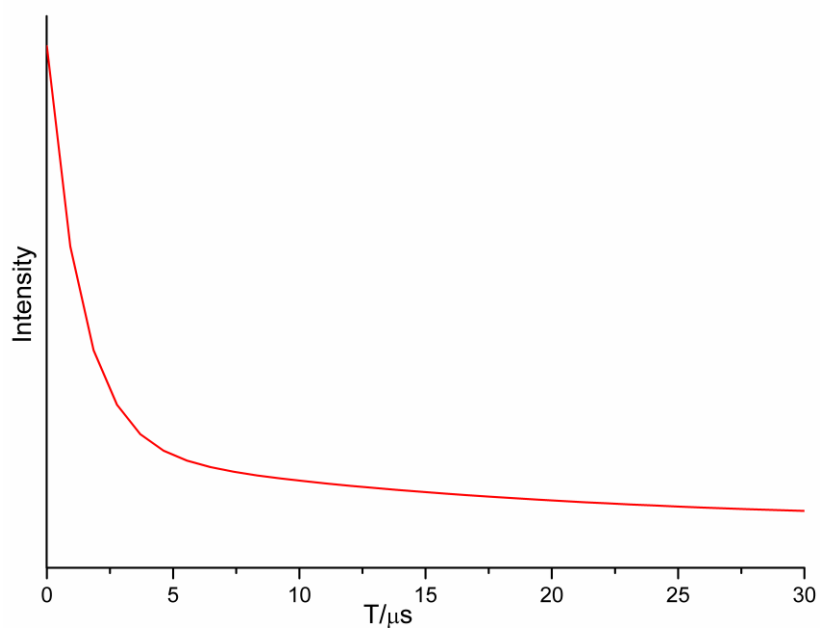
Figure S4. The PL spectra of the **L-H** ligand.



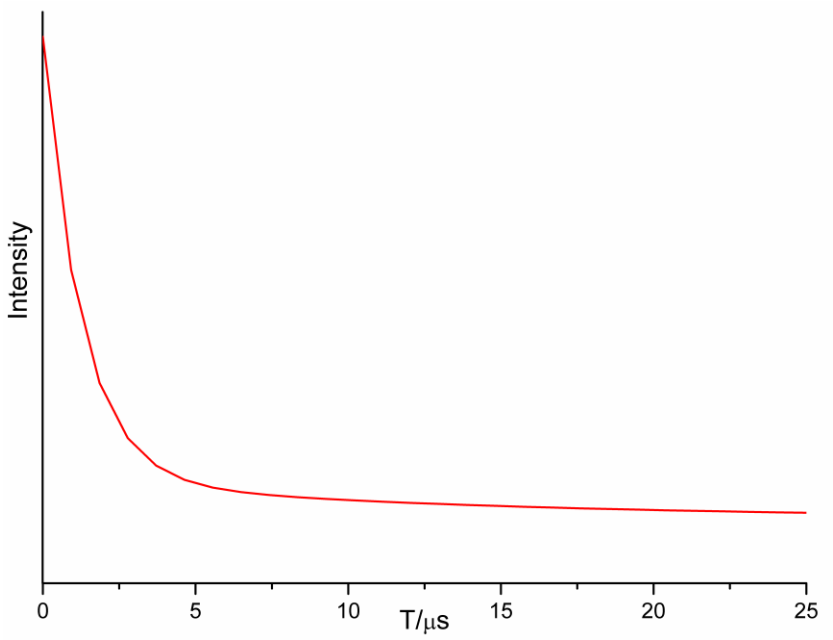
(a)



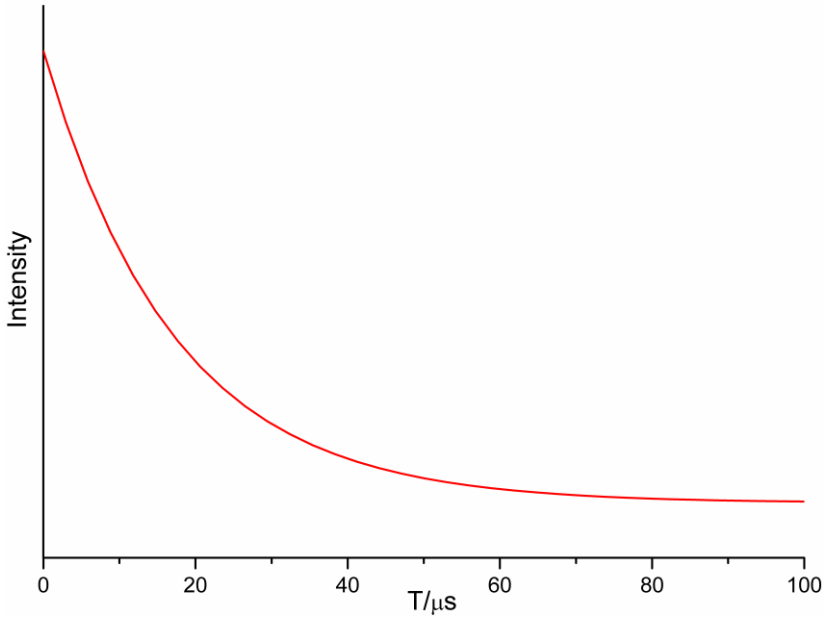
(b)



(c)



(d)



(e)

Figure S5. Transient NIR emission decay profiles of **L-H** ligand (a), **Ir-Gd** (b), **Ir-Er** (c), **Ir-Nd** (d), **Ir-Yb** (e) in solid powder.

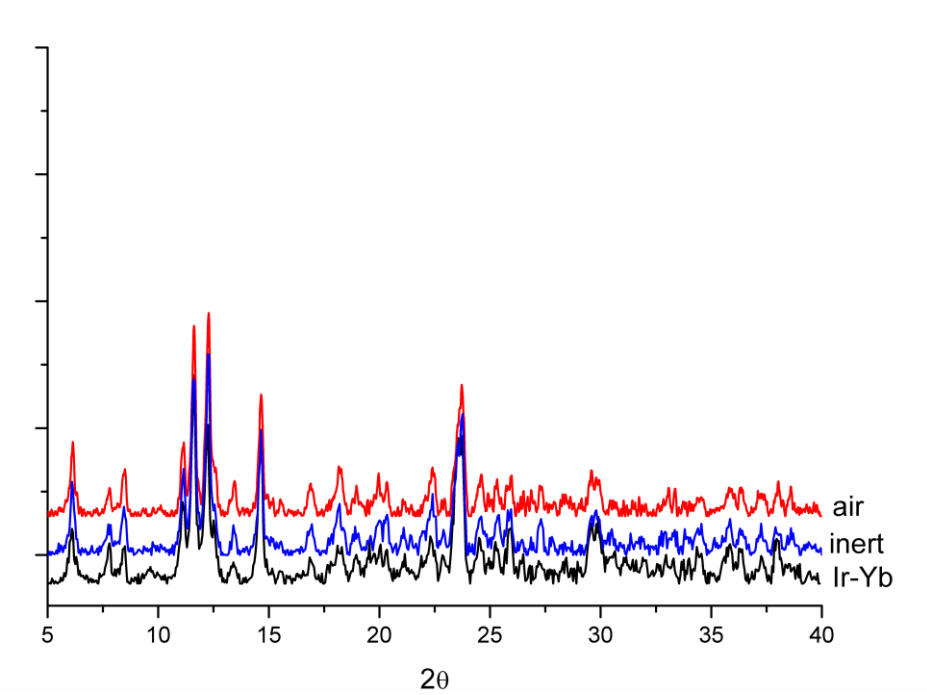


Figure S6. Powder X-ray diffraction (PXRD) patterns of the original sample and the light-exposed samples of **Ir-Yb** complex.