Supplementary Information

Enhanced near-infrared luminescence in Ln_2Cd_2 (Ln = Nd, Yb) heterotetranuclear complexes

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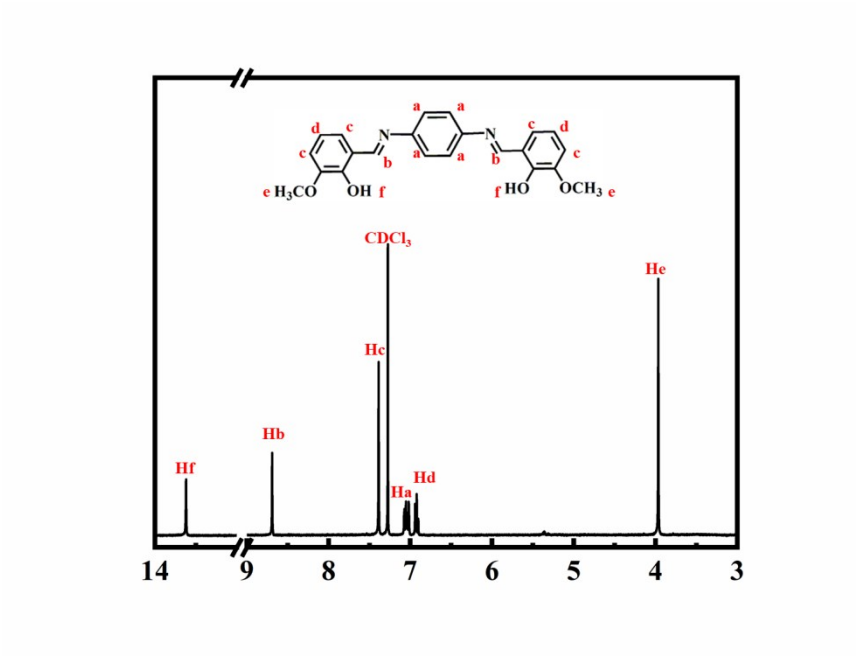

Fig. S1. ^{1}H NMR spectrum of H_2L in $CDCl_3$.

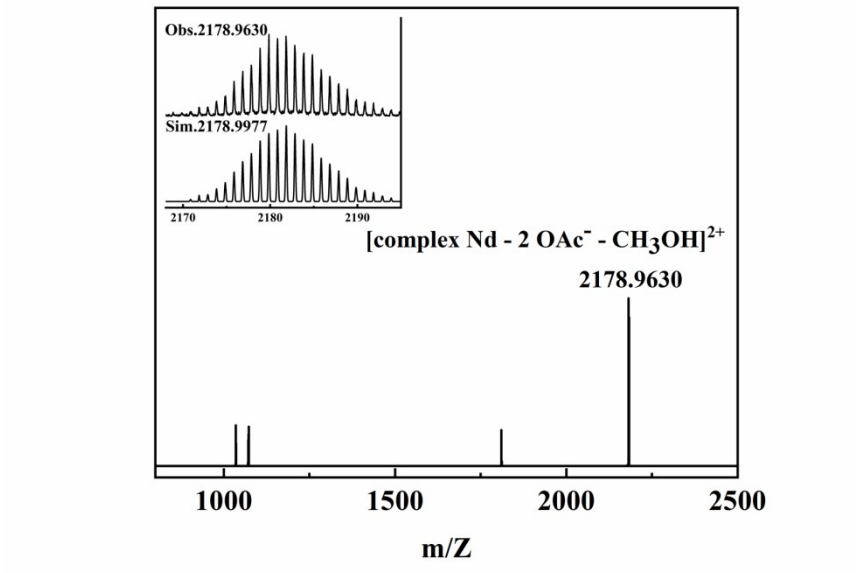

Fig. S2. ESI-TOF-MS of complex 1.

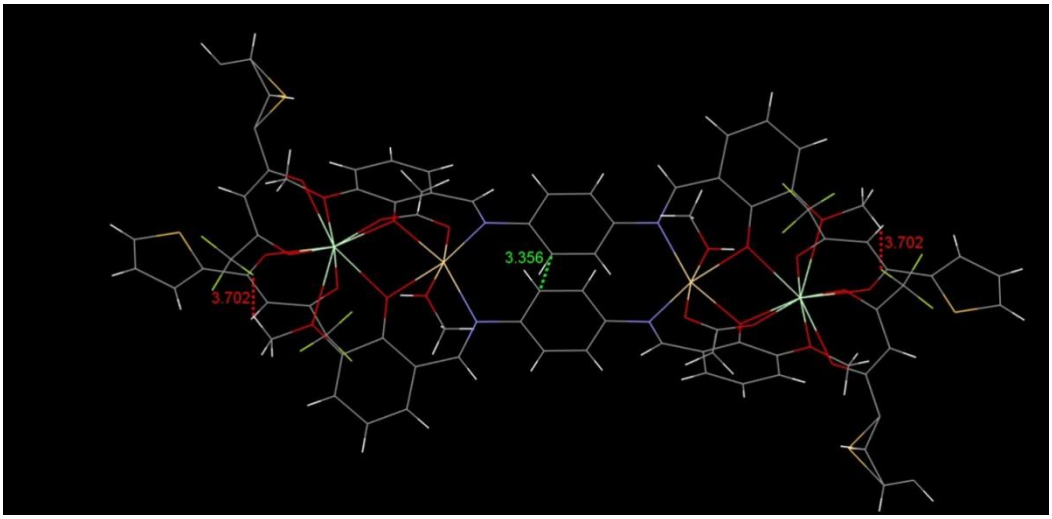

Fig. S3. The intramolecular C–H···F interactions between the F atoms of TTA and H atoms of L and π - π conjugate effect for complex 2.

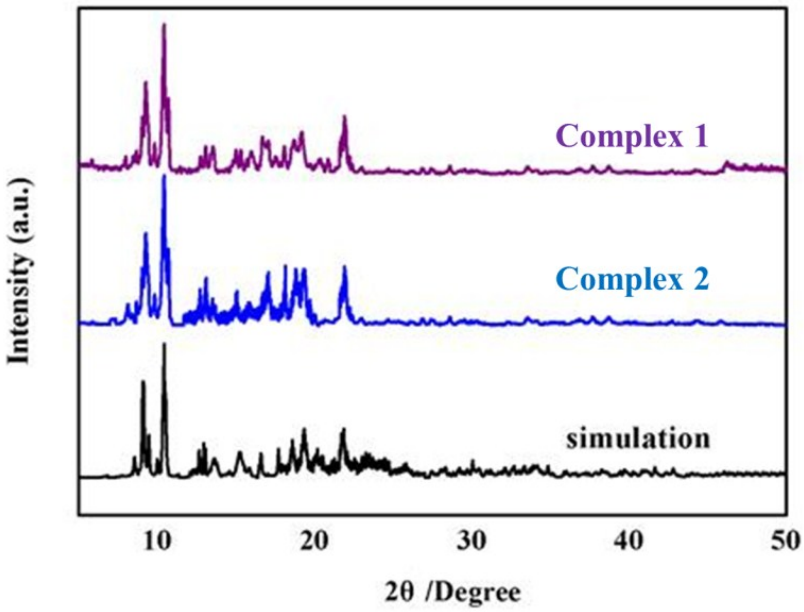

Fig. S4. The powder X-ray diffraction (PXRD) patterns of complexes **1** and **2**

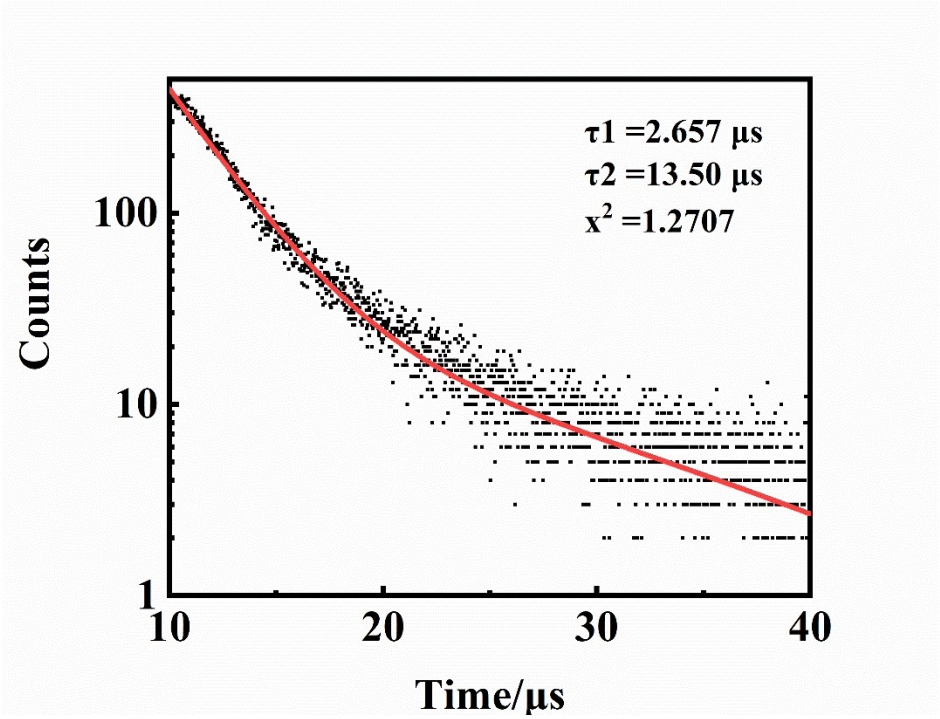

Fig. S5 Luminescence decay curves of **1** in CH_3CN.

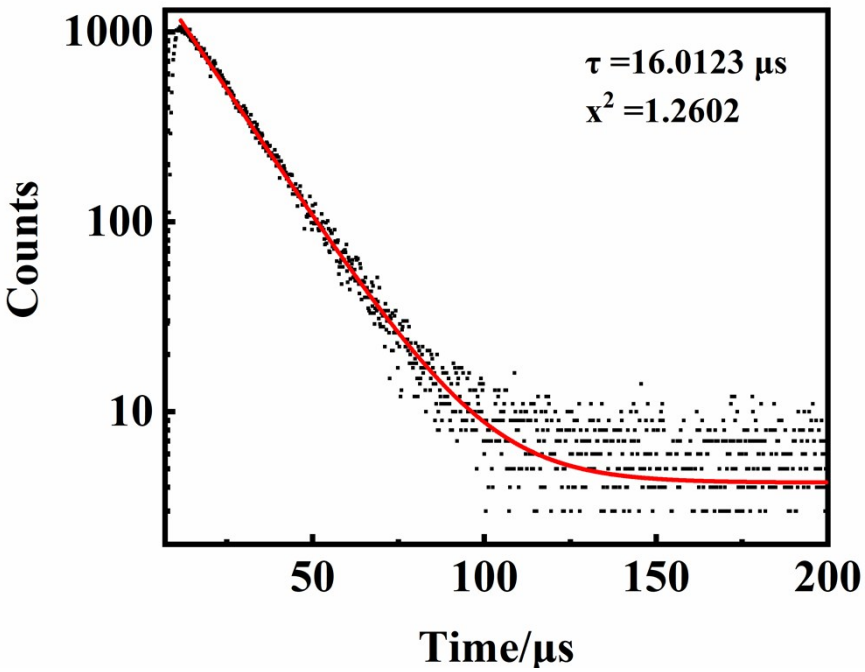

Fig. S6. Luminescence decay curves of **2** in CH_3CN.

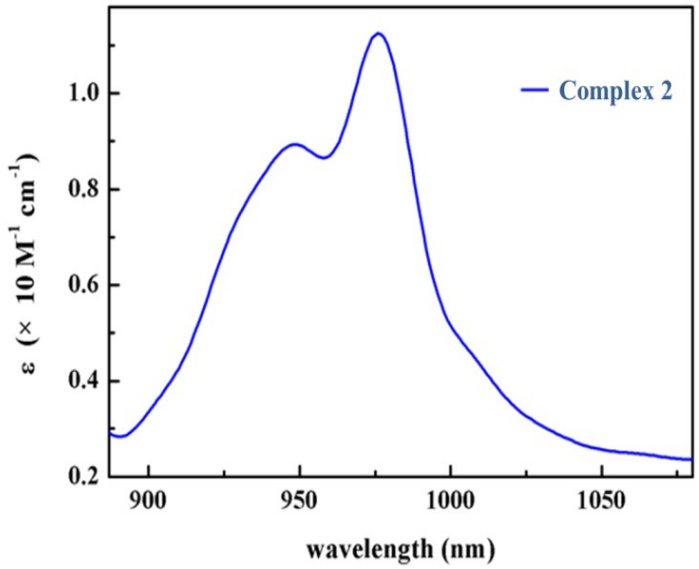

Fig. S7. Near-infrared spectrum of f–f absorption transition for **2** in CH_3CN.

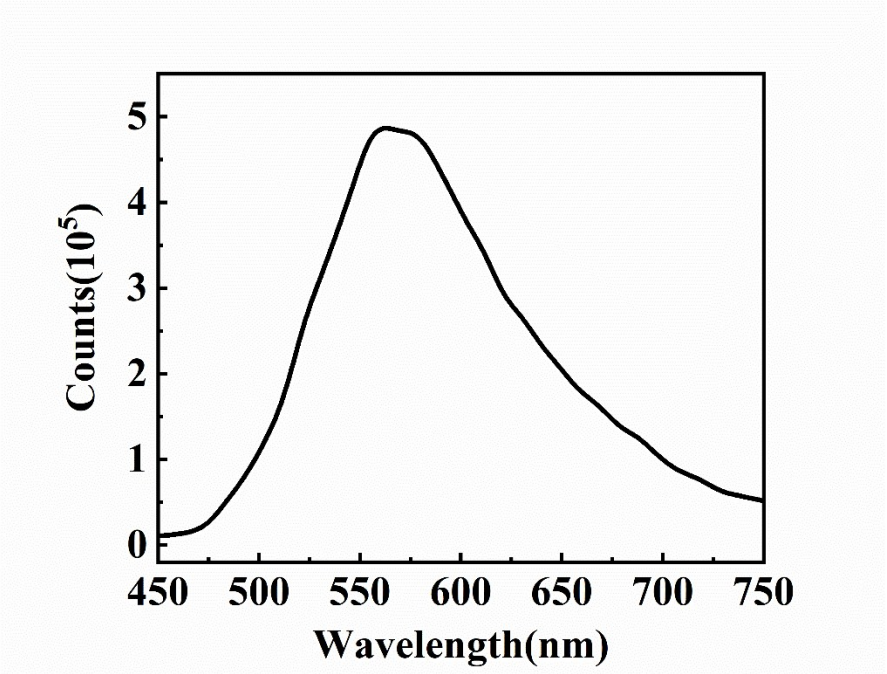

Fig. S8. Emission spectrum of $\mathbf{Gd_2L_2}$ in CH_3CN at 77 K.

Table S1.Some absolute quantum yields of related literatures.

References	Complex	Φem (%)
This text	Yb^{3+}	2.13
	Nd^{3+}	0.34
16(a)	Yb^{3+}	0.04
16(b)	Nd^{3+} (1)	0.17
	Nd^{3+} (2)	0.46
16(c)	Yb^{3+}	1.07
	Nd^{3+}	0.36
16(d)	Nd^{3+}	0.56
	Yb^{3+}	1.32
16(e)	Nd^{3+}(1)	0.45
	Nd^{3+}(2)	1.07
	Yb^{3+} (1)	1.69
	Yb^{3+} (2)	3.08
16(f)	Nd^{3+}	0.62
	Yb^{3+}	0.79
16(g)	Yb^{3+}	0.41

Table S2. Crystallographic data for **1**.

Complex	1
CCDC number	1977217
Empirical formula	$C_{86}H_{74}N_4O_{22}F_{12}S_4Cl_8Nd_2Cd_2$
Formula weight	2668.61
Temperature (K)	100
Crystal system	triclinic
Space group	P-1
a (Å)	10.7102(8)
b (Å)	12.4241(9)
c (Å)	18.9297(14)
α (°)	88.674(2)
β (°)	81.057(3)
γ (°)	77.969(2)

V (Å^3)	2433.5(3)
Z	1
ρ_{calc}g/cm^{-3}	1.821
μ (mm^{-1})	1.880
F(000)	1318.0
θ range	5.84 to 56.58
Index ranges	-14 ⩽ h ⩽ 14
	-16 ⩽ k ⩽ 16
	-25 ⩽ l ⩽ 25
Reflections collected	127756
Completeness to theta =	99.3%
Data/restraints/parameters	12059/207/658
Goodness-of-fit on F^2	1.070
Final R indexes [I>=2σ (I)]	R_1 = 0.0516
	wR_2 = 0.1321
Final R indexes [all data]	R_1 = 0.0543
	wR_2 = 0.1346

Table S3. Purity and producing factory of reagents

Reagents and chemicals	Purity	Manufacturer
CH_3OH	Analytical pure	Tianjin Kemiou Chemical Reagent Development Center
CH_3CN	⩾99.5%	Tianjin Kemiou Chemical Reagent Development Center
CH_2Cl_2	⩾99.5%	Tianjin Kemiou Chemical Reagent Development Center
$Cd(OAc)_2$	99.9%	Shanghai Yuelong Chemical Co., Ltd.
NaOH	99.9%	Shanghai Yuelong Chemical Co., Ltd.
2-Hydroxy-3-methoxy-benzaldehyde	98%	Aladdin Chemical Reagent Co., Ltd.
2-thenoyltrifluoroacetone	98%	Aladdin Chemical Reagent Co., Ltd.
p-phenylenediamine	98%	Aladdin Chemical Reagent Co., Ltd.