Supplementary Information

Sensitization of NIR luminescence of Yb^{3+} by Zn^{2+} chromophores in heterometallic complexes with bridging Schiff-base ligand

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Table S1. Details of crystallographic, collection and refinement data for complexes **1**-**4**.

Complex	**1 + 2**	**3**	**4**
Empirical formula	$C_{106}H_{82}F_{36}N_8O_{24}Yb_2Zn_4$	$C_{60}H_{48}F_{24}N_6O_{14}Yb_2Zn_2$	$C_{66}H_{56}N_6O_{13}Yb_2$
Formula weight	3143.35	2009.86	1487.24
Temperature [K]	100(2)	100(2)	100(2)
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$
Unit cell dimensions			
a[Å]	18.1681(5)	15.4896(2)	13.1157(5)
b[Å]	13.5223(4)	21.0187(2)	19.4737(7)
c[Å]	22.7668(7)	22.5205(2)	23.2334(3)
α[°]	90	90	90
β[°]	96.9370(10)	109.7990(10)	99.043(2)
γ[°]	90	90	90
Volume [$Å^3$]	5552.3(3)	6898.60(13)	5860.3(3)

Z	2	4	4
Calculated density [Mg/m^3]	1.880	1.935	1.686
Absorption coefficient [mm^{-1}]	2.655	3.505	3.244
Crystal size [mm]	0.340×0.18×0.10	0.30×0.15×0.10	0.40×0.20×0.20
θ [°]	1.802 - 29.130	2.900 - 30.508	3.021 - 28.000
Reflections collected / unique	60046 / 14939	142215 / 21020	32714 / 14043
R_{int}	0.0266	0.0304	0.0249
Final R indices [I>2sigma(I)]	R_1=0.0348, wR_2=0.0829	R_1=0.0227, wR_2=0.0507	R_1=0.0246, wR_2=0.0473
R indices (all data)	R_1=0.0406, wR_2=0.0882	R_1=0.0298, wR_2=0.0529	R_1=0.0366, wR_2=0.0498
S	1.033	1.053	1.024
Largest diff. peak and hole [$e/Å^3$]	2.017 / -1.103	0.933 / -0.748	0.723 / -0.661

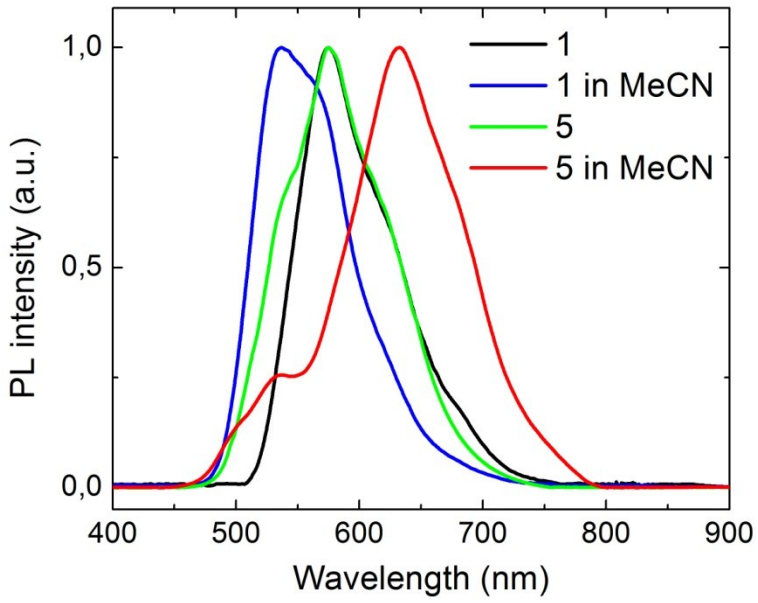

Fig. S1. PL spectra of **1** and **5** in solid state and MeCN solution under 380 nm excitation at room temperature.

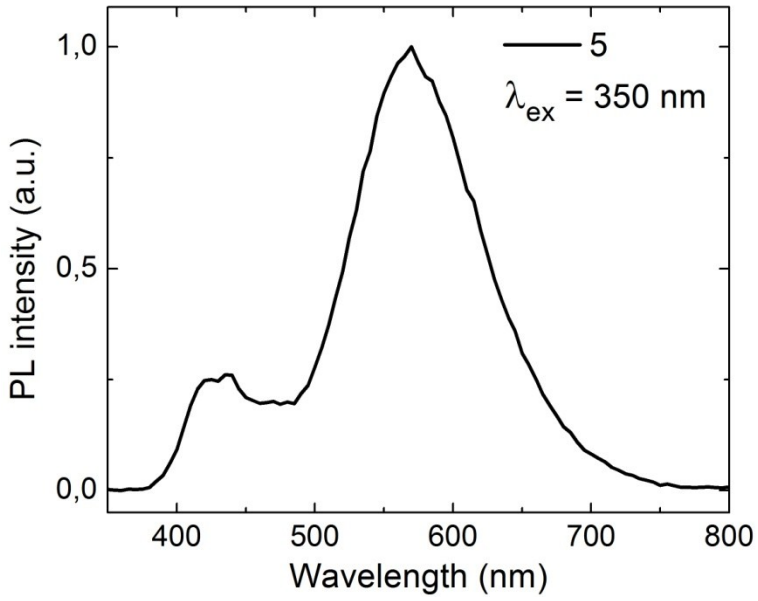

Fig. S2. PL of **5** under 350 nm excitation. The band at ca. 440 nm was observed for all complexes and corresponds to $^1S_1 \rightarrow {}^1S_0$ transition in the Schiff-base.

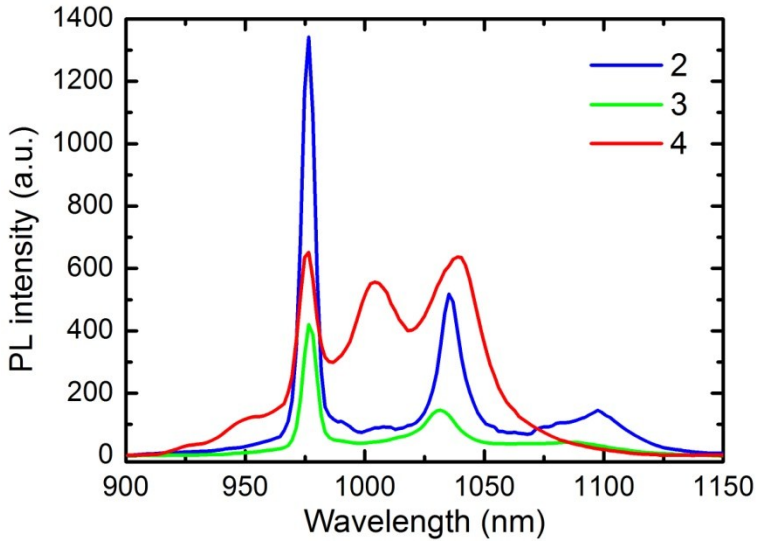

Fig. S3. NIR PL of ytterbium complexes **2-4** in MeCN solution (O.D. = 0.1 at 405 nm) under 405 nm laser diode excitation.

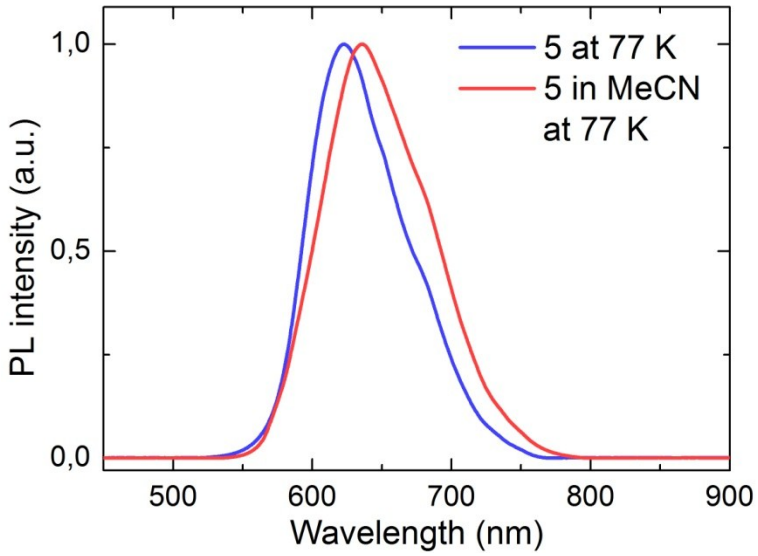

Fig. S4. Phosphorescence spectra of the Gd derivative **5** in solid state and MeCN solution at 77K.

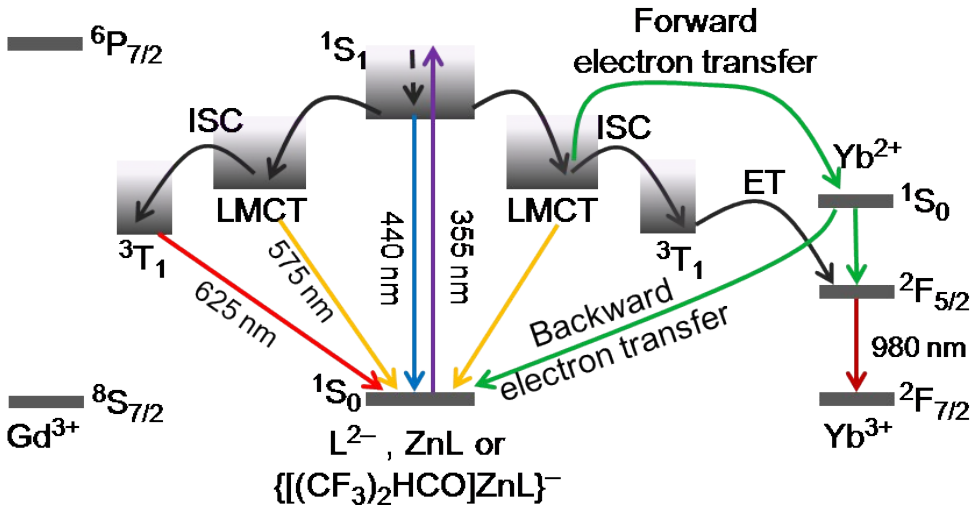

Fig. S5. Energy diagram showing transfer of excitation energy in the complexes **2**-**5**.