Electronic Supplementary Material (ESI) for Materials Advances.

pH Dependent Sensitization of Europium in a Hydrogen Bonded Three-Dimensional Metal-Organic Compounds with $(4^96^6)_2(4^46^2)_3$ Topology: Luminescence Titration and Time-resolved Studies

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ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1. Selected bond distances (Å) observed in $[Y_2(pydc)_6(H_2pip)_3]\cdot 20H_2O$ (pydc = 2,6-pyridine dicarboxylate, H_2pip = diprotonated piperazine), **1**.

Bond	Distances, Å	Bond	Distances, Å
Y(1)-O(1)	2.397(2)	Y(1)-O(3) #2	2.406(2)
Y(1)-O(1)#1	2.397(2)	Y(1)-N(1)	2.484(2)
Y(1)-O(1) #2	2.397(2)	Y(1)-N(1) #1	2.484(2)
Y(1)-O(3)	2.406(2)	Y(1)-N(1) #1	2.484(2)
Y(1)-O(3) #1	2.406(2)		

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

Table S2. Selected bond angles observed in $[Y_2(pydc)_6(H_2pip)_3]\cdot 20H_2O$ (pydc = 2,6-pyridine dicarboxylate, H_2pip = diprotonated piperazine), **1**.

Angle	Amplitude (º)	Angle	Amplitude (º)
O(1)#1-Y(1)-O(1)#2	77.36(8)	O(3)-Y(1)-N(1)	64.41(7)
O(1)#1-Y(1)-O(1)	77.36(8)	O(3)#1-Y(1)-N(1)	133.68(8)
O(1)#2-Y(1)-O(1)	77.36(8)	O(3)#2-Y(1)-N(1)	71.34(7)
O(1)#1-Y(1)-O(3)	89.14(8)	O(1)#1-Y(1)-N(1)#1	64.21(7)
O(1)#2-Y(1)-O(3)	147.64(7)	O(1)#2-Y(1)-N(1)#1	76.31(7)
O(1)-Y(1)-O(3)	128.58(7)	O(1)-Y(1)-N(1)#1	137.09(7)
O(1)#1-Y(1)-O(3)#1	128.58(7)	O(3)-Y(1)-N(1)#1	71.34(7)
O(1)#2-Y(1)-O(3)#1	89.14(8)	O(3)#1-Y(1)-N(1)#1	64.41(7)
O(1)-Y(1)-O(3)#1	147.64(7)	O(3)#2-Y(1)-N(1)#1	133.68(8)
O(3)-Y(1)-O(3)#1	76.43(9)	N(1)-Y(1)-N(1)#1	119.915(6)
O(1)#1-Y(1)-O(3)#2	147.64(8)	O(1)#1-Y(1)-N(1)#2	137.09(7)
O(1)#2-Y(1)-O(3)#2	128.58(7)	O(1)#2-Y(1)-N(1)#2	64.21(7)
O(1)-Y(1)-O(3)#2	89.14(8)	O(1)-Y(1)-N(1)#2	76.31(7)
O(3)-Y(1)-O(3)#2	76.43(9)	O(3)-Y(1)-N(1)#2	133.68(8)
O(3)#1-Y(1)-O(3)#2	76.43(9)	O(3)#1-Y(1)-N(1)#2	71.34(7)
O(1)#1-Y(1)-N(1)	76.31(7)	O(3)#2-Y(1)-N(1)#2	64.41(7)
O(1)#2-Y(1)-N(1)	137.09(8)	N(1)-Y(1)-N(1)#2	119.916(6)
O(1)-Y(1)-N(1)	64.20(7)	N(1)#1-Y(1)-N(1)#2	119.915(6)

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

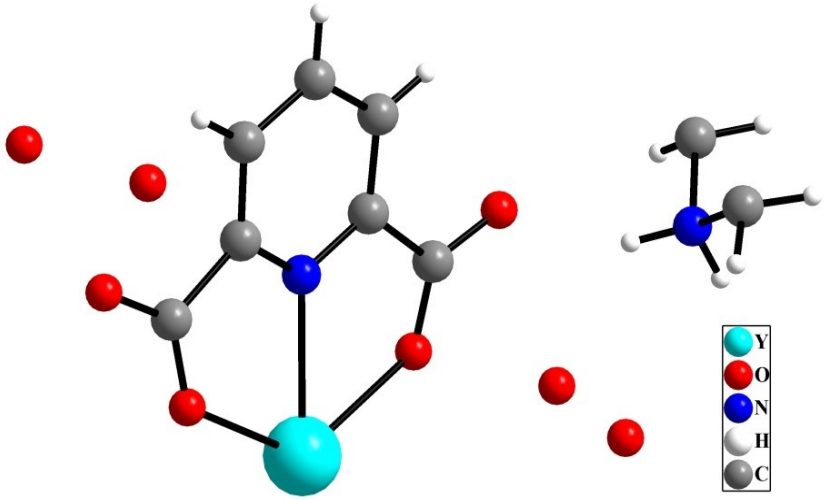

Figure S1. Figure shows the assymetric unit in $[Y_2(pydc)_6(H_2pip)_3]\cdot 20H_2O$ (pydc = 2,6-pyridine dicarboxylate, H_2pip = diprotonated piperazine), **1**. The hydrogen atoms in water molecules have not been located.

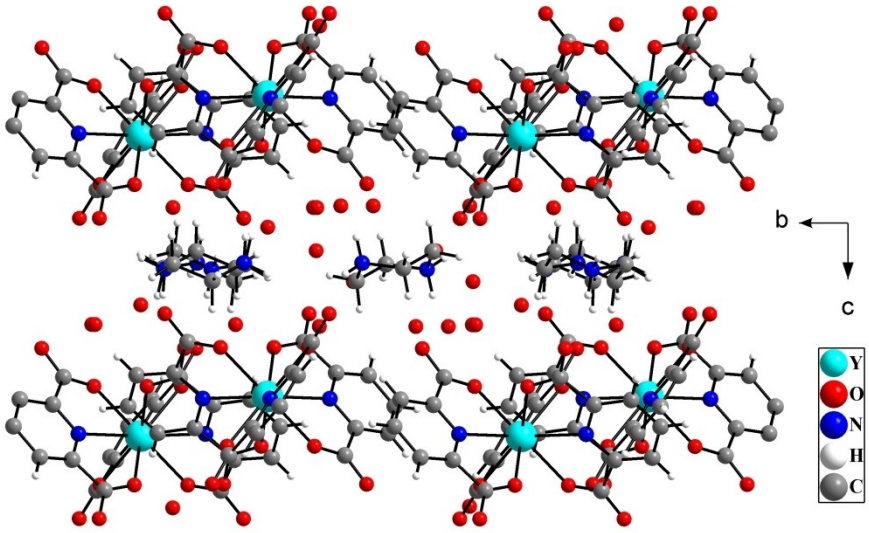

Figure S2. Figure shows the three-dimensional arrangement in *bc* in $[Y_2(pydc)_6(H_2pip)_3]\cdot 20H_2O$ (pydc = 2,6-pyridine dicarboxylate, H_2pip = diprotonated piperazine), **1**. The hydrogen atoms in water molecules have not been located.

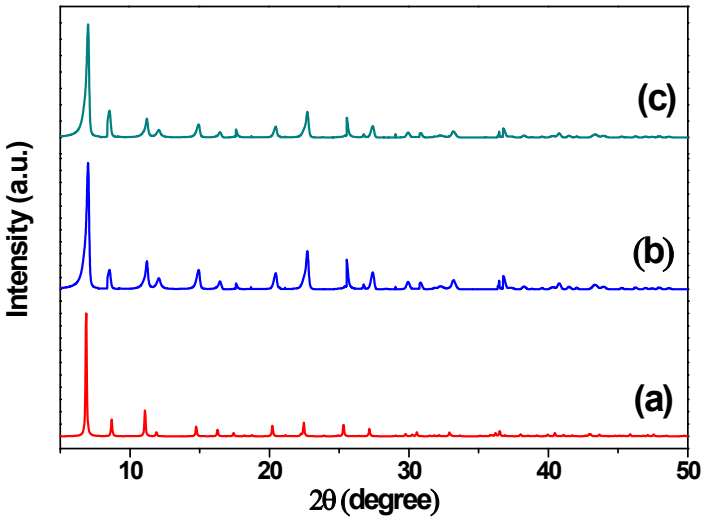

Figure S3. Powder XRD (Cu Kα) patterns of (a) **1** (simulated from single-crystal X-ray data), (b) as synthesized **1** (experimental) and (c) as synthesized **1a (**experimental).

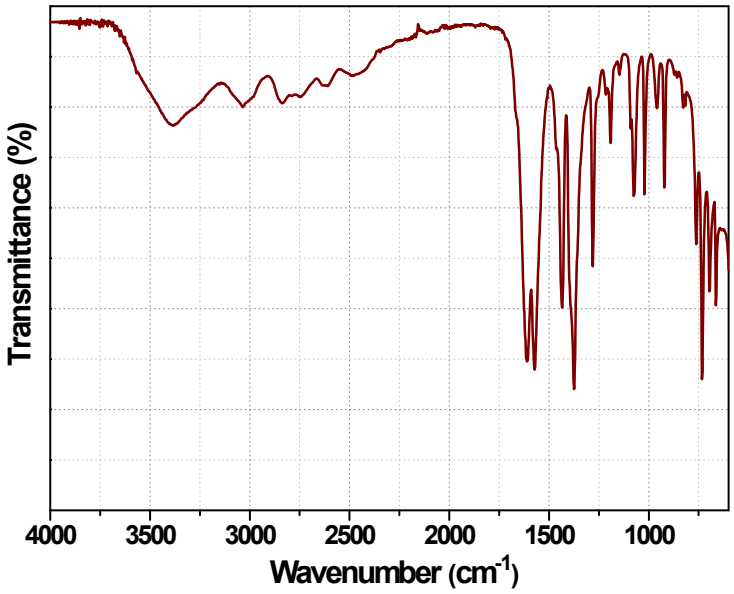

Figure S4. FTIR spectrum of **1**.

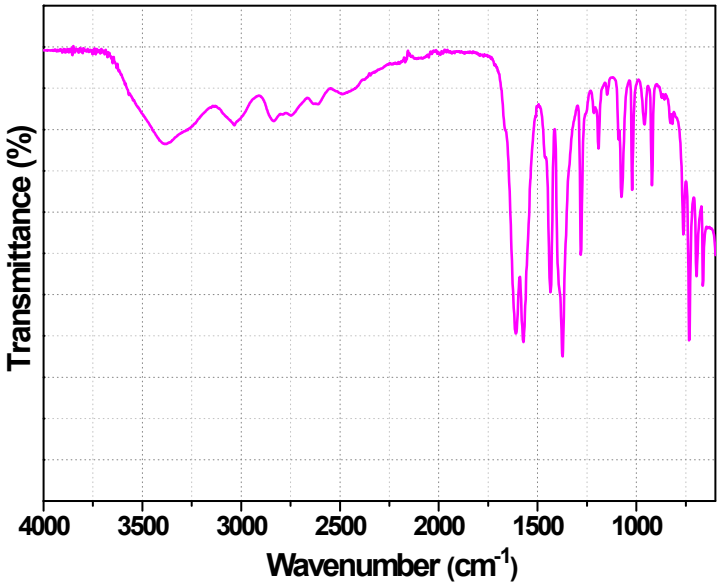

Figure S5. FTIR spectrum of **1a**.

Table S3. The observed IR bands for compounds **1** and **1a**.

Bands	Wavenumber (cm^{-1})	Bands	Wavenumber (cm^{-1})
$\upsilon_{asy.\ str}$(aromatic N-H)	3387(m)	$\upsilon_{sy.\ str}$(carboxylate)	1435(s), 1372(s)
υ_{str}(aromatic C-H)	3034(w)	υ_{str}(C-N)	1574(s), 1280(s), 1214(m)
$\upsilon_{asy.str}$(sp^3 C-H)	2972(w)	δ(aromatic C-H)$_{in\ plane\ bending}$	1193(s), 1147(m), 1074(m)
$\upsilon_{sy.str}$(sp^3 C-H)	2832(w), 2742(w)	δ(aromatic C-H)$_{out\ of\ plane\ bending}$	920(s). 875(w), 858(w), 825(w), 758(w)
$\upsilon_{asy.\ str}$(carboxylate)	1606(s)	δ(carboxylate)$_{bending}$	728(s), 695(w)

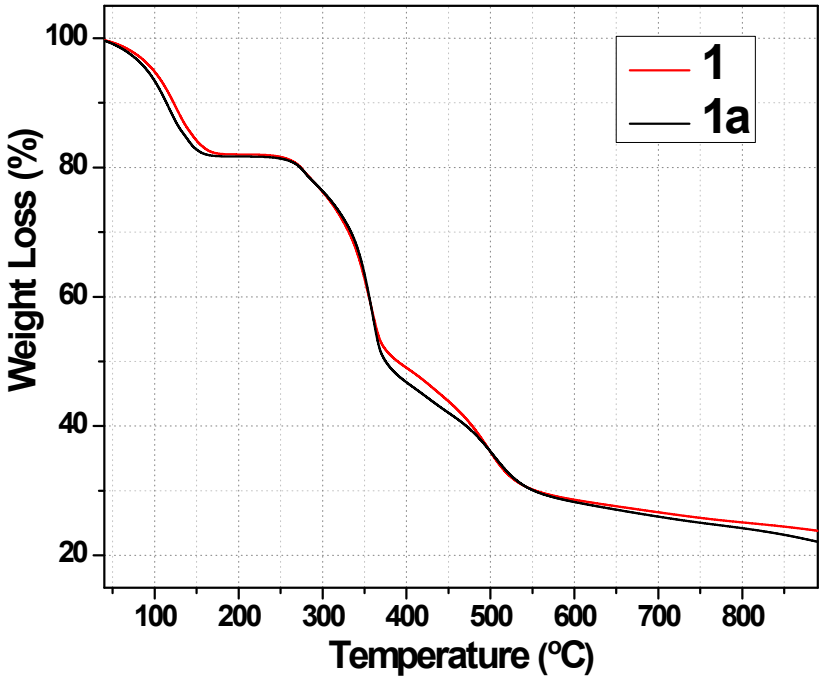

Figure S6. Thermogravimetric analysis (TGA) data of **1** and **1a**, in a nitrogen atmosphere. The plot shows % weight loss of **1** and **1a** with the increase in temperature.

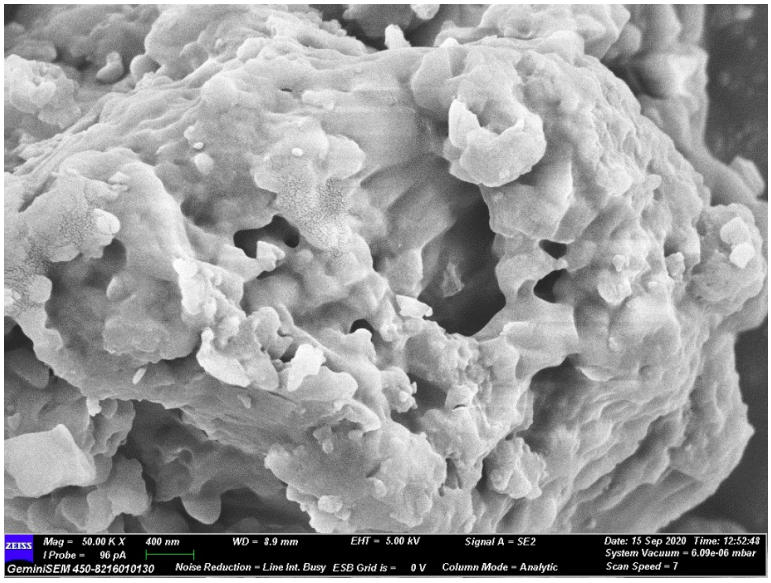

Figure S7. SEM image of **1a**.

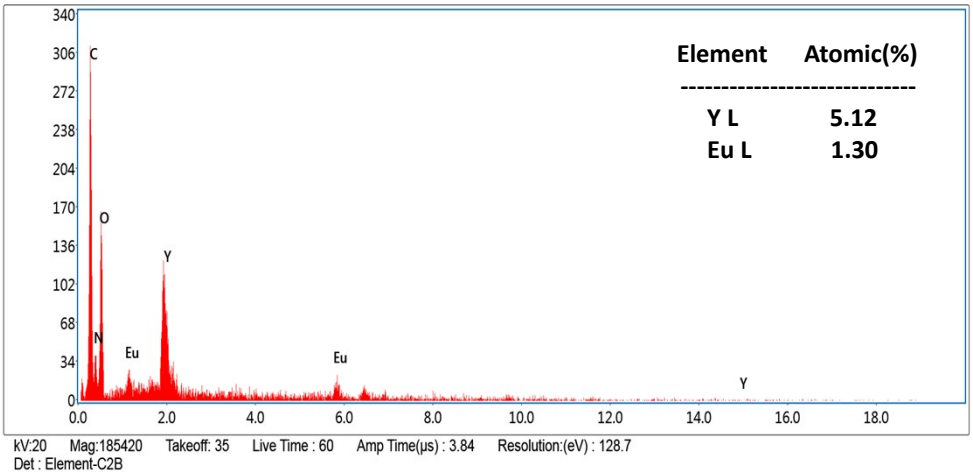

Figure S8. Representative EDX plot of **1a.** The figure demonstrates that Eu and Y are present in the molar ratio of ~ 1:4.

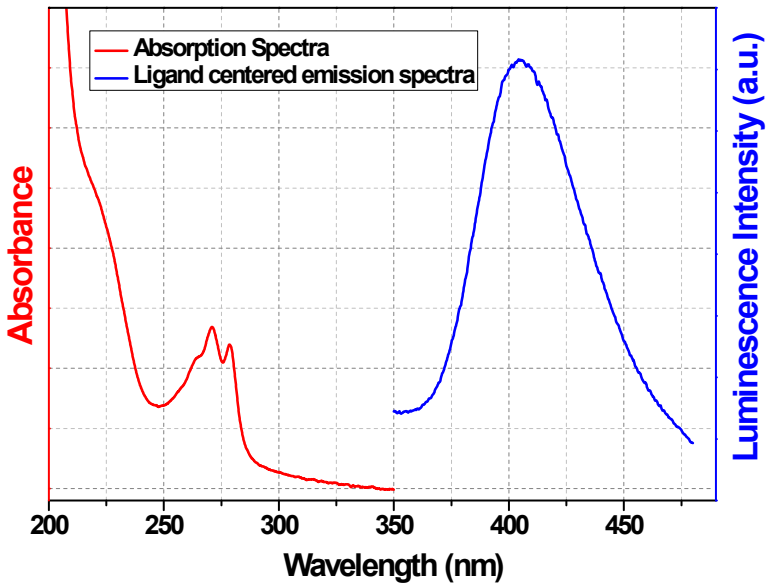

Figure S9. UV-Visible absorption spectrum of **1a** and ligand-centered emission spectra of **1a.**

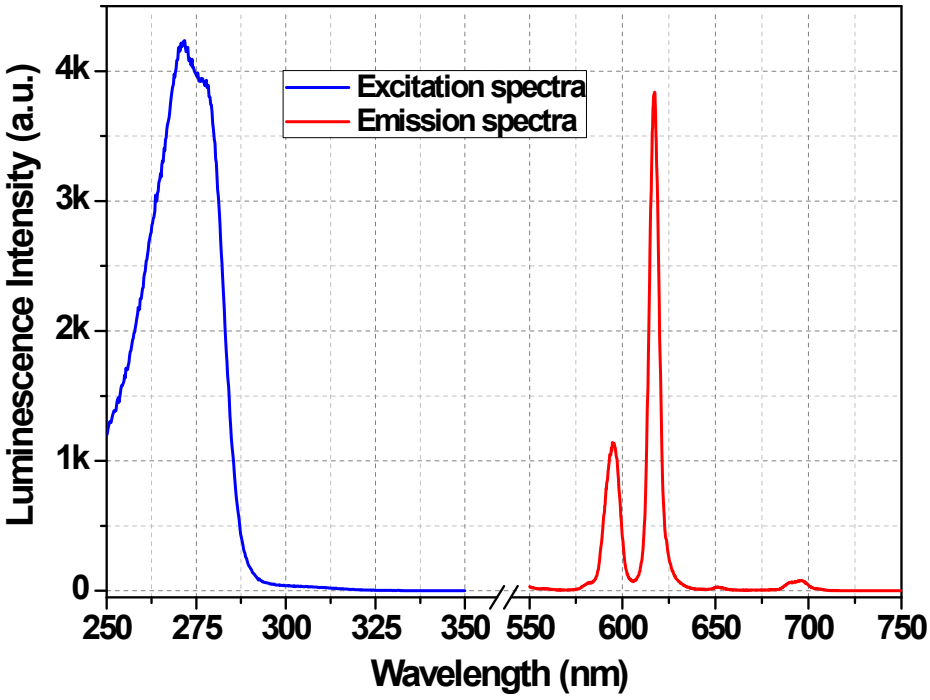

Figure S10. Excitation and emission spectra of **1a.** The excitation wavelength was chosen at 280 nm for emission spectra and for the excitation spectra, emission was fixed at 616 nm.

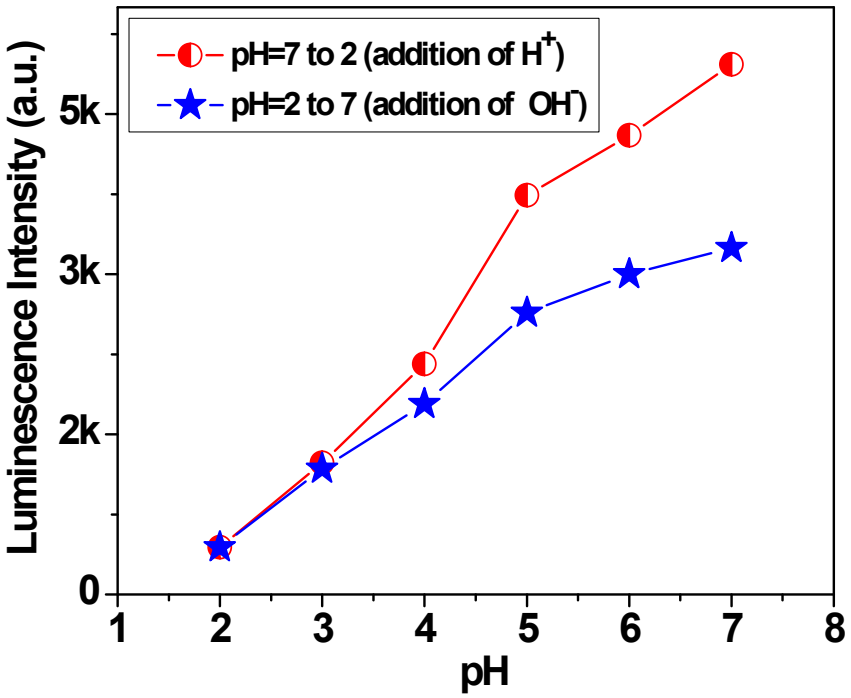

Figure S11. Plot of luminescence intensity (monitored at 616 nm) *vs* pH. The plot indicates the partial reversible pH response of compound **1a** in the pH range of 2–7.

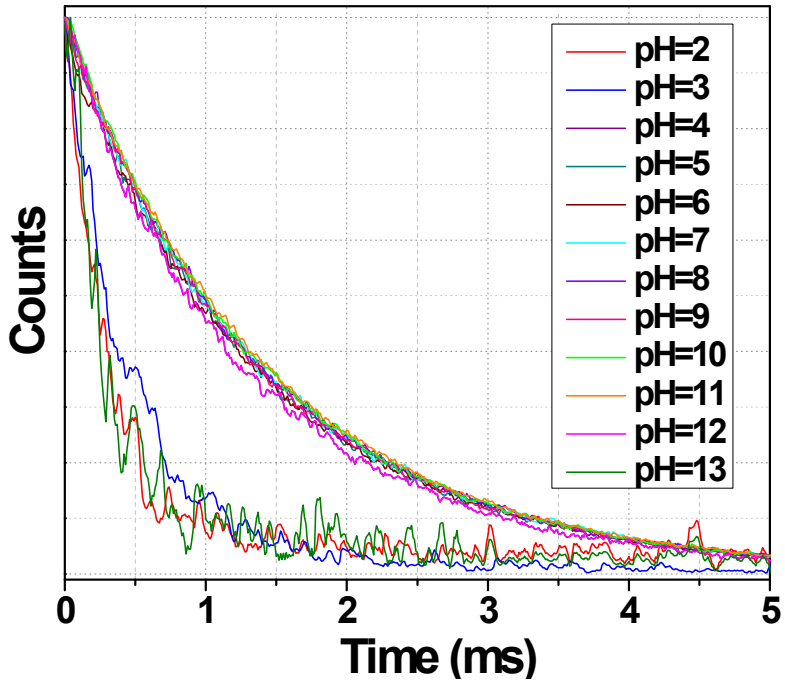

Figure S12. Luminescence lifetime decay observed at λ_{ex} = 280 nm and λ_{em} = 616 nm at different pH values.