Electronic Supplementary Material (ESI) for New Journal of Chemistry.

pH Response of a Hydroxyl-FunctionalizedLuminescent Metal-Organic Framework based Phosphor

Sayani Hui,[a] Prakash Majee,[b] Debal Kanti Singha,[a] PoojaDaga,[b] Sudip Kumar Mondal[b*]and Partha Mahata[a*]

[a]Department of Chemistry, Jadavpur University, Kolkata-700032, India. Email: parthachem@gmail.com

[b]Department of Chemistry, Siksha-Bhavana, Visva-Bharati University, Santiniketan-731235, West Bengal, India. Email: sudip.mondal@visva-bharati.ac.in

ELECTRONIC SUPPLEMENTARY INFORMATION

* Corresponding Authors, E-mail: parthachem@gmail.com, sudip.mondal@visva-bharati.ac.in

Discussion on the B level alerts on Single crystal X-ray data obtained from checkCIF

Group 1

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O100 Check

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O200 Check

Explanation:

Hydrogen atoms of the solvate/lattice water molecules were not located but are included in the formula. The location of hydrogen atoms were not possible in disordered oxygen atoms [O100 and O200} of water molecules.

Group 2

PLAT430_ALERT_2_B Short Inter D...A Contact O18 ..O100…….2.81 Ang.

PLAT430_ALERT_2_B Short Inter D...A Contact O19 ..O200 . …….2.77 Ang.

Explanation:

The presence of disordered oxygen atoms of lattice water molecules [O100 and O200] and coordinated water molecules [O18 and O19] is responsible for the observed short distances.

Group 3

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers

PLAT939_ALERT_3_B Large Value of Not (SHELXL) Weight Optimized S

Explanation:

This is due to weak quality of the data and refinement statistics if compared to that expected for small molecule structures from highly diffracting crystals. The ALERT reports the S value based on the supplied sigma(I) only. A large value of S generally indicates the presence of large outliers in the data set.

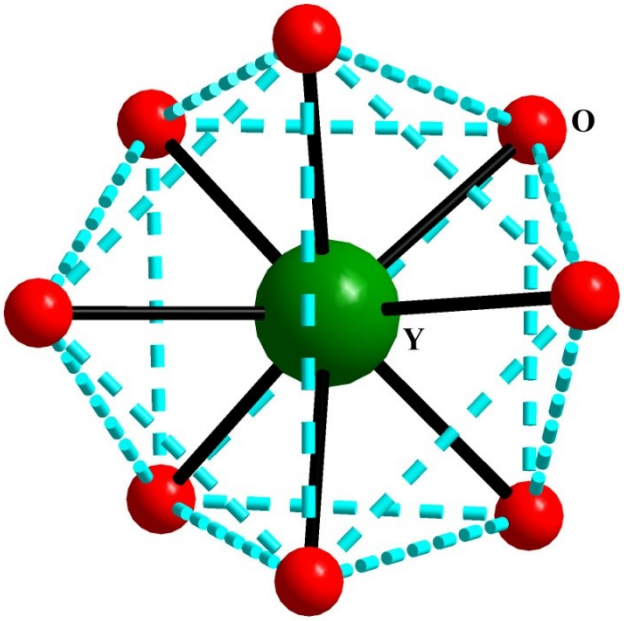
Table S1: Selected bond distances (Å) observed in $[Y_2(CAM)_3(H_2O)_4].2H_2O$, **1a**

Bond	Distances, Å	Bond	Distances, Å
Y(1)-O(1)	2.380(2)	Y(2)-O(3)#2	2.381(2)
Y(1)-O(4)#1	2.343(2)	Y(2)-O(6)	2.402(2)
Y(1)-O(7)	2.369(2)	Y(2)-O(8)	2.397(2)
Y(1)-O(11)	2.336(3)	Y(2)-O(12)#3	2.437(2)
Y(1)-O(16)	2.373(3)	Y(2)-O(13)#3	2.420(3)
Y(1)-O(17)	2.405(3)	Y(2)-N(1)#2	2.460(3)
Y(1)-O(18)	2.382(3)	Y(2)-N(2)	2.478(3)
Y(1)-O(19)	2.376(2)	Y(2)-N(3)#3	2.467(3)
Y(2)-O(2)#2	2.368(2)		

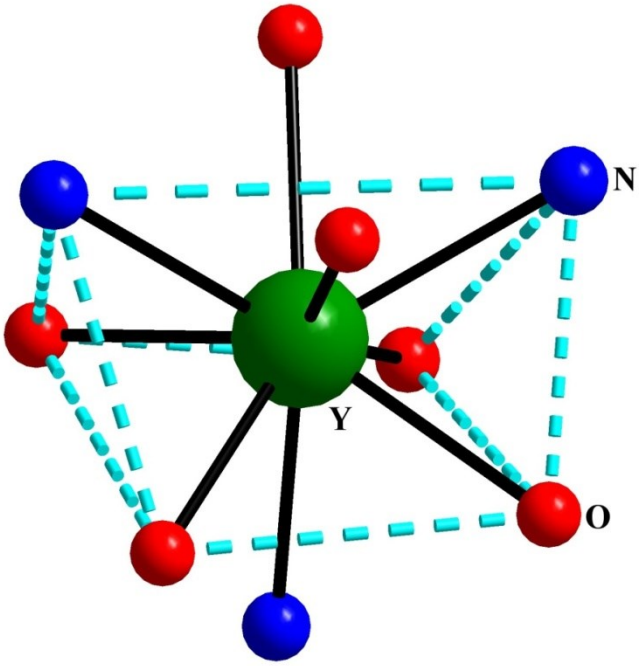
Table S2: Selected bond angles observed in $[Y_2(CAM)_3(H_2O)_4].2H_2O$, **1a**

Angle	Amplitude (º)	Angle	Amplitude (º)
O(11)-Y(1)-O(4)#1	117.15(9)	O(19)-Y(1)-O(1)	80.46(9)
O(11)-Y(1)-O(7)	78.00(9)	O(11)-Y(1)-O(18)	76.72(9)
O(4)#1-Y(1)-O(7)	139.73(9)	O(4)#1-Y(1)-O(18)	142.11(9)
O(11)-Y(1)-O(16)	144.09(9)	O(7)-Y(1)-O(18)	75.45(9)
O(4)#1-Y(1)-O(16)	77.78(8)	O(16)-Y(1)-O(18)	112.52(10)
O(7)-Y(1)-O(16)	71.62(9)	O(19)-Y(1)-O(18)	82.45(10)
O(11)-Y(1)-O(19)	71.35(9)	O(1)-Y(1)-O(18)	72.08(9)
O(4)#1-Y(1)-O(19)	70.86(9)	O(11)-Y(1)-O(17)	73.12(9)
O(7)-Y(1)-O(19)	145.54(9)	O(4)#1-Y(1)-O(17)	72.18(9)
O(16)-Y(1)-O(19)	142.34(8)	O(7)-Y(1)-O(17)	78.19(9)
O(11)-Y(1)-O(1)	140.16(9)	O(16)-Y(1)-O(17)	82.19(10)
O(4)#1-Y(1)-O(1)	77.24(9)	O(19)-Y(1)-O(17)	106.72(10)
O(7)-Y(1)-O(1)	116.20(9)	O(1)-Y(1)-O(17)	143.75(9)
O(16)-Y(1)-O(1)	72.60(9)	O(18)-Y(1)-O(17)	143.28(9)
O(2)#2-Y(2)-O(3)#2	129.30(8)	O(2)#2-Y(2)-O(8)	147.07(9)
O(3)#2-Y(2)-O(8)	76.49(9)	O(2)#2-Y(2)-O(6)	79.90(9)
O(3)#2-Y(2)-O(6)	84.85(9)	O(8)-Y(2)-O(6)	127.69(8)
O(2)#2-Y(2)-O(13)#3	79.41(9)	O(3)#2-Y(2)-O(13)#3	144.10(9)
O(8)-Y(2)-O(13)#3	87.92(9)	O(6)-Y(2)-O(13)#3	79.47(9)
O(2)#2-Y(2)-O(12)#3	83.79(9)	O(3)#2-Y(2)-O(12)#3	81.01(9)

O(8)-Y(2)-O(12)#3	80.68(9)	O(6)-Y(2)-O(12)#3	143.95(9)
O(13)#3-Y(2)-O(12)#3	128.61(8)	O(2)#2-Y(2)-N(1)#2	64.37(8)
O(3)#2-Y(2)-N(1)#2	64.97(8)	O(8)-Y(2)-N(1)#2	134.05(9)
O(6)-Y(2)-N(1)#2	74.14(9)	O(13)#3-Y(2)-N(1)#2	138.02(9)
O(12)#3-Y(2)-N(1)#2	69.82(9)	O(2)#2-Y(2)-N(3)#3	77.85(9)
O(3)#2-Y(2)-N(3)#3	134.06(9)	O(8)-Y(2)-N(3)#3	69.27(9)
O(6)-Y(2)-N(3)#3	140.63(9)	O(13)#3-Y(2)-N(3)#3	64.81(9)
O(12)#3-Y(2)-N(3)#3	64.28(9)	N(1)#2-Y(2)-N(3)#3	122.55(9)
O(2)#2-Y(2)-N(2)	136.32(9)	O(3)#2-Y(2)-N(2)	73.16(9)
O(8)-Y(2)-N(2)	63.93(8)	O(6)-Y(2)-N(2)	63.96(8)
O(13)#3-Y(2)-N(2)	70.94(9)	O(12)#3-Y(2)-N(2)	139.87(9)
N(1)#2-Y(2)-N(2)	122.28(9)	N(3)#3-Y(2)-N(2)	115.03(9)



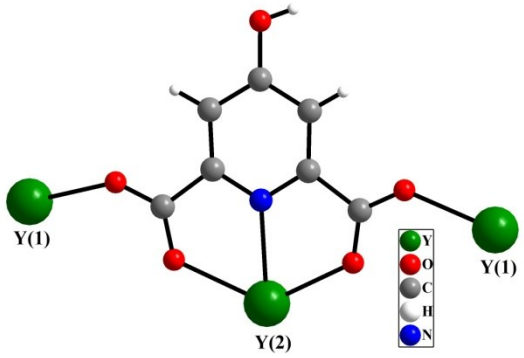
(a)



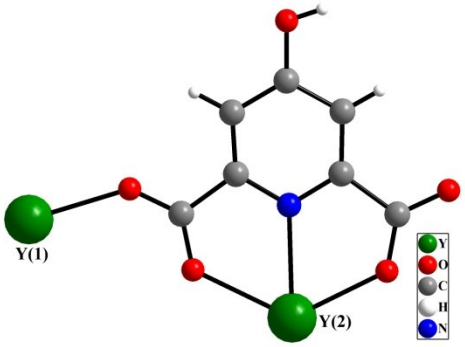
(b)

Fig. S1: Figure show (a) distorted square anti-prism geometry observed in Y(1) and (b) distorted tricapped trigonal prism geometry observed in Y(2) in $[Y_2(CAM)_3(H_2O)_4].2H_2O$, **1a**.

(a)



(b)



(c)

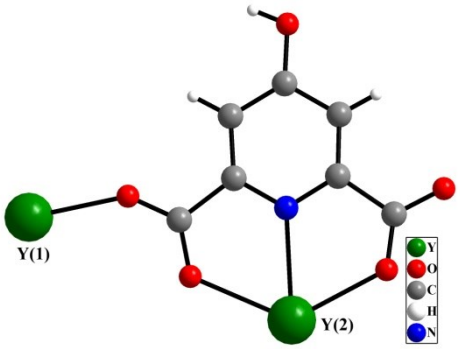


Fig. S2: Figure show the connectivities with the Y^{3+} ions- (a) CAM(1), (b) CAM(2), (c) CAM(3) in $[Y_2(CAM)_3(H_2O)_4].2H_2O$, **1a**.

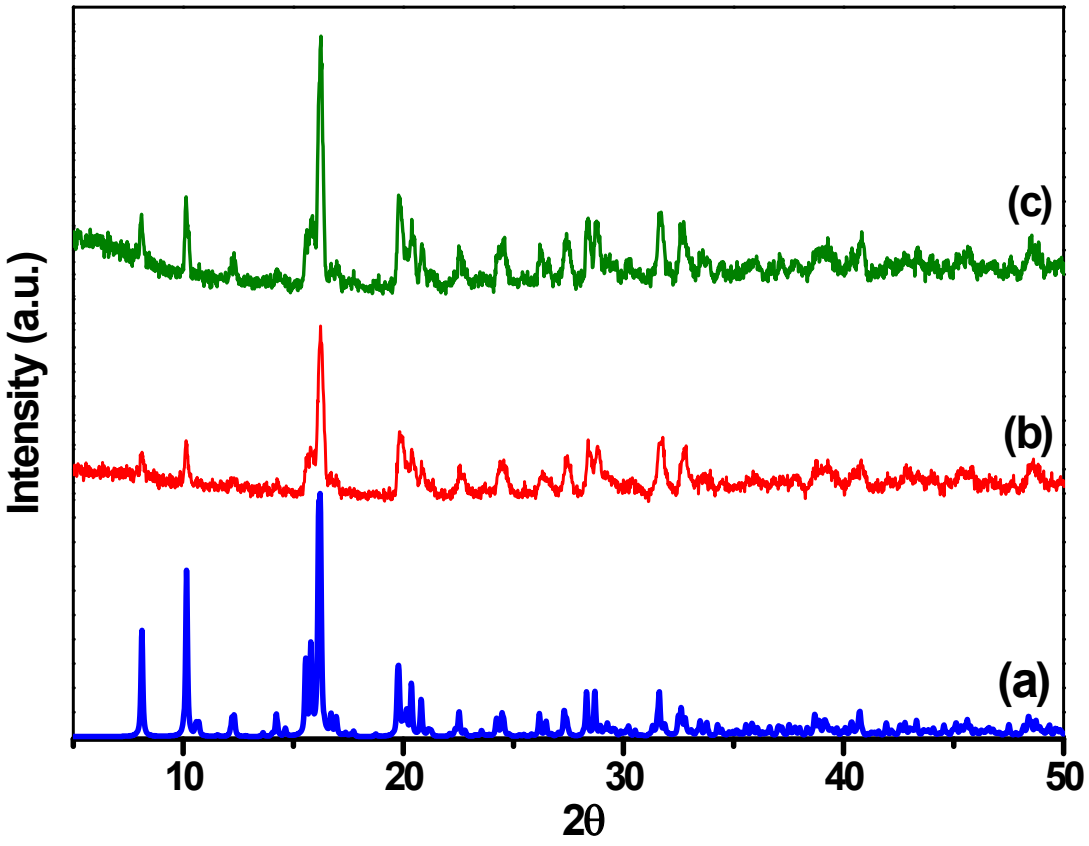


Fig. S3: Powder XRD (CuKα) patterns: (a) simulated from single crystal X-ray data of $[Y_2(CAM)_3(H_2O)_4].2H_2O$, **1a,** (b) hydrothermally synthesized $[Y_2(CAM)_3(H_2O)_4].2H_2O$, **1a,** and (c) hydrothermally synthesized $[Y_{1.8}Tb_{0.2}(CAM)_3(H_2O)_4].2H_2O$, **1.**

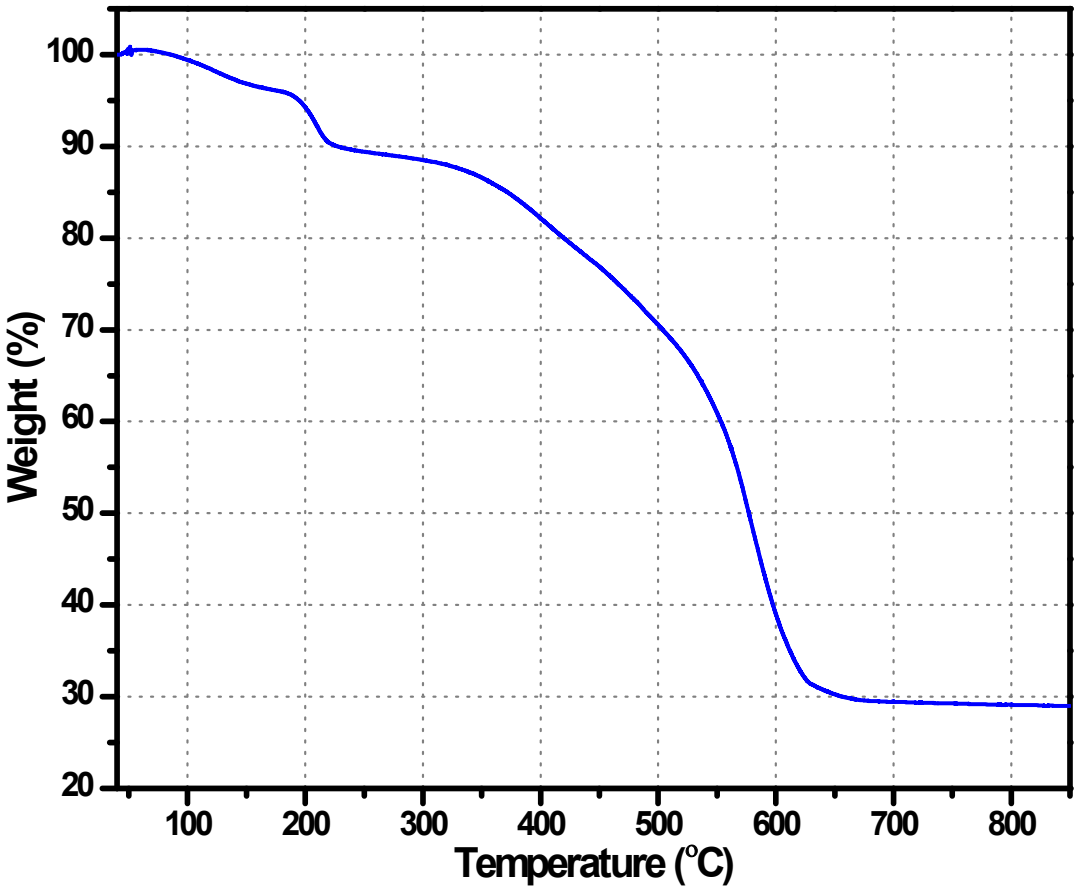


Fig. S4: Thermogravimetric analysis (TGA) of compound **1** in nitrogen atmosphere.

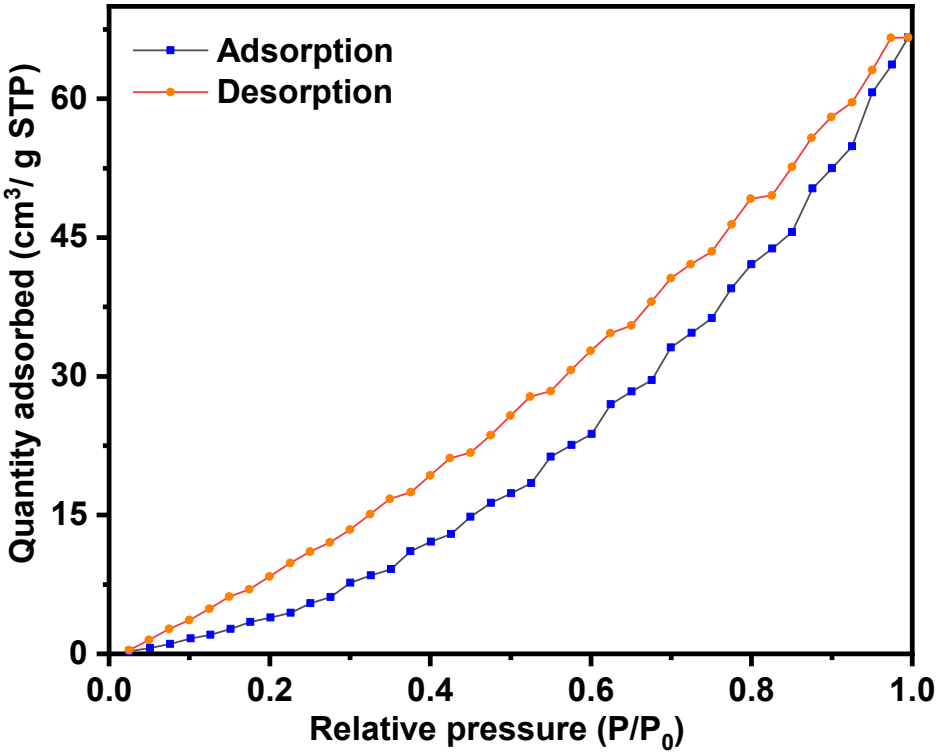


Fig. S5: N_2 sorption plot of compound **1.**

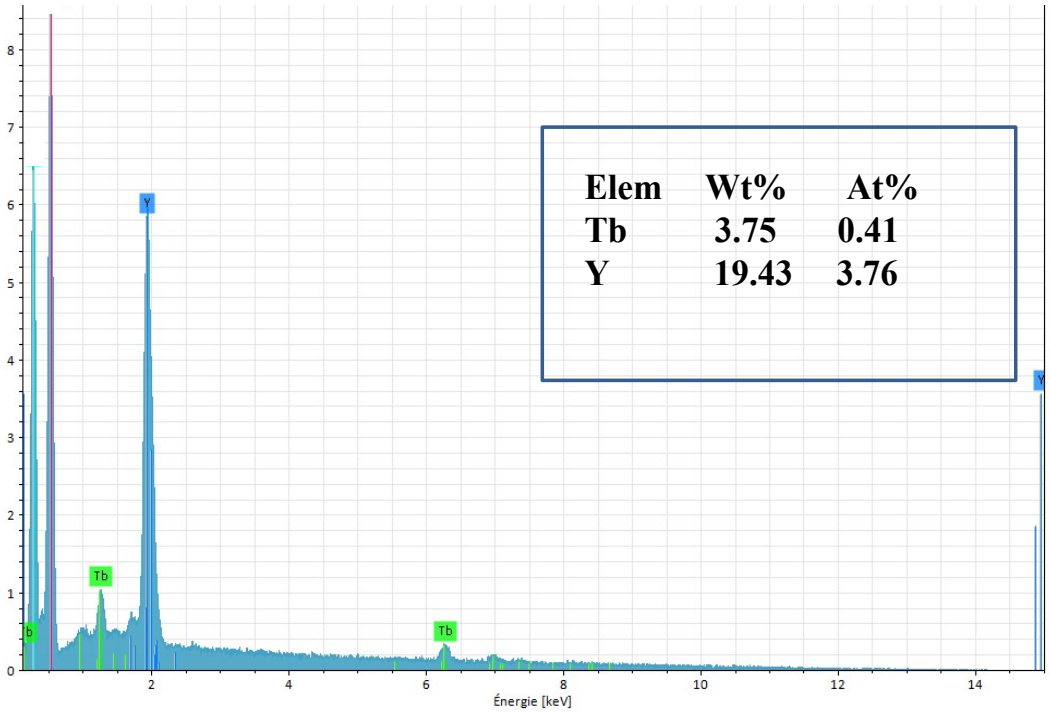


Fig. S6: Representative EDX plot of compound **1.** Note the presence of Tb and Y are in molar ratio of ~ 1:9.

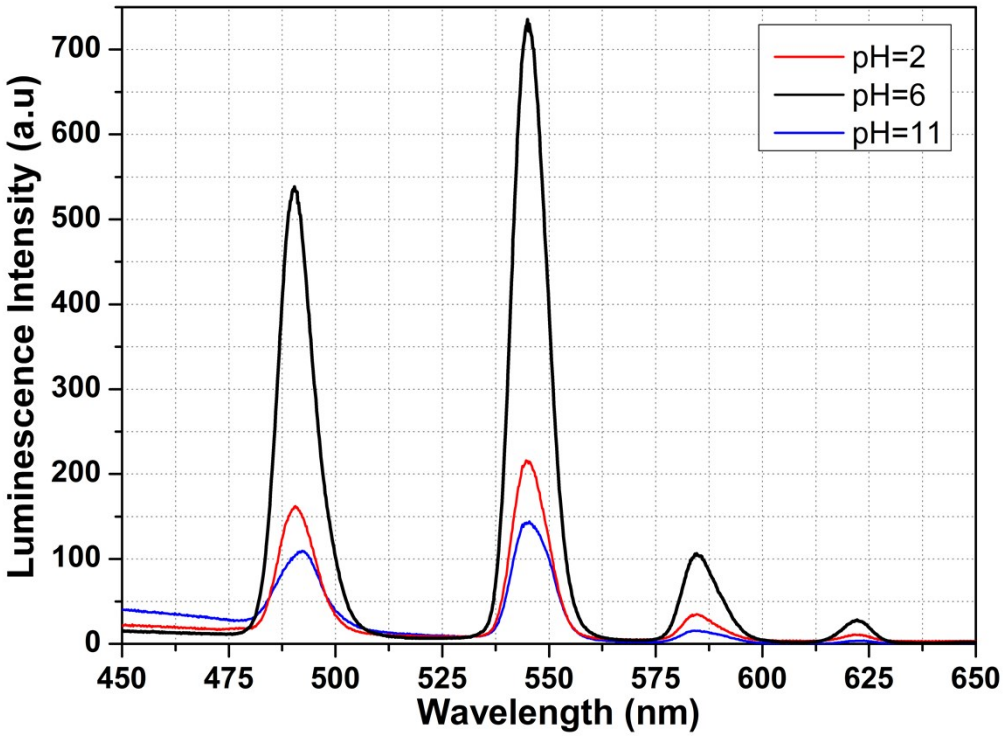


Fig. S7: Figure shows luminescence spectra of aqueous solution of compound **1** at pH 6, pH 2 and pH 11 upon excitation at 280 nm.

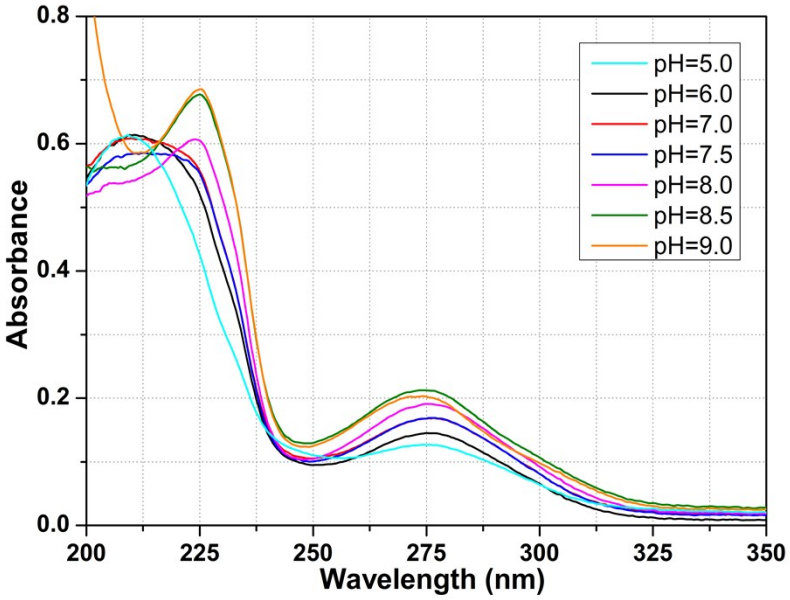


Fig.S8: Absorption spectra of compound **1** at different pH (5-9).

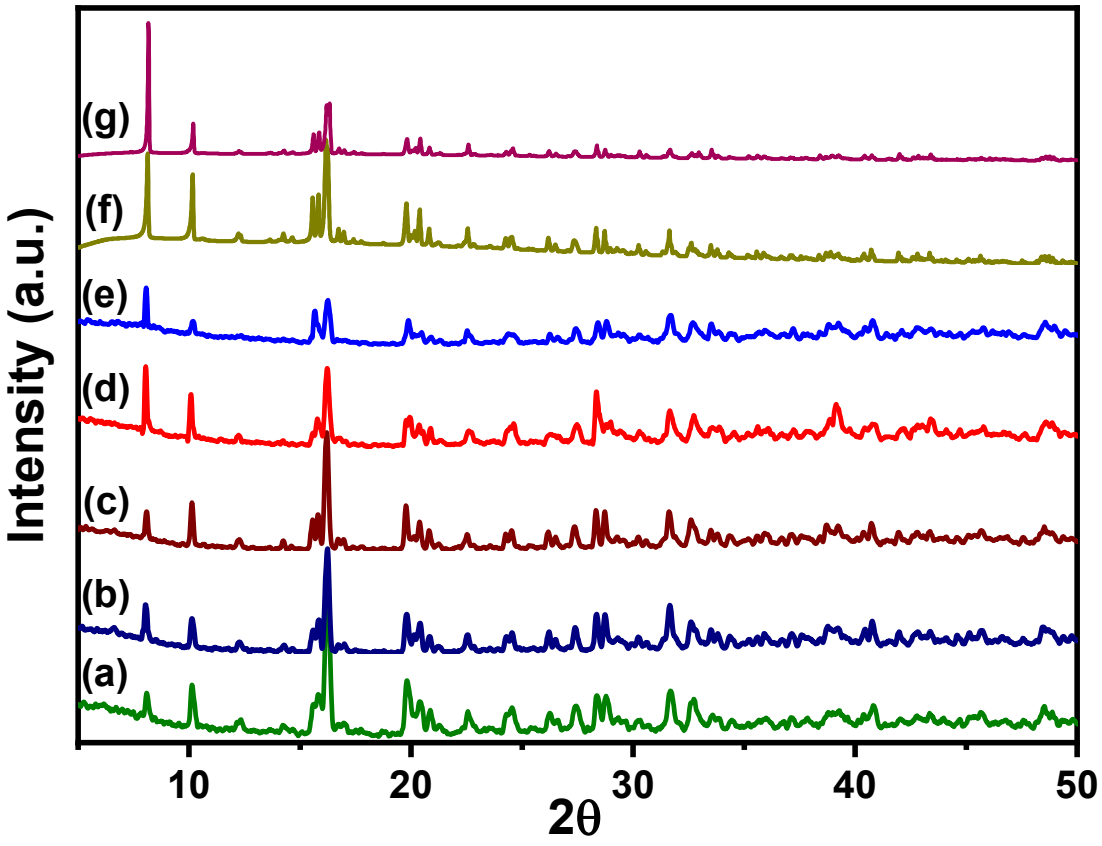


Fig.S9: Powder XRD (CuKα) patterns: (a) hydrothermally synthesized $[Y_{1.8}Tb_{0.2}(CAM)_3(H_2O)_4].2H_2O$, **1,** (b) pH= 4, (c) pH= 5, (d) pH=6, (e) pH=7, (f) pH= 8 and (g) pH= 9**.**

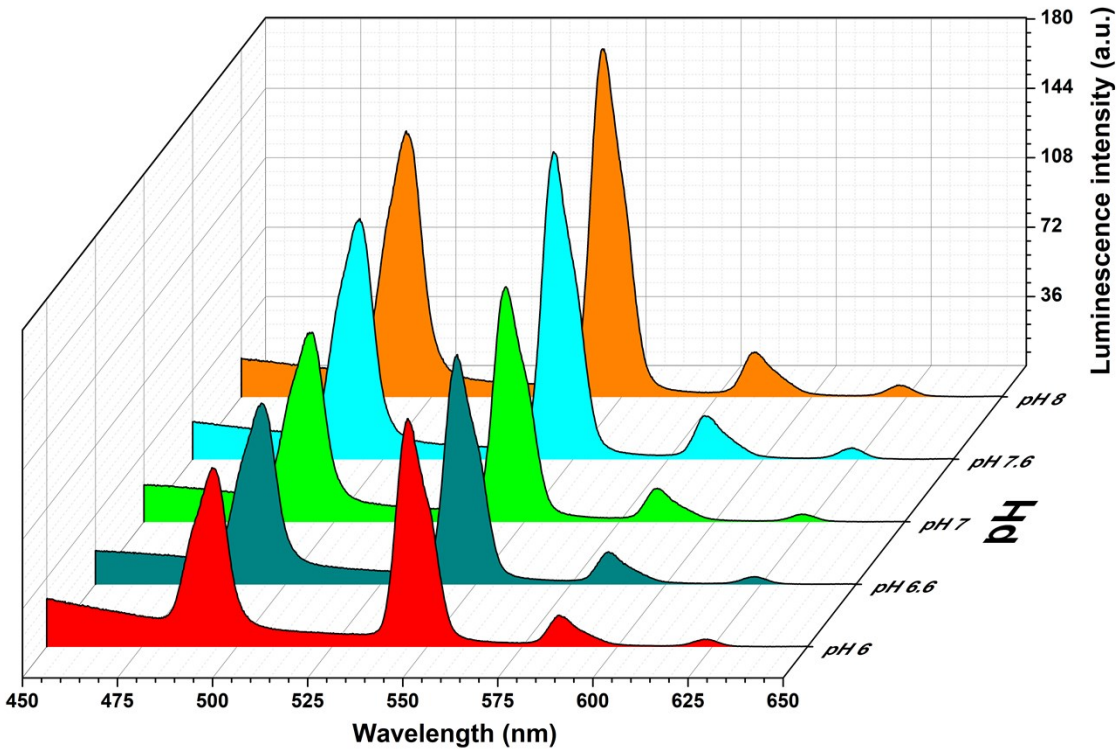


Fig. S10: Figure shows luminescence spectra of compound **1** in phosphate buffer solution at different pH values upon excitation at 280 nm.

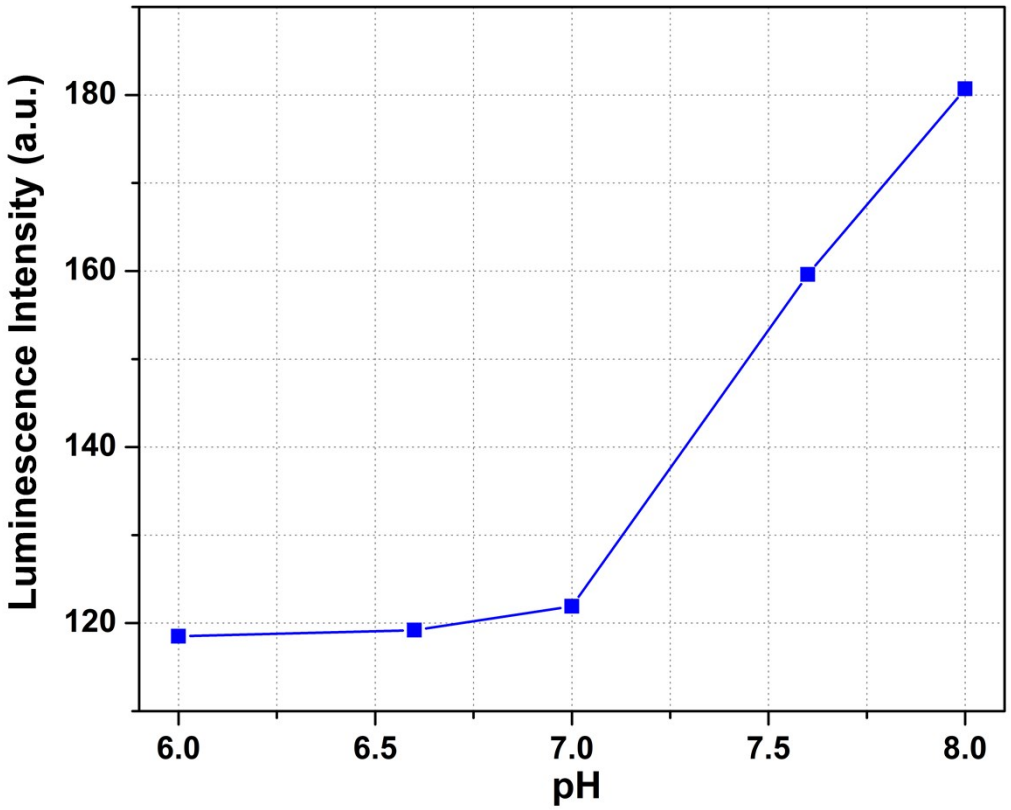


Fig. S11: Changes in luminescence intensity of **1** at different pH values in phosphate buffer, obtained by monitoring the luminescence intensity at λ_{em} = 545 nm.