Supporting Information

Multidimensional (0D to 3D) Alkaline-Earth Metal Diphosphonates: Synthesis, Structural Diversity, and Luminescence Properties

Duraisamy Senthil Raja,[a+] Pin-Chun Lin,[b] Wei-Ren Liu,[b*] Jun-Xiang Zhan,[a] Xin-Yi Fu,[a] and Chia-Her Lin[a*]

[a] Department of Chemistry, Chung-Yuan Christian University, Chung Li 320, Taiwan;
[b] Department of Chemical Engineering, Chung-Yuan Christian University, Chung Li 320, Taiwan

* To whom correspondence should be addressed. E-mail: wrliu1203@gmail.com (W. R. Liu) chiaher@cycu.edu.tw (C. H. Lin)

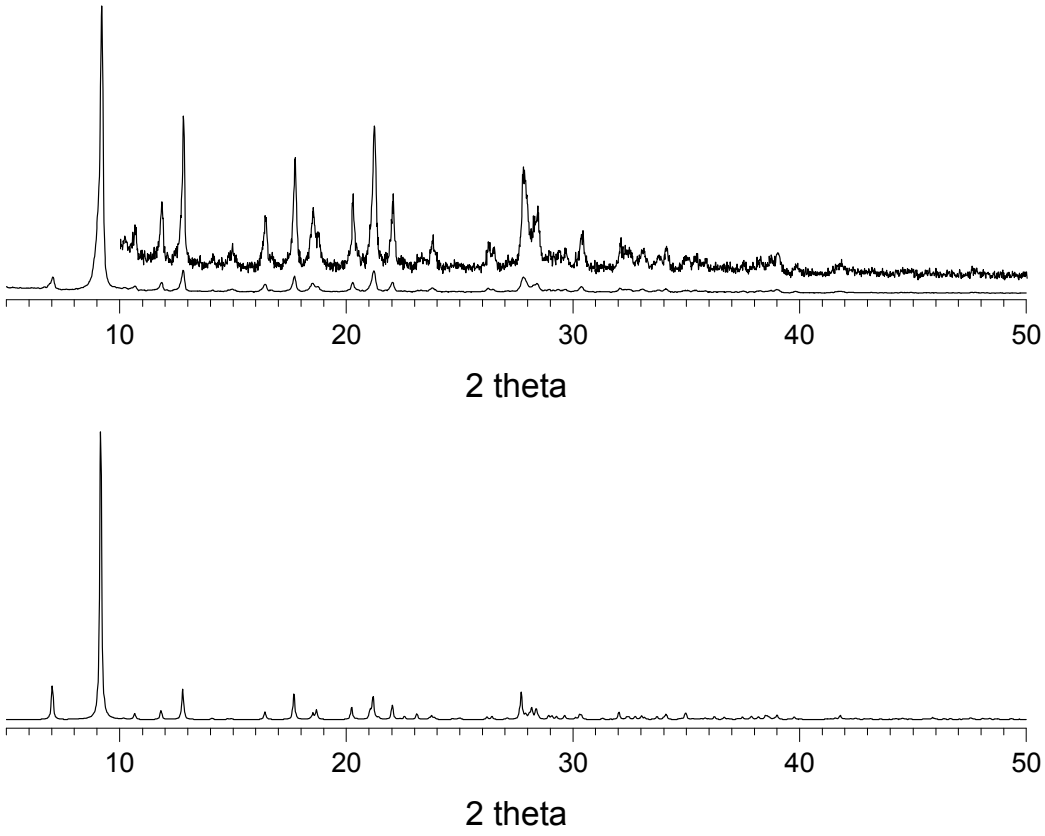


Fig. S1 PXRD patterns of **1** (measured, top (inset: without the first strong intensity peak for better clarity); calculated, bottom).

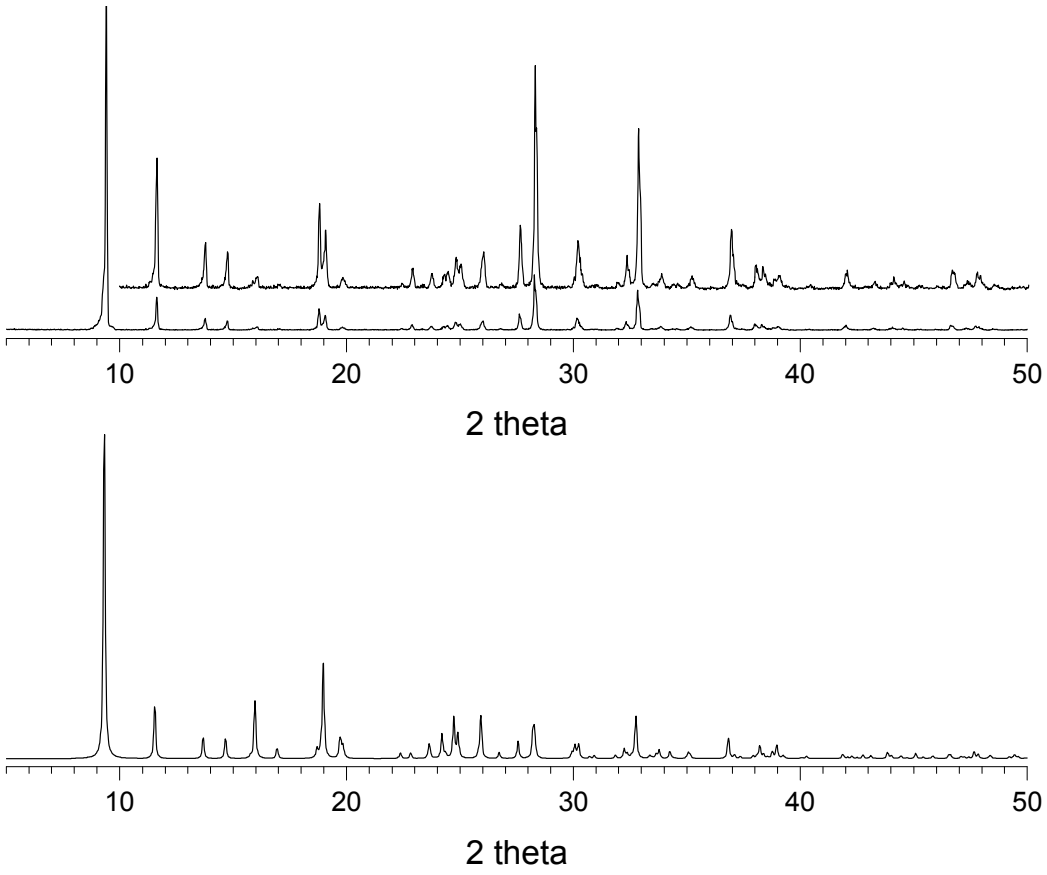


Fig. S2 PXRD patterns of **2** (measured, top (inset: without the first strong intensity peak for better clarity); calculated, bottom).

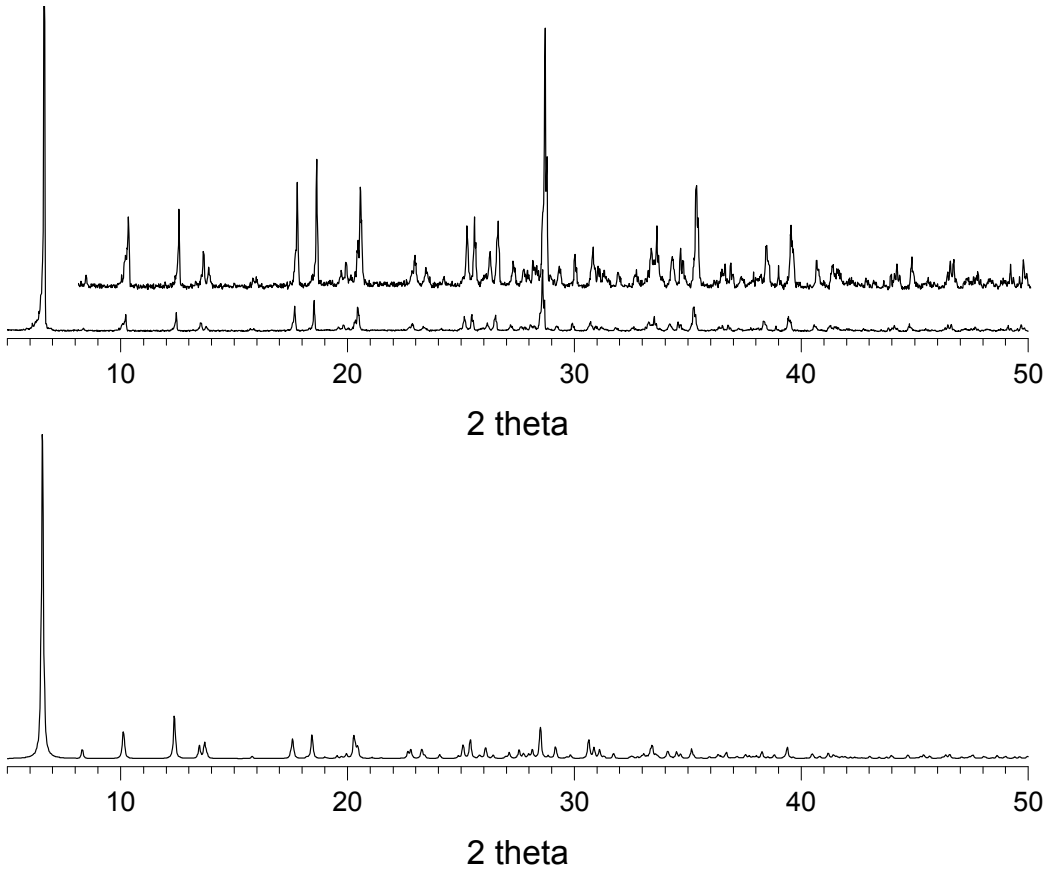


Fig. S3 PXRD patterns of **3** (measured, top (inset: without the first strong intensity peak for better clarity); calculated, bottom).

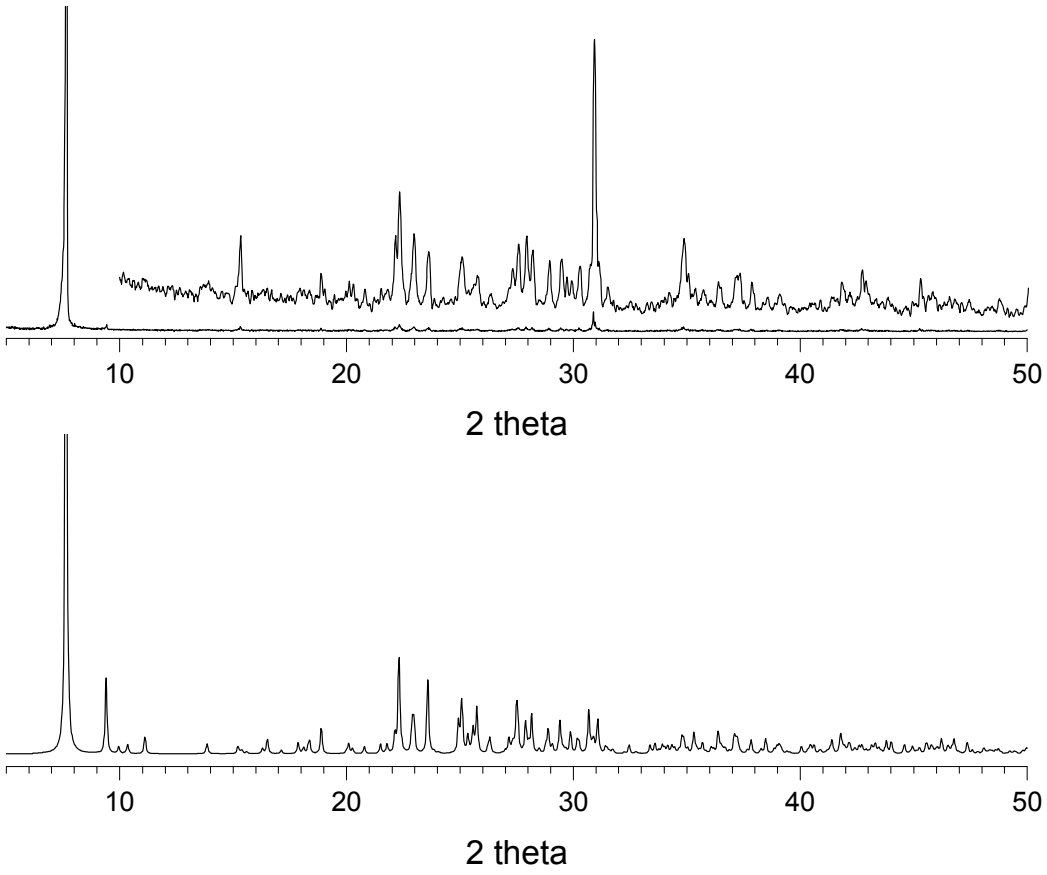


Fig. S4 PXRD patterns of **4** (measured, top (inset: without the first strong intensity peak for better clarity); calculated, bottom).

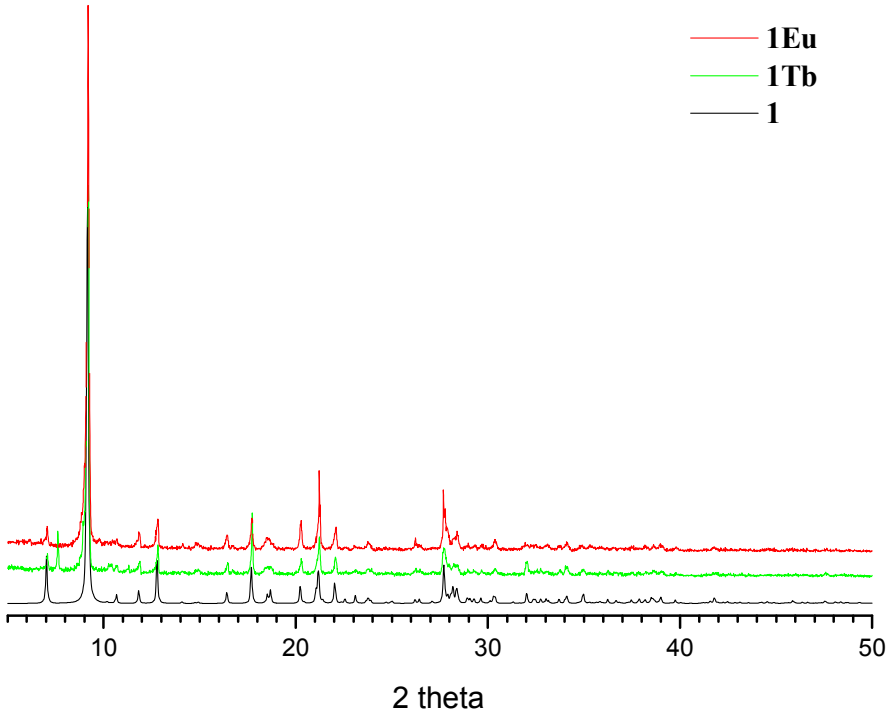


Fig. S5 PXRD patterns of as synthesized compounds of **1**, **1Eu**, and **1Tb**

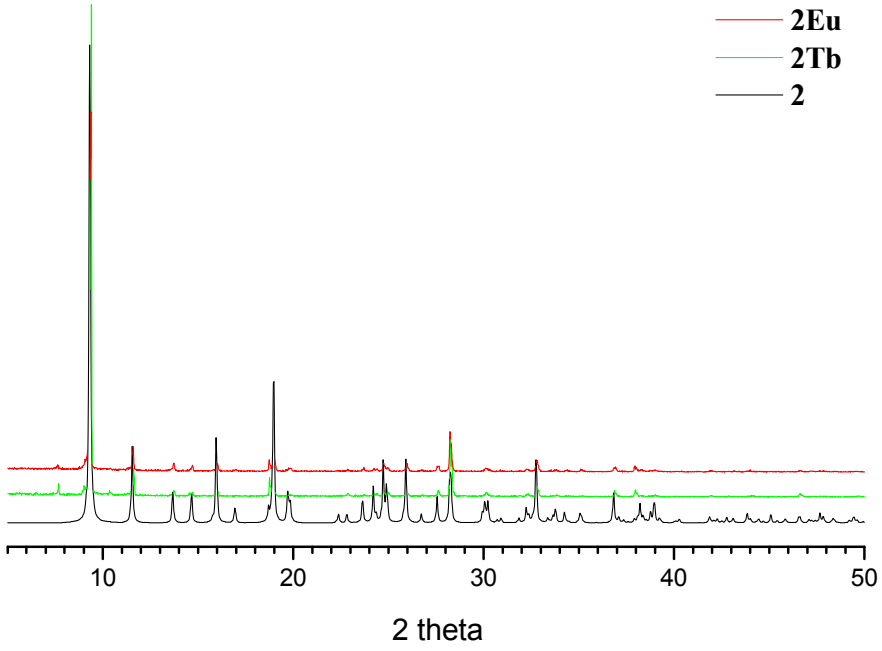


Fig. S6 PXRD patterns of as synthesized compounds of **2**, **2Eu**, and **2Tb**

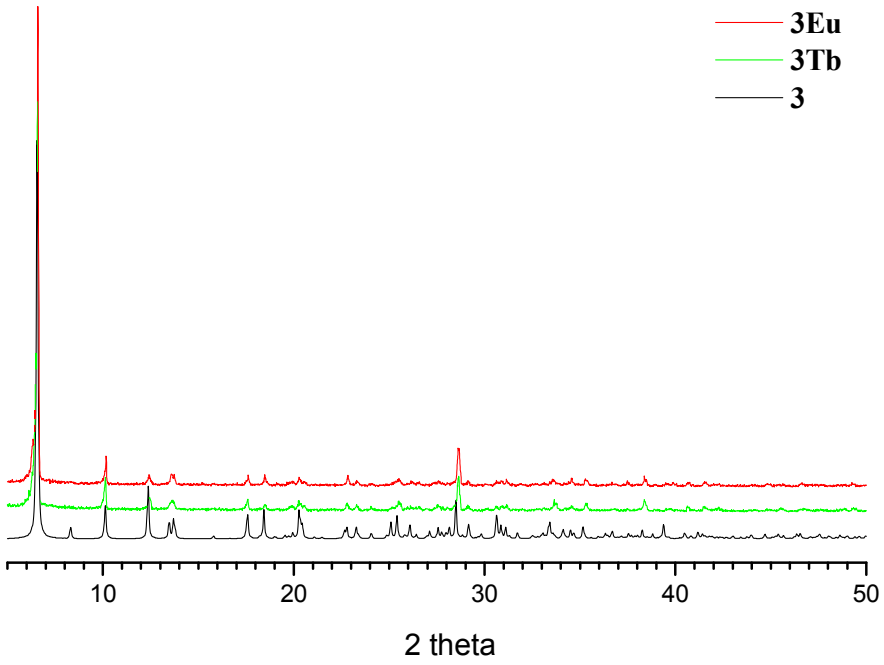


Fig. S7 PXRD patterns of as synthesized compounds of **3**, **3Eu**, and **3Tb**

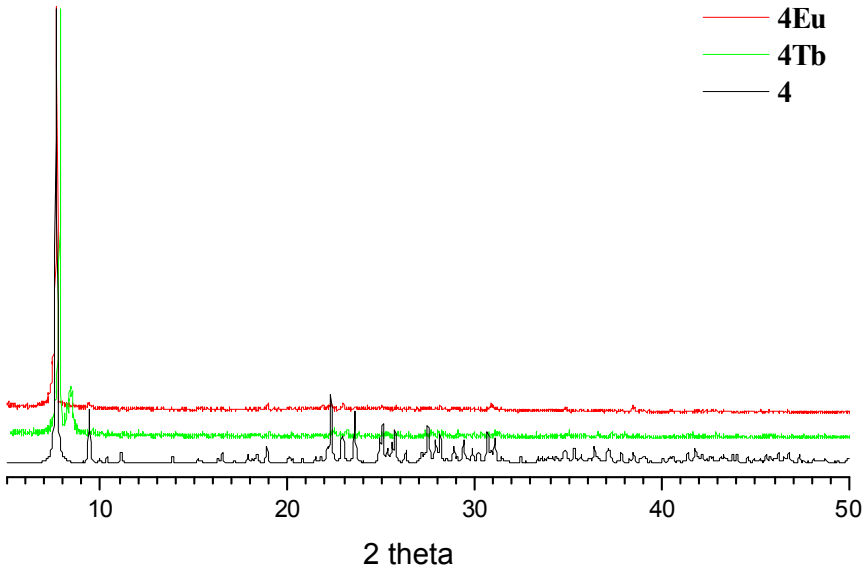


Fig. S8 PXRD patterns of as synthesized compounds of **4**, **4Eu**, and **4Tb**.

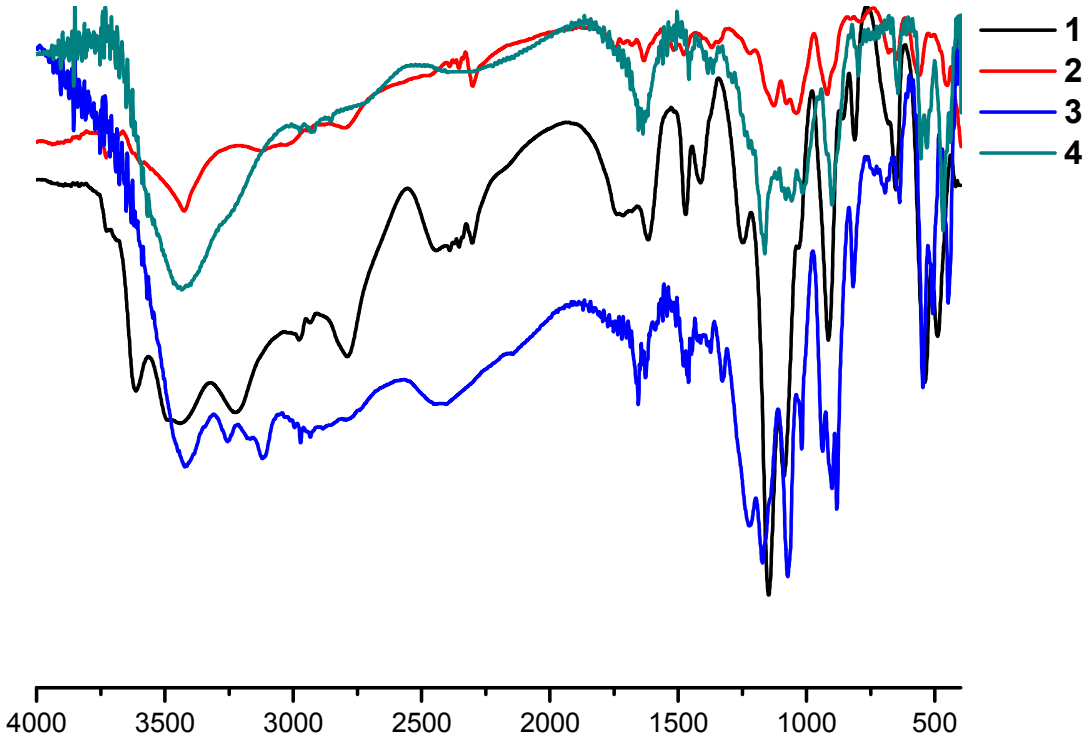


Fig. S9. FT-IR spectra of compounds **1-4**.

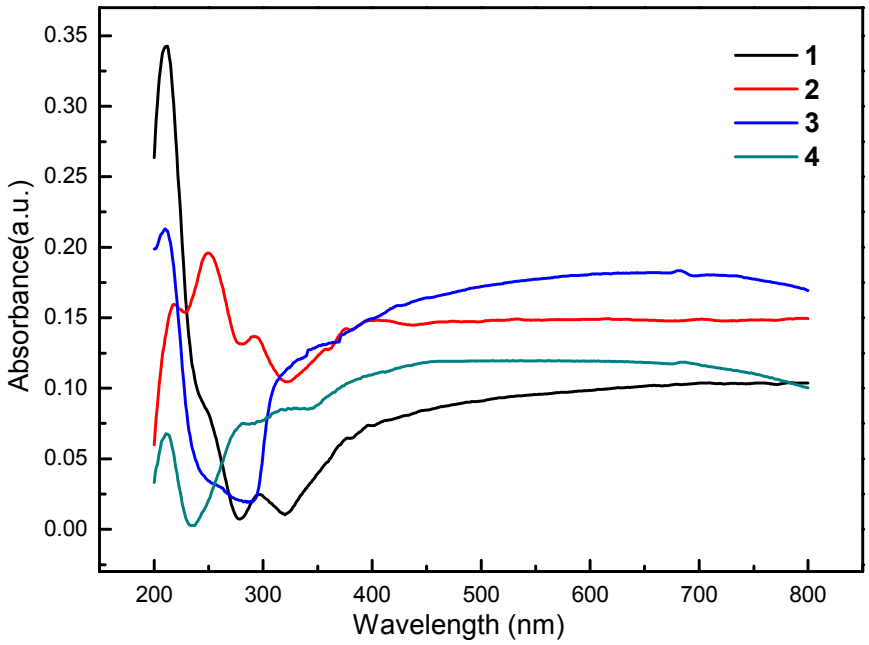


Fig. S10 UV-vis absorption spectra of compounds **1-4**.

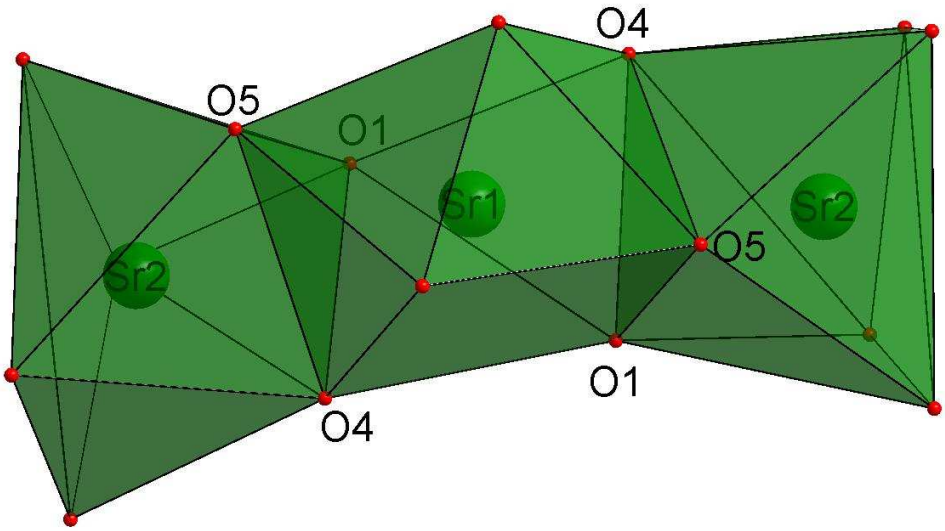
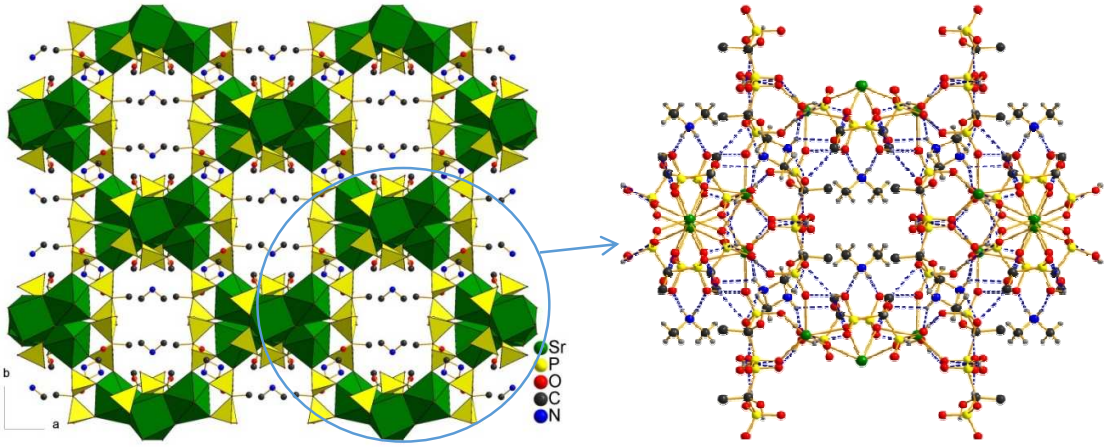


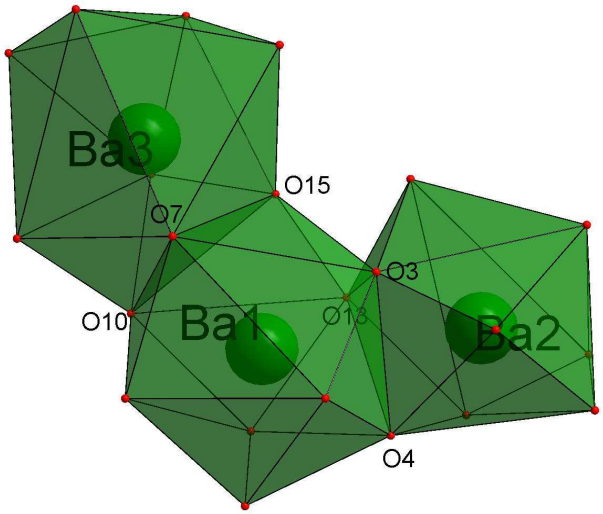
Fig. S11 The face sharing diagram of Sr1-polyhedron with Sr2-polyhedra.



(a) (b)

Fig. S12 (a) The 3D structural view of **3** along the c-axis (left). (b) The view of different modes of H-bonding interaction in **3**.

(a)



(b)

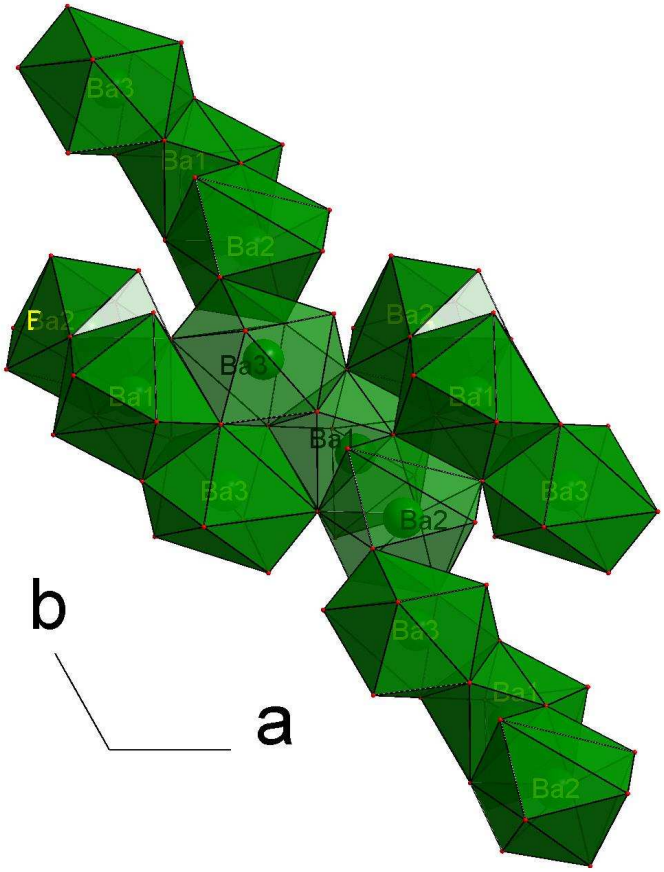


Fig. S13 (a) The face sharing diagram of Ba1-polyhedron with Ba2-and Ba3-polyhedron. (b) The connection of trinuclear Ba_3O_{22} unit with four of their neighboring units.

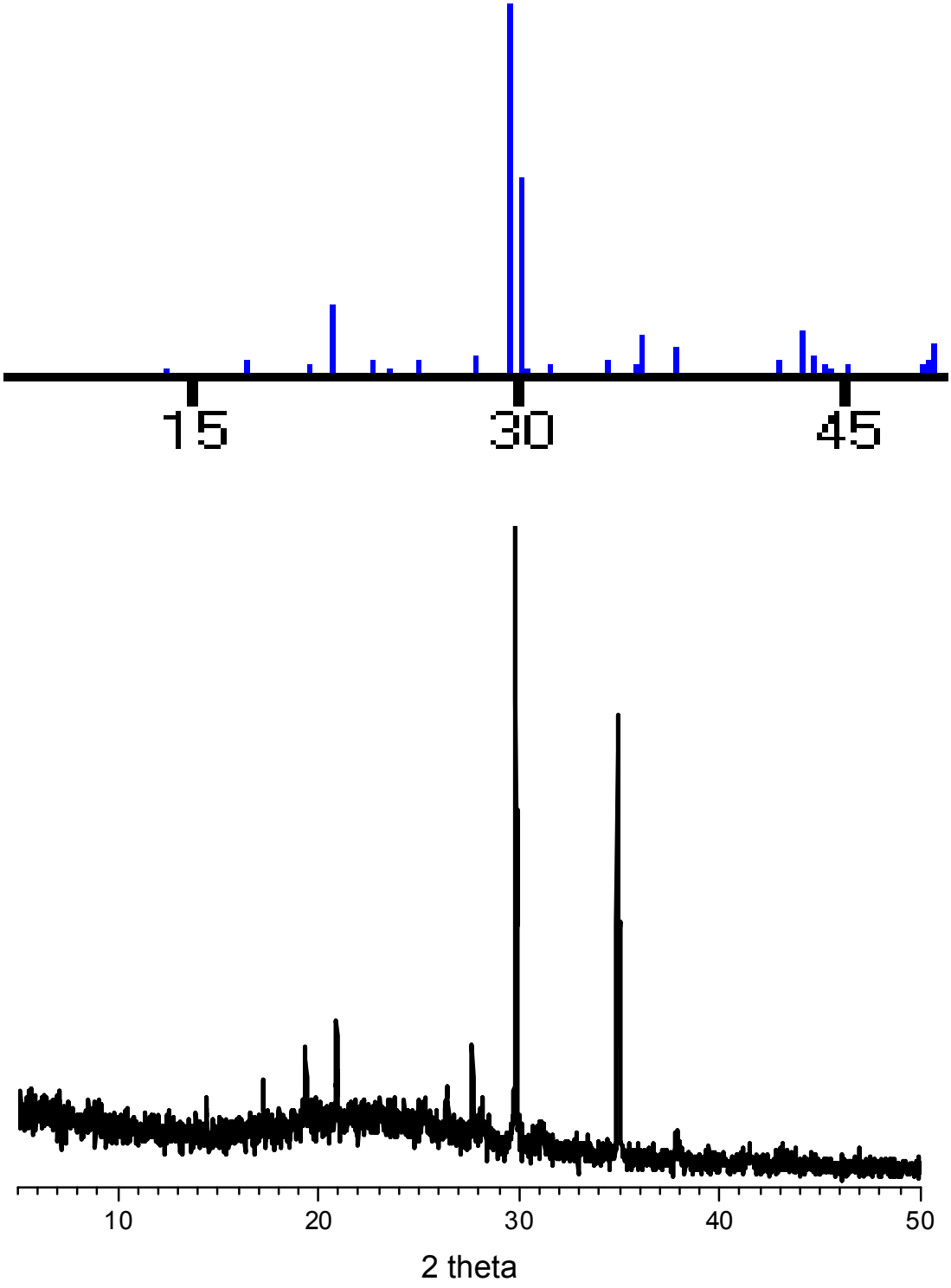


Fig. S14 PXRD patterns of JCPDF- (#751055) $Mg_2P_2O_7$ (top) and complex **1** after 800 ^oC (bottom).

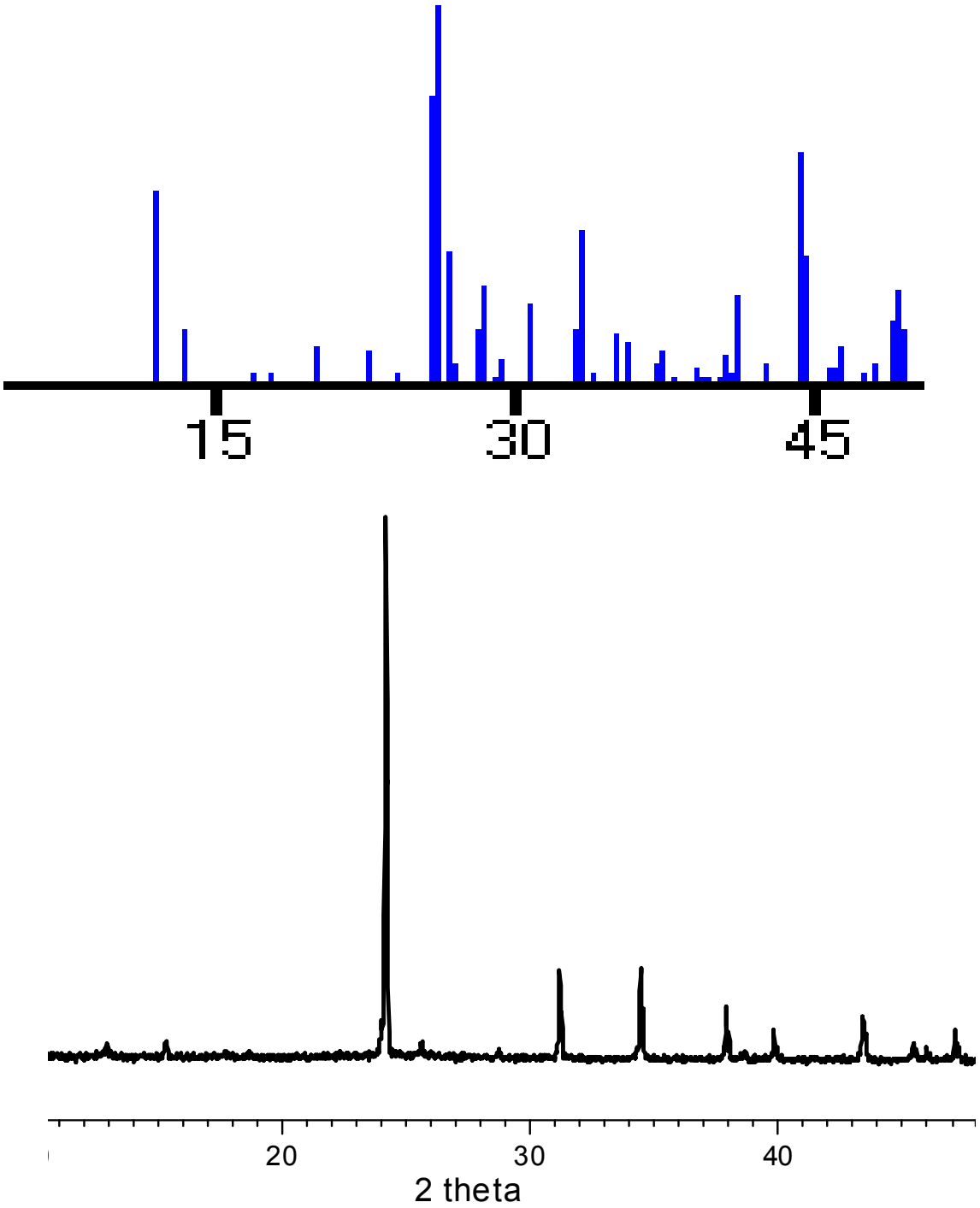


Fig. S15 PXRD patterns of JCPDF- (#721419) $Sr_2P_2O_7$ (top) and complex **3** after 800 ^oC (bottom).

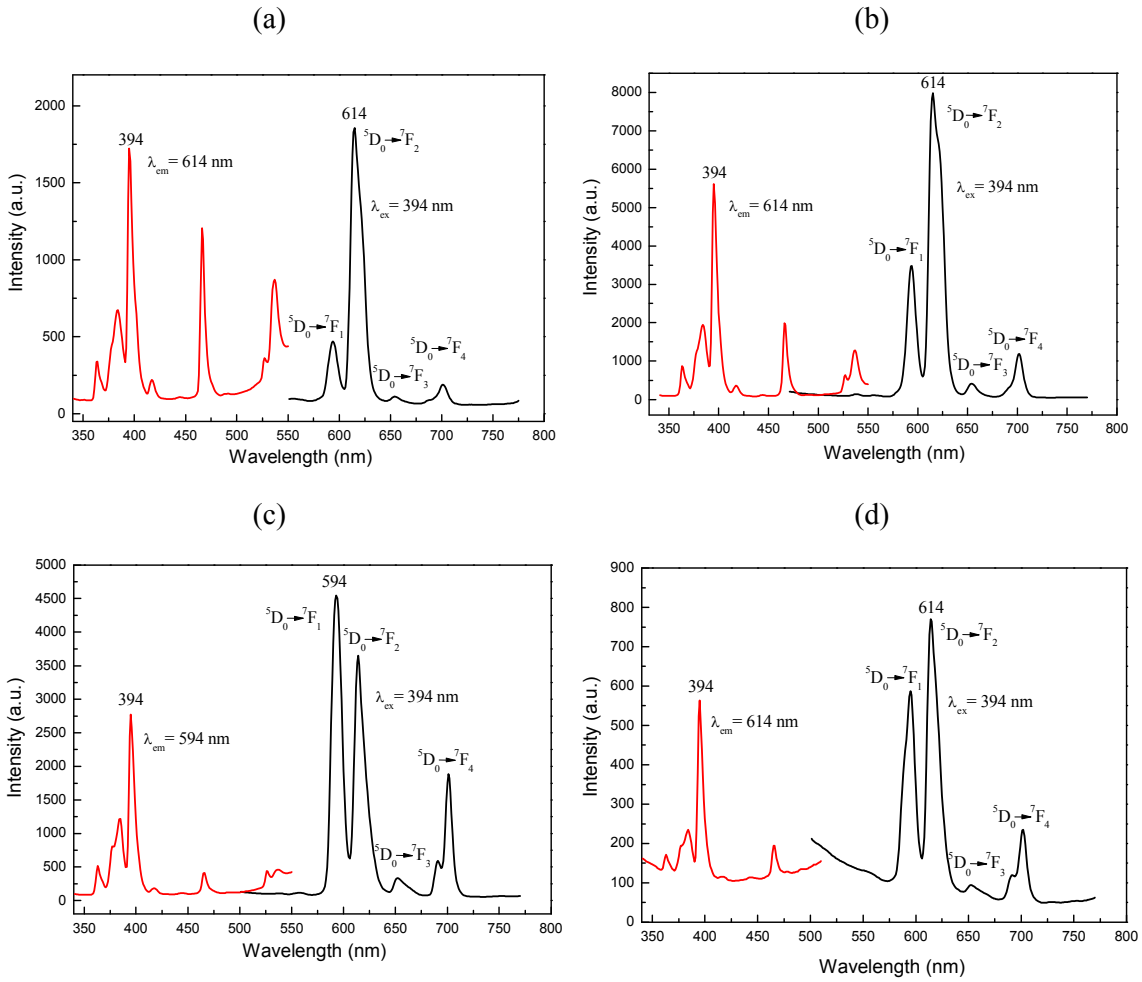


Fig. S16 Photoluminescence spectra of: **1Eu** (a), **2Eu** (b), **3Eu** (c), and **4Eu** (d).

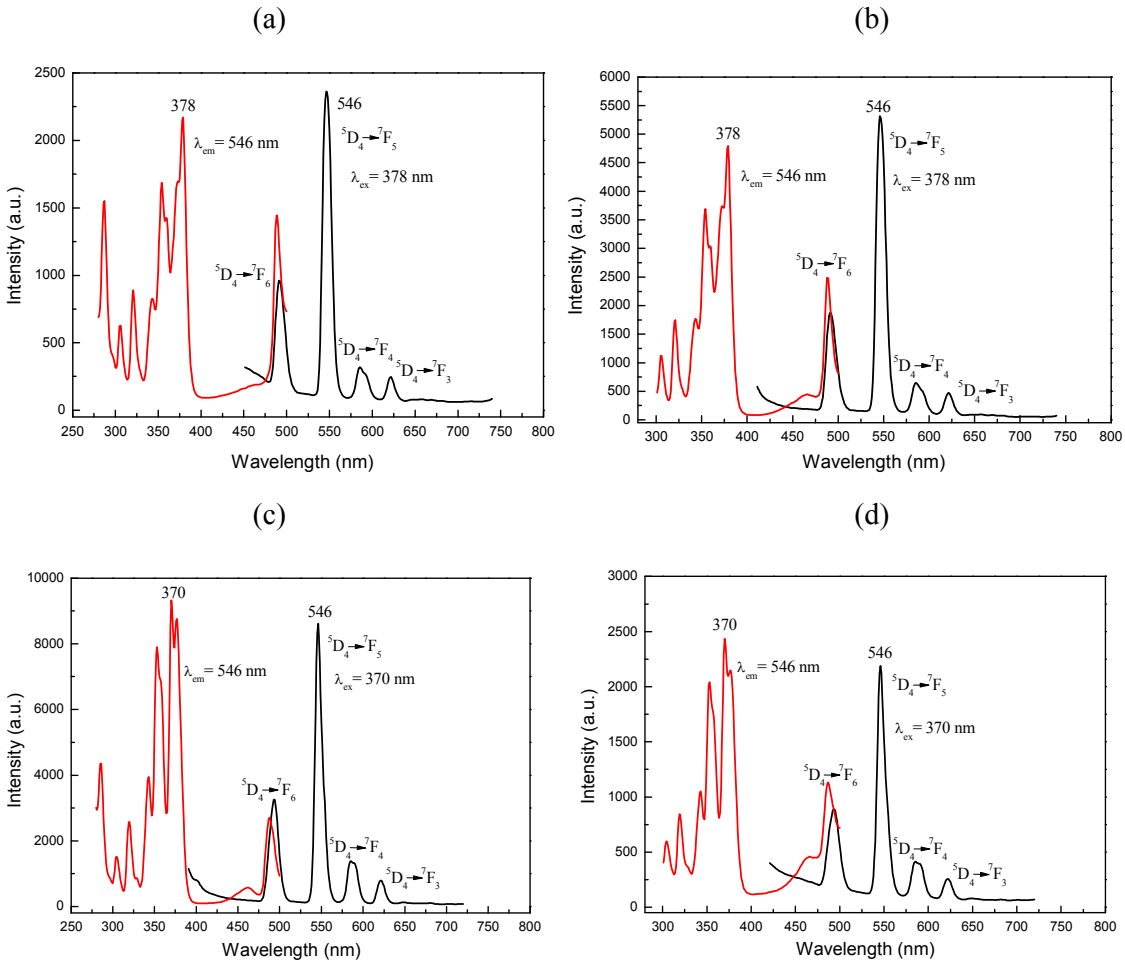


Fig. S17 Photoluminescence spectra of: **1Tb** (a), **2Tb** (b), **3Tb** (c), and **4Tb** (d).

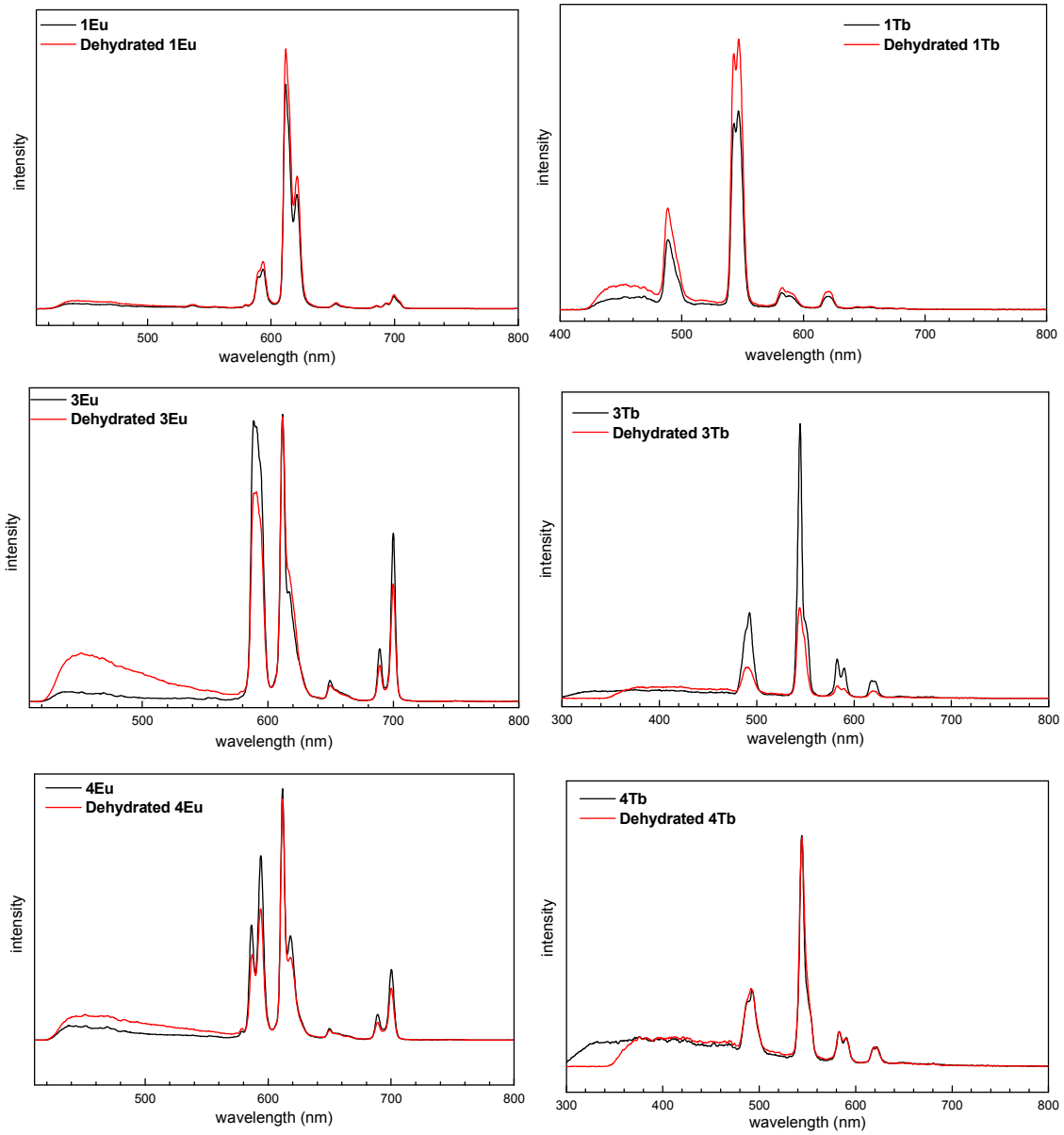


Fig. S18 Emission spectra of dehydrated **1Ln**, **3Ln**, and **4Tb** and their corresponding original compounds.

Table S1. Selected bond lengths (Å) for **1**-**4**.

1			
Mg(1)-O(4)	2.046(2)	Mg(1)-O(1)	2.110(2)
Mg(1)-O(4)#1	2.046(2)	Mg(1)-O(1)#2	2.110(2)
Mg(1)-O(4)#2	2.046(2)	Mg(1)-O(1)#1	2.110(2)
2			
Ca(1)-O(1)#1	2.3230(13)	Ca(1)-O(6)#1	2.3487(13)
Ca(1)-O(1)	2.3230(13)	Ca(1)-O(2)	2.3605(12)
Ca(1)-O(6)	2.3487(13)	Ca(1)-O(2)#1	2.3606(12)
3			
Sr(1)-O(2)#1	2.5462(18)	Sr(2)-O(7)	2.478(2)
Sr(1)-O(2)	2.5462(18)	Sr(2)-O(1W)	2.555(2)
Sr(1)-O(4)#1	2.5901(18)	Sr(2)-O(4)	2.5827(19)
Sr(1)-O(4)	2.5902(18)	Sr(2)-O(1)	2.5879(18)
Sr(1)-O(5)#1	2.6113(19)	Sr(2)-O(8)	2.5993(19)
Sr(1)-O(5)	2.6113(19)	Sr(2)-O(5)#1	2.7334(19)
Sr(1)-O(1)#1	2.6253(19)	Sr(2)-O(13)#2	2.7448(19)
Sr(1)-O(1)	2.6253(19)	Sr(2)-O(9)	3.008(2)
4			
Ba(1)-O(3)	2.758(2)	Ba(2)-O(13)	2.756(2)
Ba(1)-O(10)	2.769(2)	Ba(2)-O(1)	2.825(2)
Ba(1)-O(13)#1	2.794(2)	Ba(2)-O(12)#1	2.920(2)
Ba(1)-O(4)	2.817(2)	Ba(2)-O(14)	3.113(2)
Ba(1)-O(21)	2.819(2)	Ba(2)-O(3)	3.121(2)
Ba(1)-O(20)	2.888(2)	Ba(3)-O(15)#4	2.614(2)
Ba(1)-O(13)	2.895(2)	Ba(3)-O(17)	2.693(2)
Ba(1)-O(19)	2.914(2)	Ba(3)-O(7)#4	2.720(2)
Ba(1)-O(7)	2.931(2)	Ba(3)-O(6)#5	2.790(2)
Ba(1)-O(15)	3.048(2)	Ba(3)-O(11)#4	2.915(2)
Ba(2)-O(4)	2.657(2)	Ba(3)-O(2)	2.968(2)
Ba(2)-O(2)#2	2.675(2)	Ba(3)-O(3)	3.017(2)
Ba(2)-O(11)#3	2.685(2)	Ba(3)-O(7)	3.232(2)
Ba(2)-O(10)#1	2.753(2)	Ba(3)-O(10)#4	3.245(2)

Table S2. Hydrogen bonding distance (Å) and angle (deg) data for **1, 2, 3**, and **4**.

D — H ··· A	d(H···A)	d(D···A)	∠DHA	Symmetry Code
		1		
O2-H1 ··· O3	1.761	2.564	168.03	[x-1/3,y+1/3,-z+1/6]
O6-H2 ··· O5	1.701	2.503	165.81	[-x+2/3,-y+1/3,-z+1/3]
O7-H3 ··· O1	1.957	2.774	175.34	[x-y,-y,z]
O1W-H6 ··· O7	1.825	2.822	172.56	
O1W-H7 ··· O6	2.002	2.918	172.56	[x-y+1/3,-y+2/3,-z+1/6]
N1-H4 ··· O5	1.873	2.746	162.88	[-x+y+2/3,y+1/3,z-1/6]
N1-H5 ··· O4	2.276	3.042	142.76	[-x+1/3,-y+2/3,z-1/6]
N1-H5 ··· O6	2.287	3.012	137.45	[-x+1/3,-y+2/3,z-1/6]
		2		
O3-H1 ··· O5	1.721	2.575	162.89	[-x+3/2,y-1/2,-z-1/2]
O4-H2 ··· O1	1.904	2.775	166.69	[-x+1,-y,-z]
O4-H2 ··· O2	2.488	3.038	120.73	[x+1,y,z]
O7-H3 ··· O6	2.181	3.091	163.40	[x+1,y,z]
N1-H4 ··· O2	2.081	2.882	147.73	[x+1/2,-y+1/2,z-1/2]
N1-H5 ··· O5	1.910	2.780	162.09	
		3		
O3-H3A ··· O8	1.852	2.670	175.59	
O3-H3A ··· O11	2.652	3.154	121.06	
O6-H6A ··· O13	1.820	2.634	111.47	[-x+1/2,-y+1/2,-z+1]
O9-H9A ··· O13	2.318	3.163	179.10	
O11-H11A ··· O10	1.803	2.525	146.00	[-x+1/2,y+1/2,-z+1/2]
O12-H12A ··· O10	1.995	2.802	167.60	[x,-y,z+1/2]
O14-H14A ··· O2	2.016	2.835	176.25	[x,-y,z-1/2]
O1W-H1WB ··· O2	2.086	2.825	145.01	[-x+1,-y,-z+1]
O1W-H1WB ··· O4	2.611	3.105	118.25	[x,-y,z-1/2]
O1W-H1WA ··· O7	2.055	2.786	143.70	[x,-y,z-1/2]
N1S-H1SD ··· O3	2.025	2.916	170.05	
N2S-H2SD ··· O6	2.153	2.940	145.59	[x,y,z-1]
N2S-H2SD ··· O14	2.428	3.064	127.80	[-x+1,y,-z+1/2]
N2S-H2SE ··· O11	2.230	3.059	153.06	
		4		
O1-H1A ··· O8	1.803	2.642	168.87	[x,y+1,z]
O5-H1 ··· O18	1.952	2.719	155.38	[-x+1,-y+2,-z+1]
O9-H2 ··· O17	1.812	2.631	178.15	
O12-H12A ··· O6	1.859	2.561	138.86	[x,y-1,z]
O14-H14A ··· O8	2.038	2.528	115.95	[-x+1,-y+1,-z]

O16-H3 ··· O2	2.430	2.895	116.86	
O19-H19A ··· O18	1.819	2.642	162.33	[-x+1,-y+2,-z+1]
O20-H20A ··· O1W	2.542	2.975	112.69	[-x,-y+1,-z+1]
O21-H21A ··· O1W	2.365	2.805	112.71	[-x,-y+1,-z+1]
O1W-H4 ··· O14	2.290	3.147	149.45	[x,y,z+1]
O1W-H5 ··· O1W	2.432	3.001	124.94	[-x,-y+1,-z+1]
O1W-H5 ··· O16	2.484	2.926	113.31	[-x+1,-y+2,-z+1]