Supporting Information

Alkaline-Earth Metal Phosphonocarboxylates: Synthesis, Structures, Chirality, and Extrinsic Luminescence Properties

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Table S2 Hydrogen bonding distances and angles for **1**, **2**, **3**, **4**, and **6**.

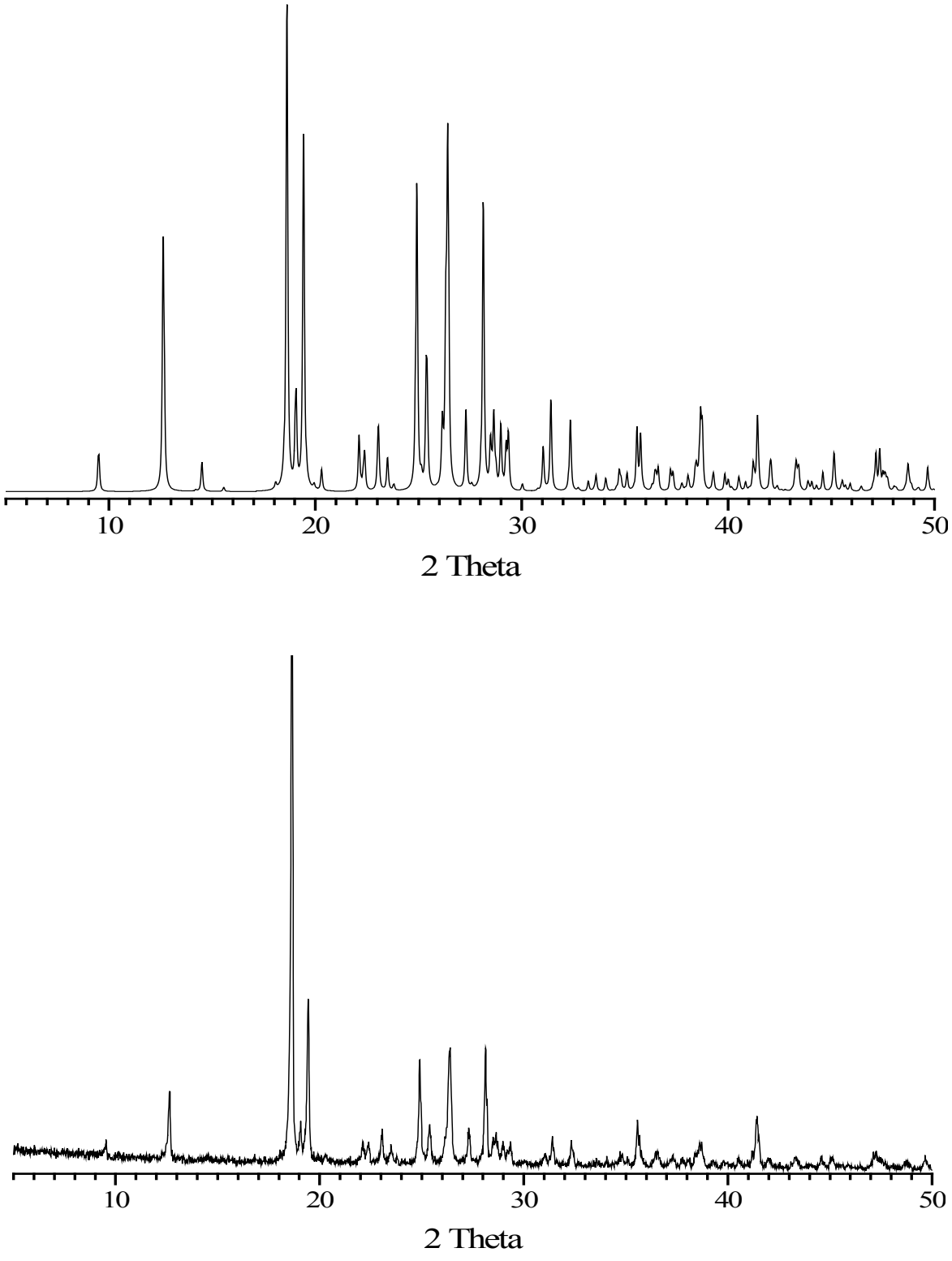


Figure. S1 Powder XRD patterns of **1** (calculated, top; measured, bottom).

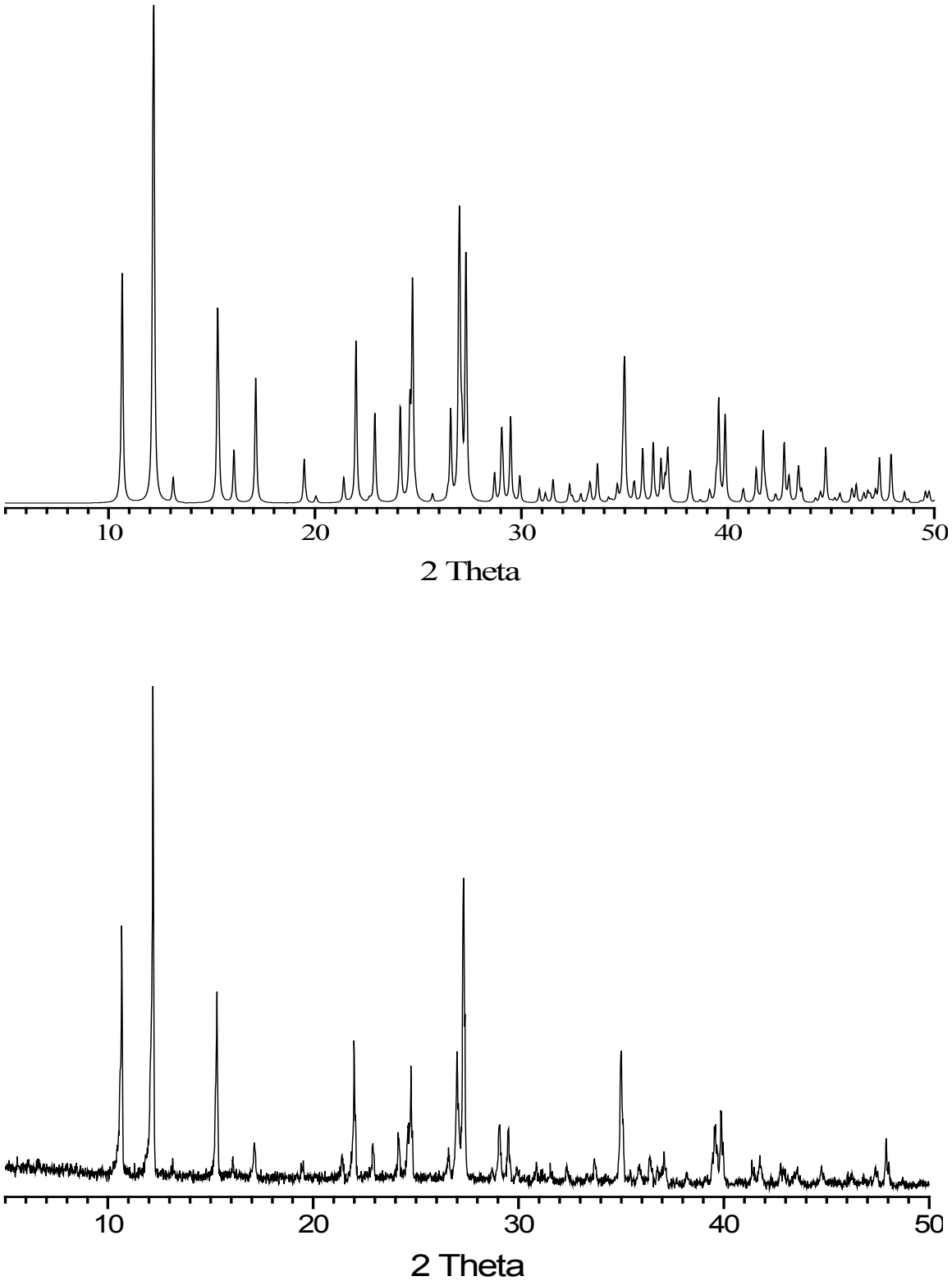


Figure. S2 Powder XRD patterns of **2** (calculated, top; measured, bottom).

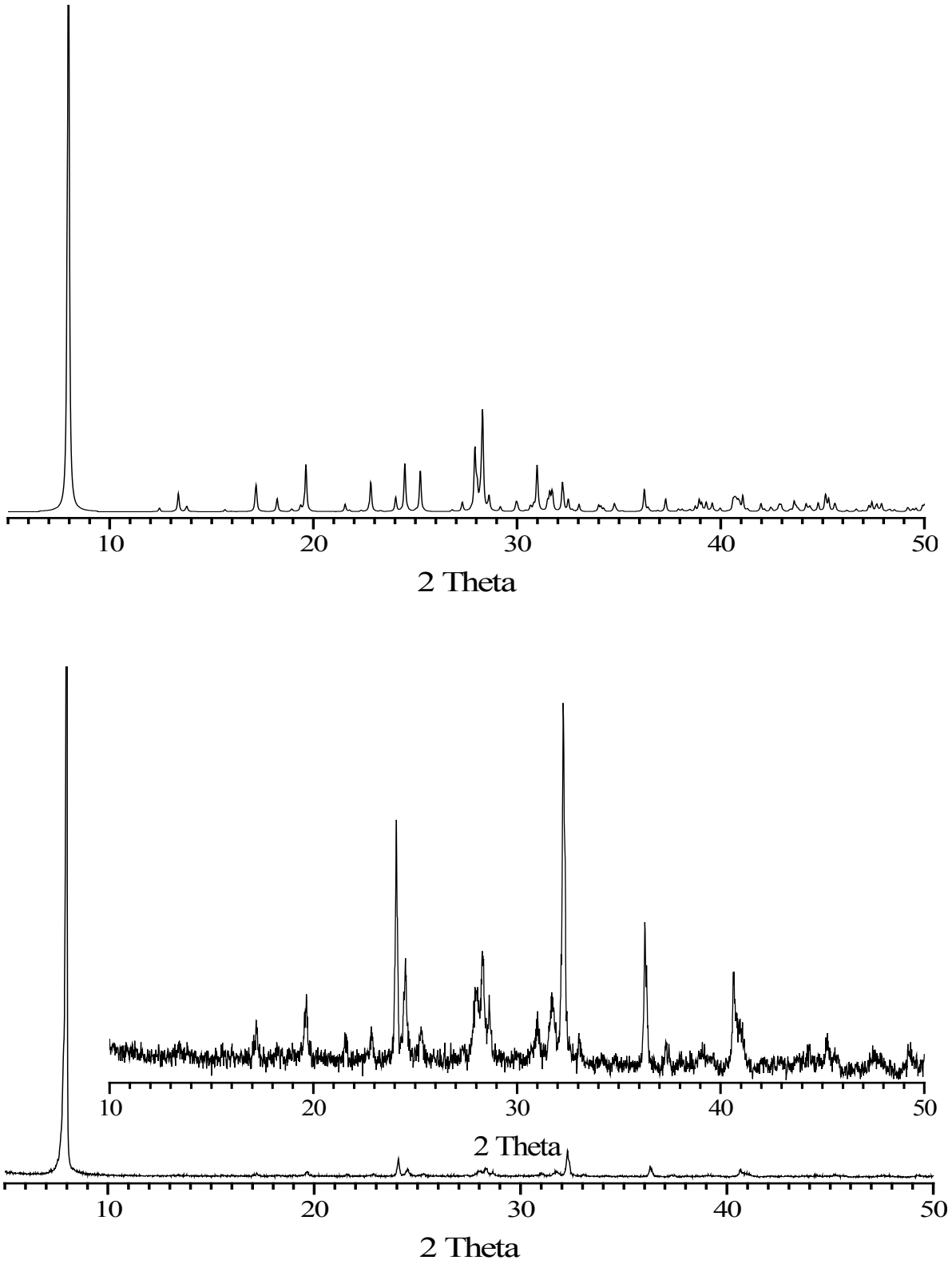


Figure. S3 Powder XRD patterns of **3** (calculated, top; measured, bottom).

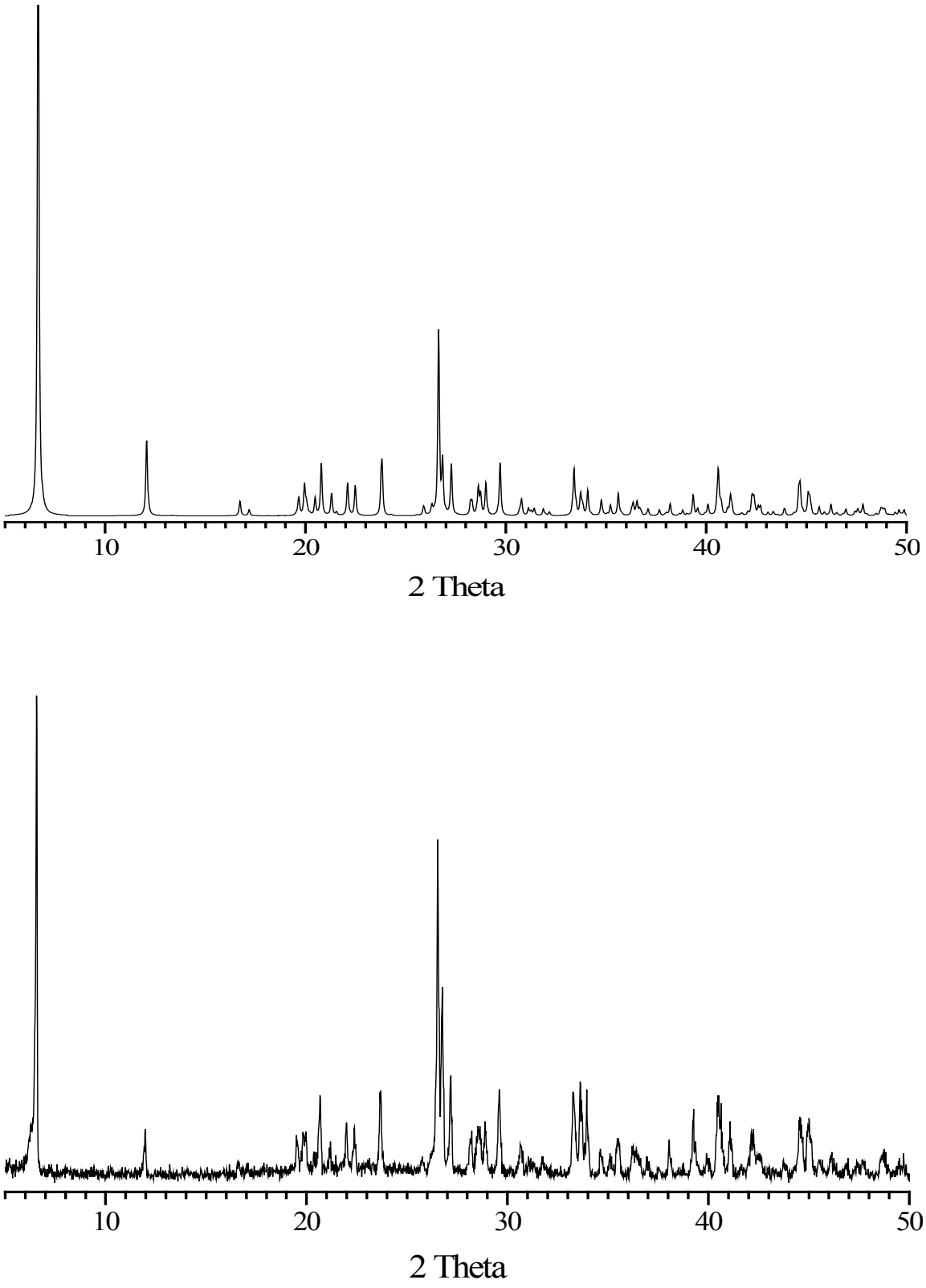


Figure. S4 Powder XRD patterns of **4** (calculated, top; measured, bottom).

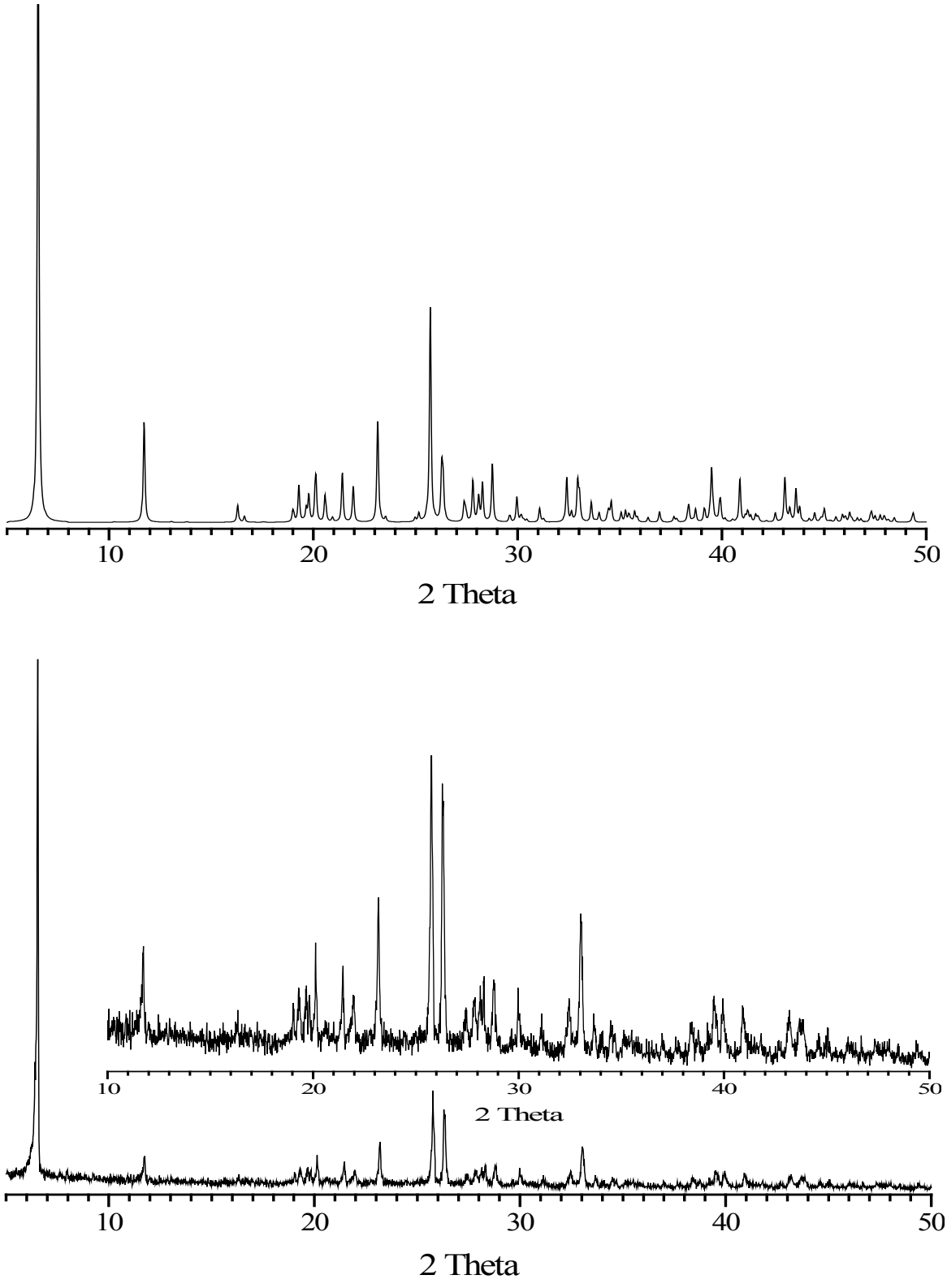


Figure. S5 Powder XRD patterns of **5** (calculated, top; measured, bottom).

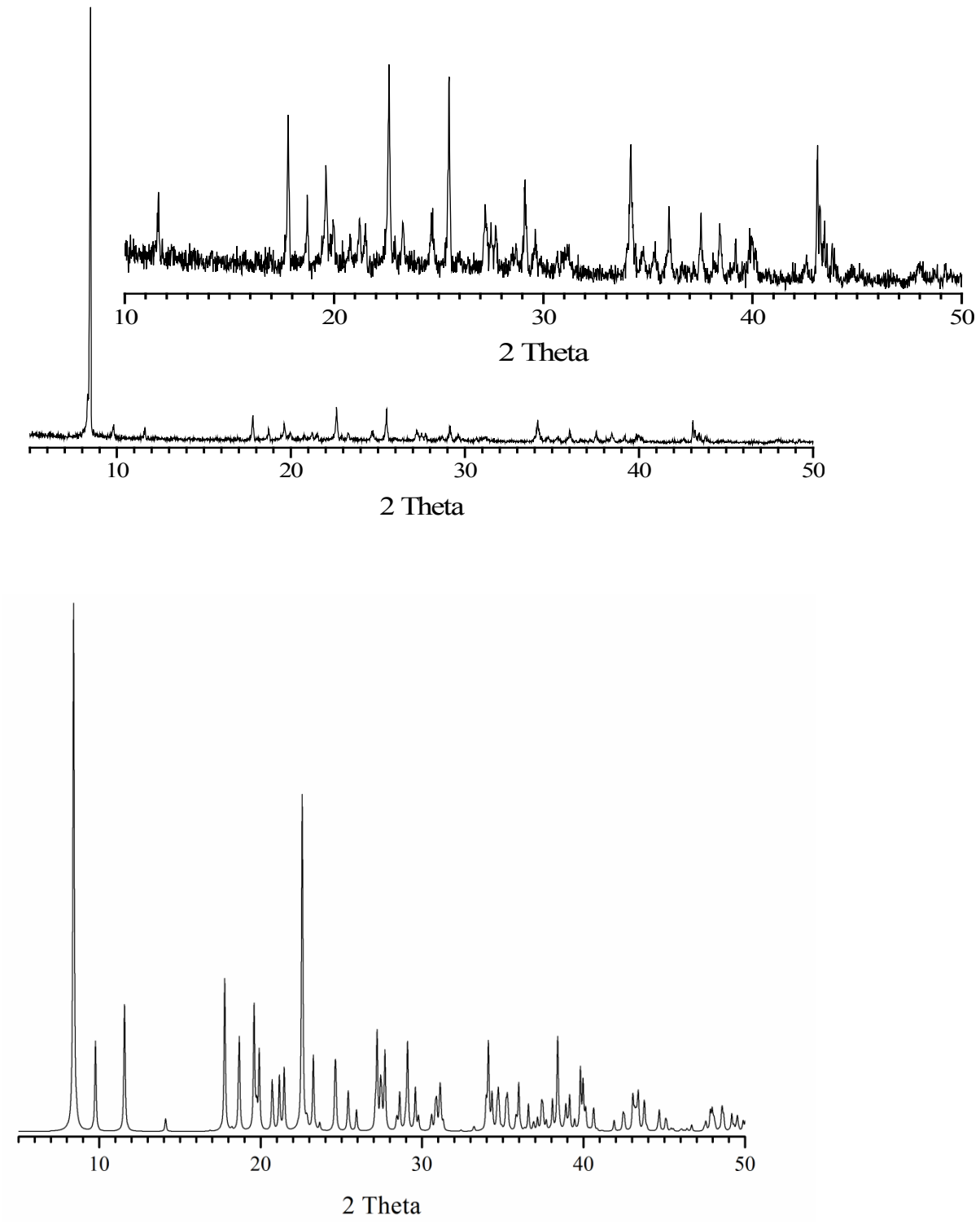


Figure. S6 Powder XRD patterns of **6** (calculated, top; measured, bottom).

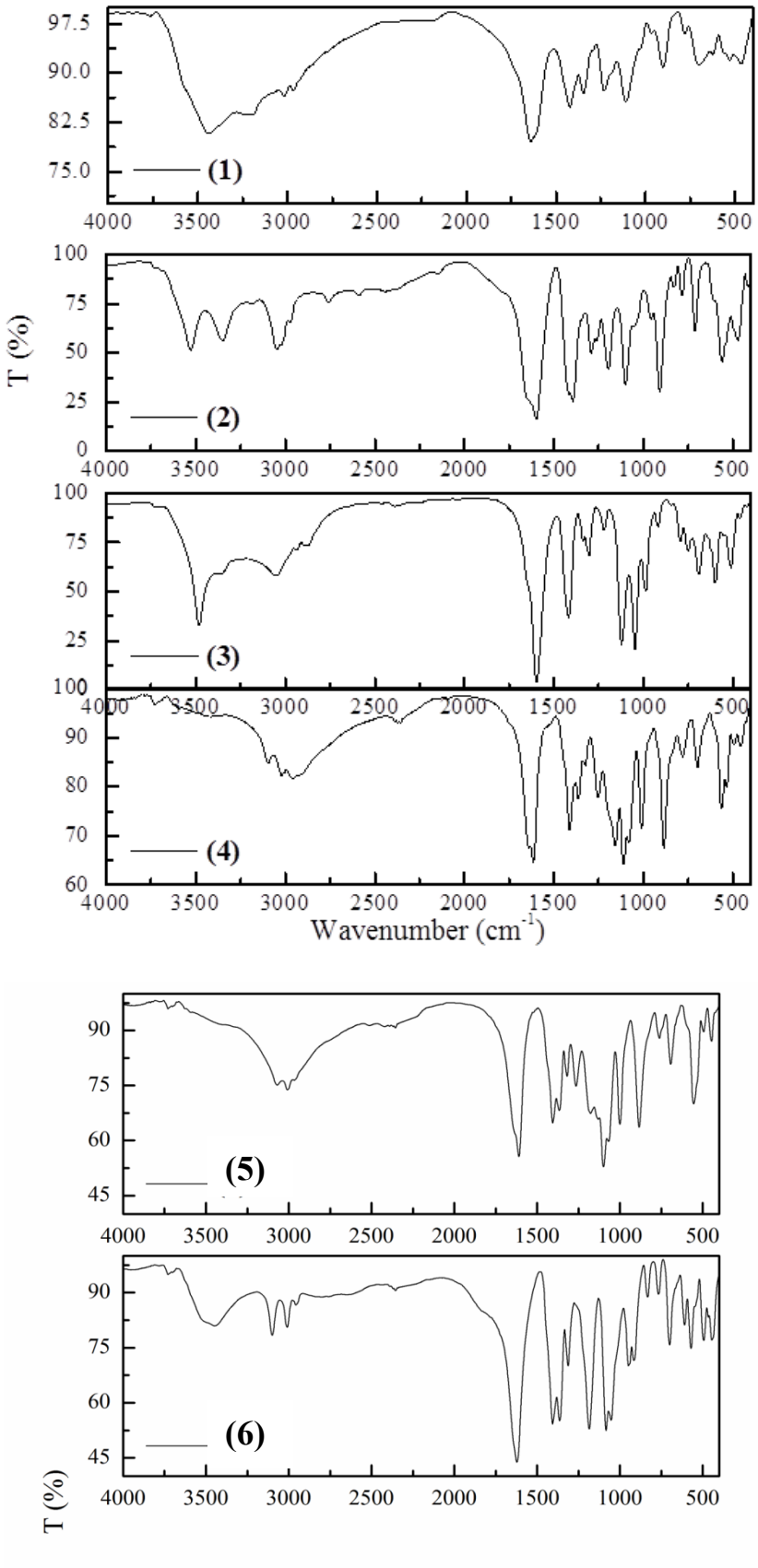


Figure. S7 FT-IR spectra of **1-6**.

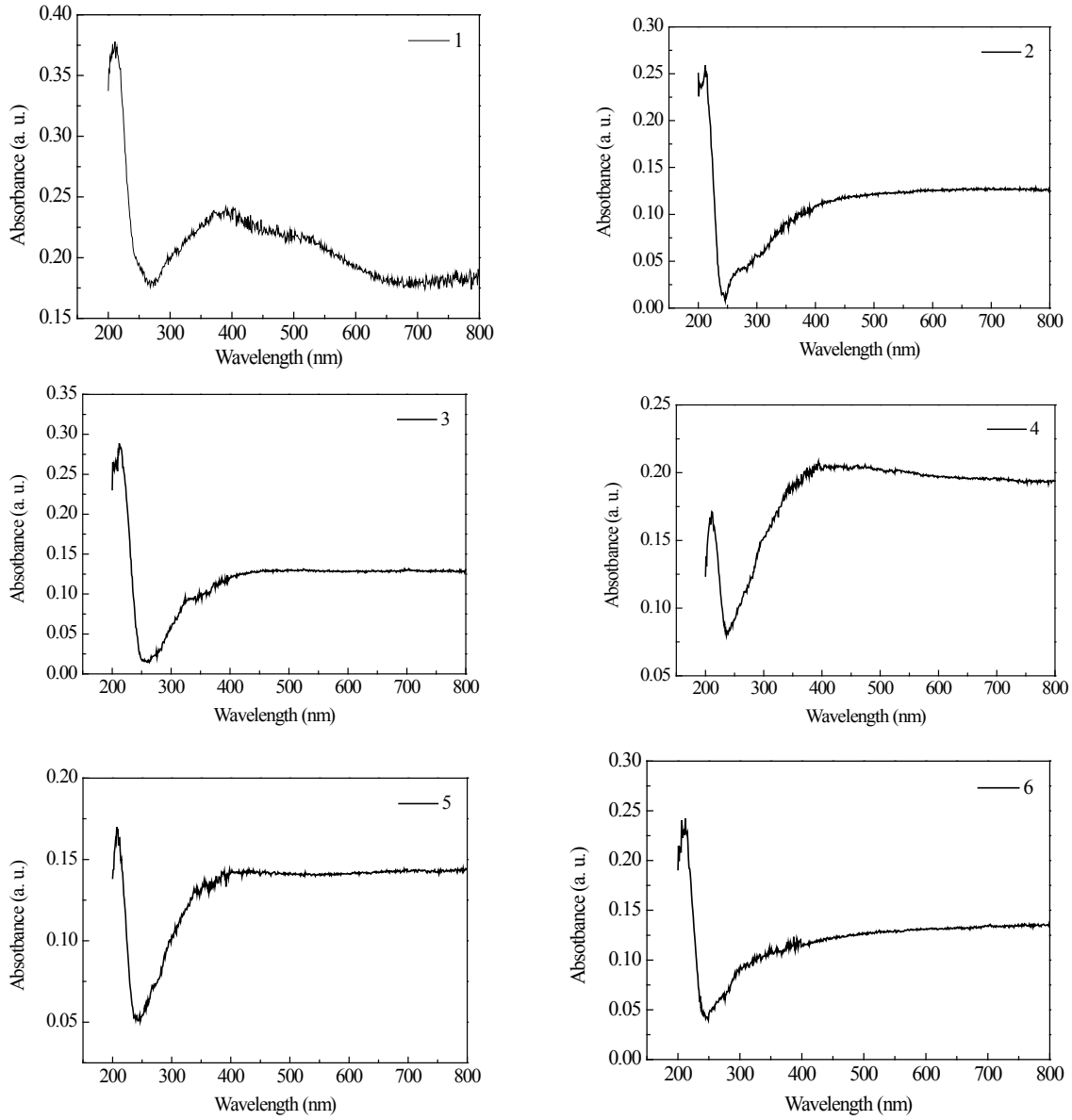


Figure. S8 UV-vis absorption spectra of compound **1-6**.

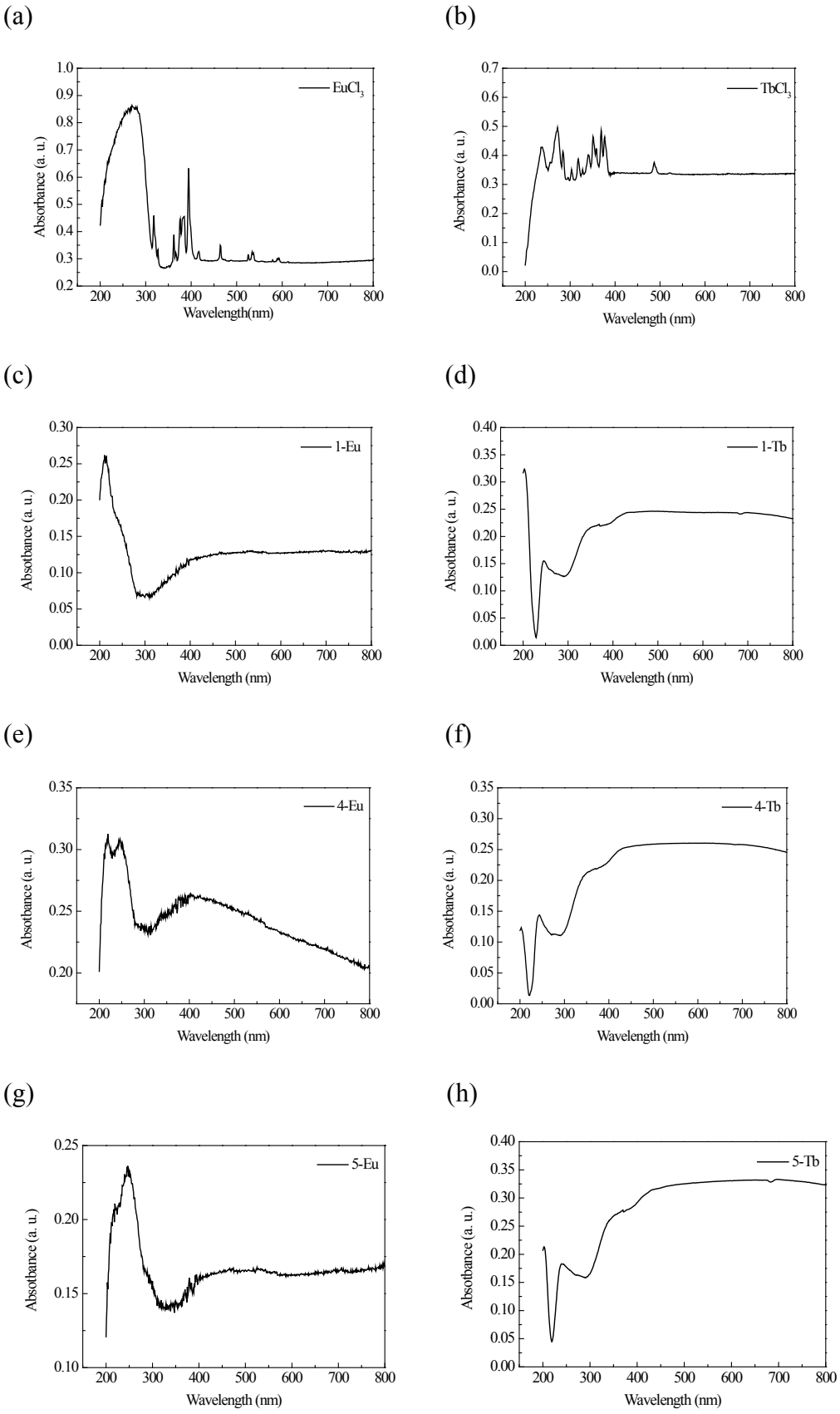


Figure. S9 UV-vis absorption spectra of: (a) $EuCl_3 \cdot 6H_2O$, (b) $TbCl_3 \cdot 6H_2O$, (c) **1-Eu**, (d) **1-Tb**, (e) **4-Eu**, (f) **4-Tb**, (g) **5-Eu**, (h) **5-Tb**.

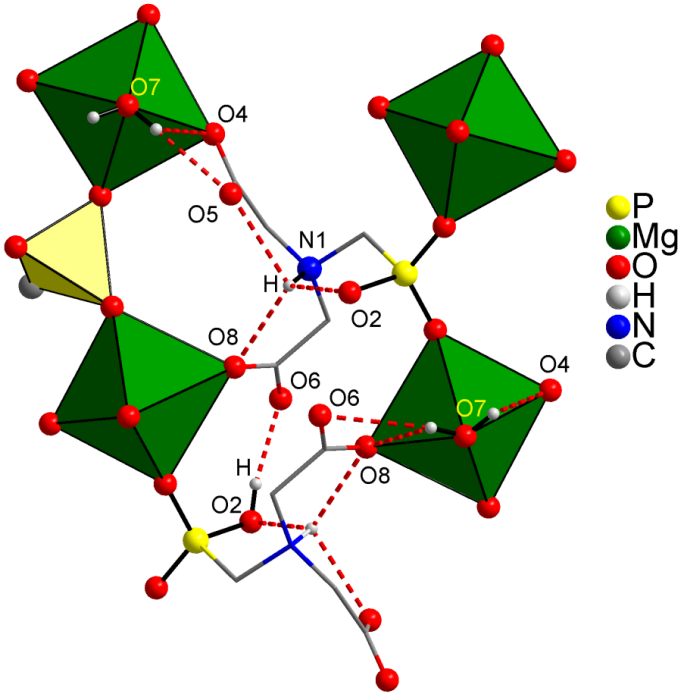


Figure. S10 Hydrogen bond system in **1**.

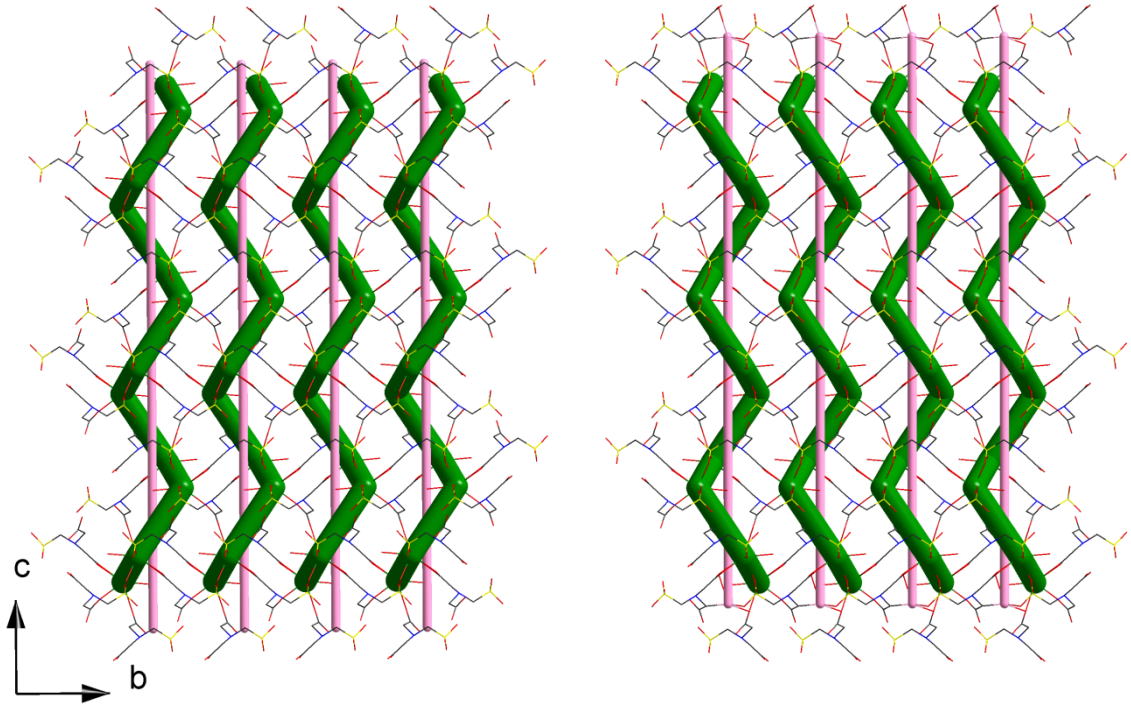


Figure. S11 Right-handed (a) and left-handed (b) helical motifs of Sr atoms in **2.**

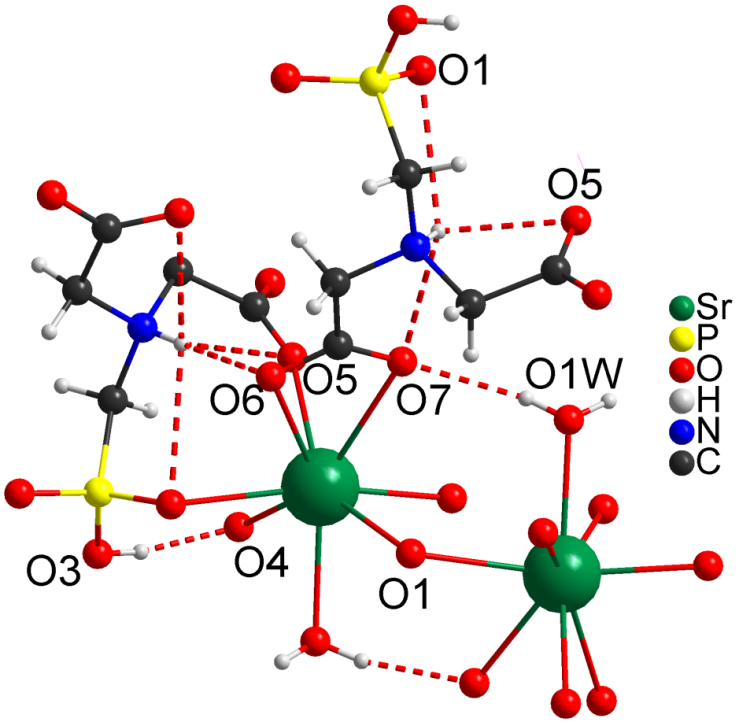


Figure. S12 Hydrogen bond system in **2**.

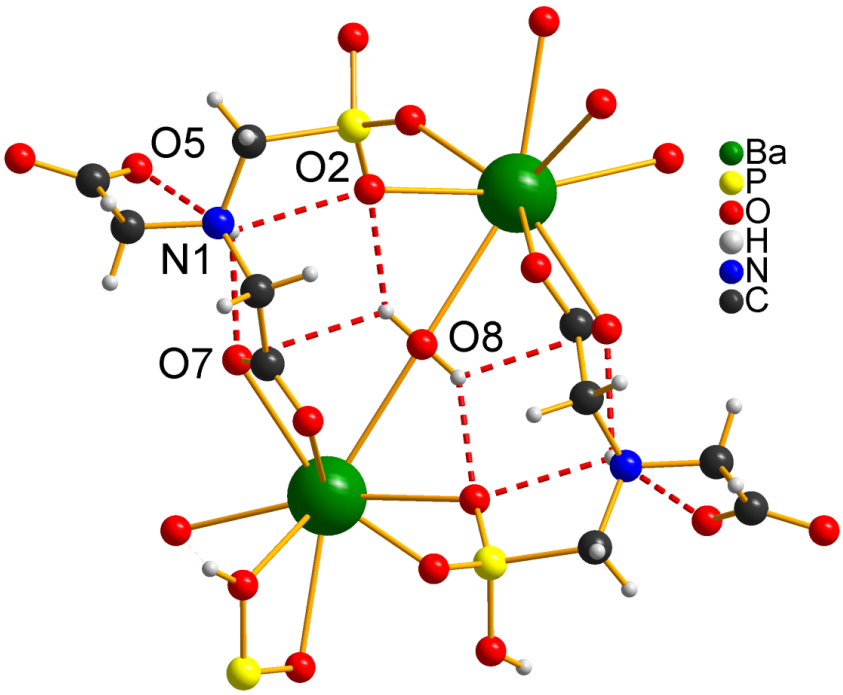


Figure. S13 Hydrogen bond system in **6**.

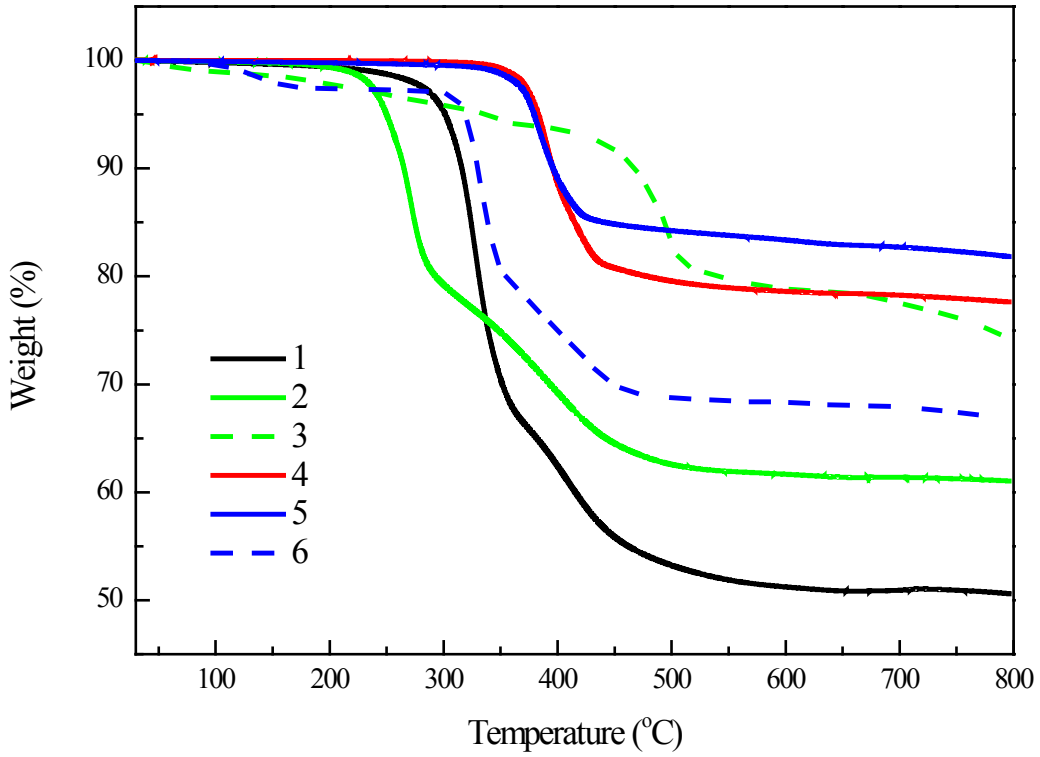


Figure. S14 TGA curves of compounds **1-6**.

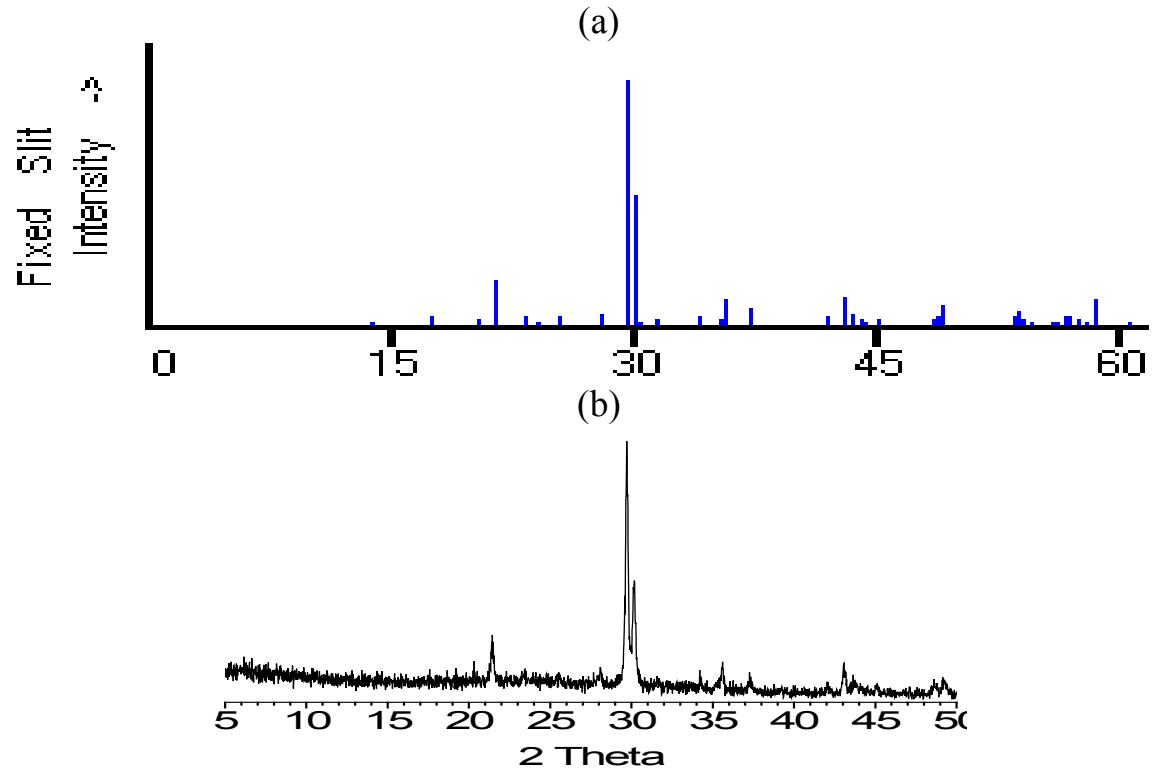


Figure S15 (a) JCPDF- (#751055) $Mg_2P_2O_7$ (b) Complex **1** after 800 °C.

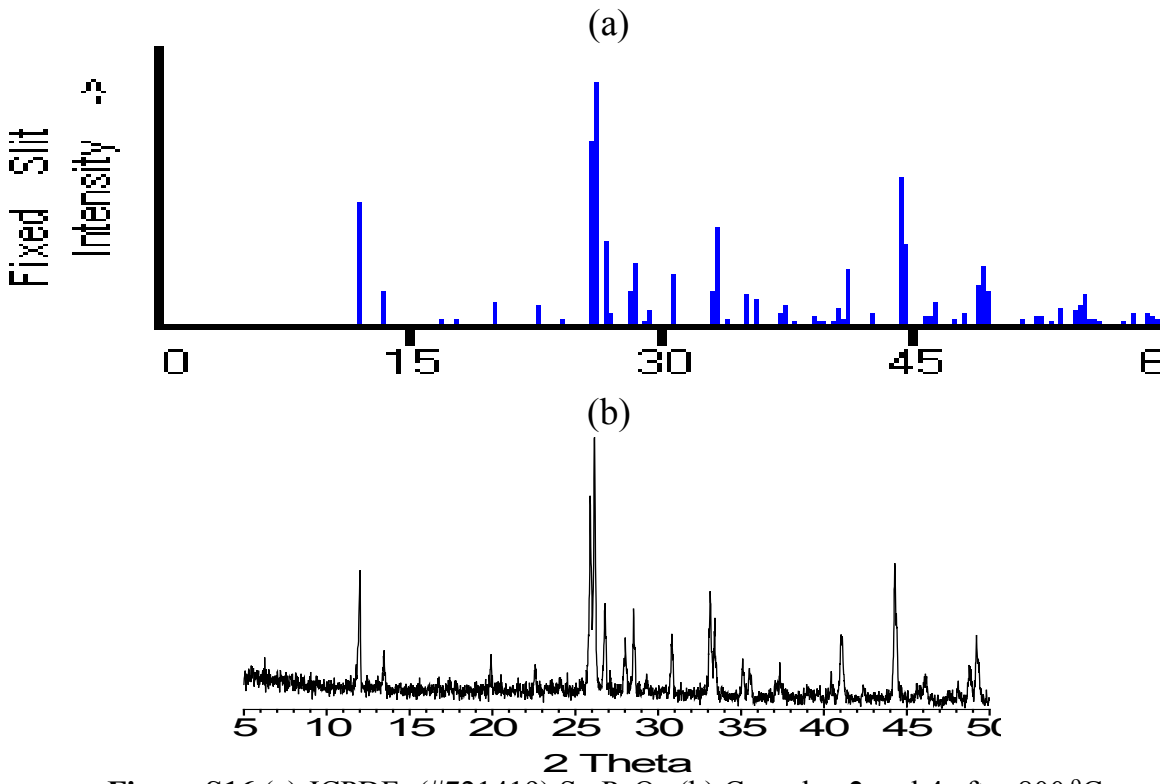


Figure S16 (a) JCPDF- (#721419) $Sr_2P_2O_7$ (b) Complex **2** and **4** after 800 °C.

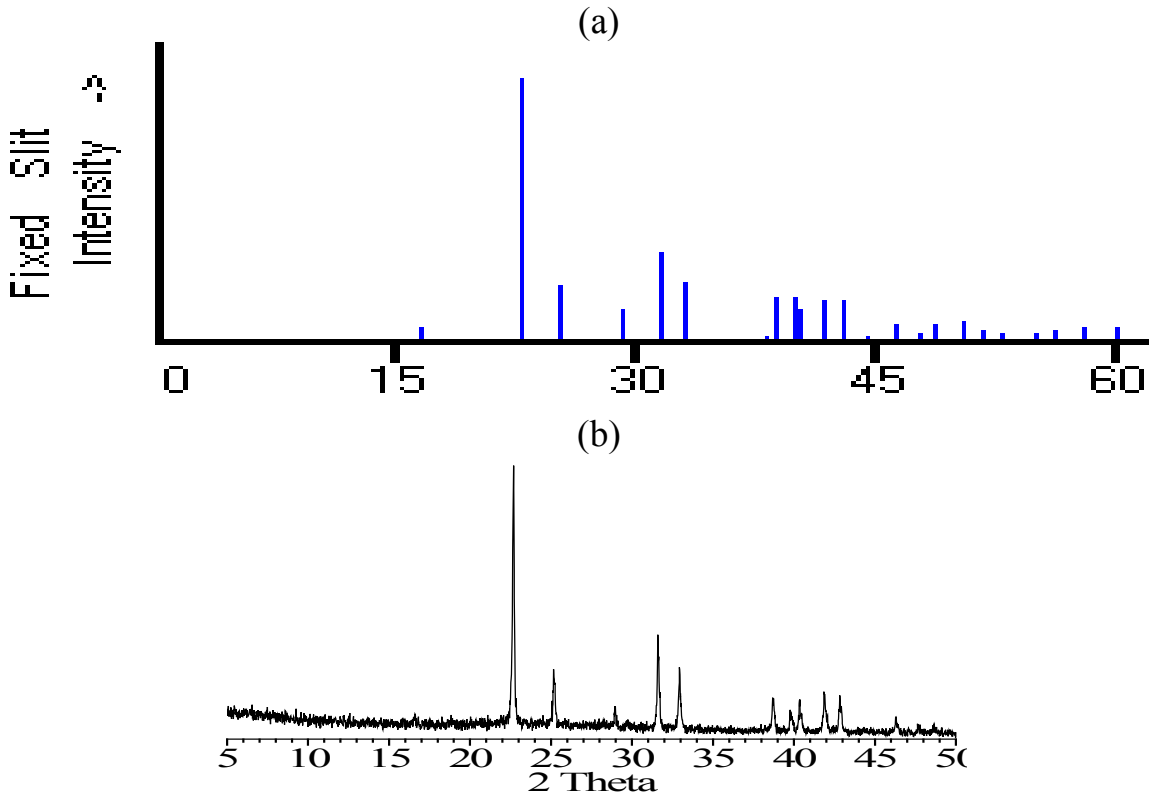
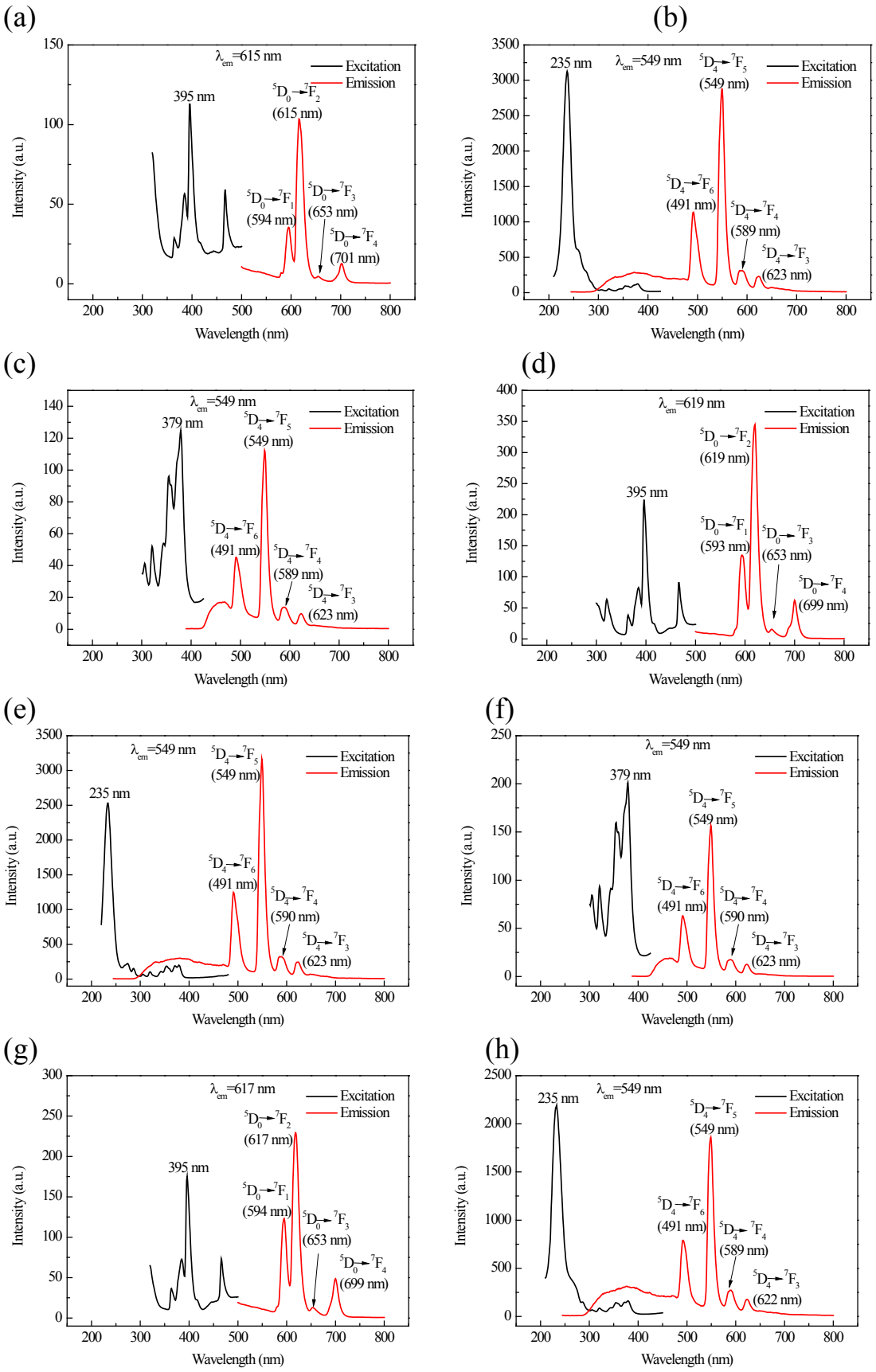


Figure S17 (a) JCPDF- (#830990) $Ba_2P_2O_7$ (b) Complex **5** after 800 °C.


(a)
λem=615 nm
Excitation
Emission
395 nm
5D0→7F2 (615 nm)
5D0→7F1 (594 nm)
5D0→7F3 (653 nm)
5D0→7F4 (701 nm)
Intensity (a.u.)
Wavelength (nm)
(b)
235 nm
λem=549 nm
5D4→7F5 (549 nm)
5D4→7F6 (491 nm)
5D4→7F4 (589 nm)
5D4→7F3 (623 nm)
(c)
λem=549 nm
379 nm
(d)
λem=619 nm
5D0→7F2 (619 nm)
395 nm
5D0→7F1 (593 nm)
5D0→7F3 (653 nm)
5D0→7F4 (699 nm)
(e)
λem=549 nm
235 nm
5D4→7F6 (491 nm)
5D4→7F4 (590 nm)
5D4→7F3 (623 nm)
(f)
λem=549 nm
379 nm
(g)
λem=617 nm
5D0→7F2 (617 nm)
395 nm
5D0→7F1 (594 nm)
5D0→7F3 (653 nm)
5D0→7F4 (699 nm)
(h)
235 nm
λem=549 nm
5D4→7F6 (491 nm)
5D4→7F4 (589 nm)
5D4→7F3 (622 nm)

(i)

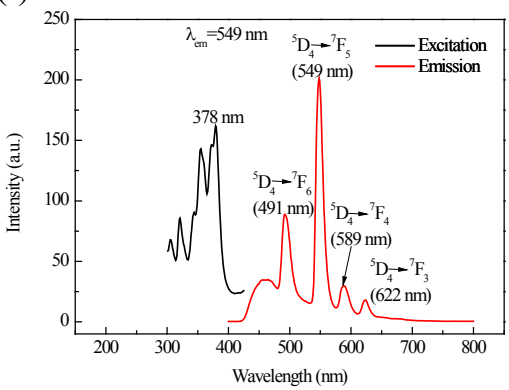


Figure S18 Photoluminescence spectra of: (a) **1Eu**, (b)(c) **1Tb**, (d) **4Eu**, (e)(f) **4Tb**, (g) **5Eu**, (h)(i) **5Tb**.

Table S1. Selected bond lengths (Å) for **1-6**.

		1	
Mg(1)-O(3)#1	2.0129(13)	Mg(1)-O(4)	2.0804(13)
Mg(1)-O(1)	2.0447(12)	Mg(1)-O(8)	2.1095(13)
Mg(1)-O(7)	2.0634(14)	Mg(1)-O(6)	2.1775(13)
		2	
Sr(1)-O(2)	2.4468(15)	Sr(1)-O(1)	2.6326(16)
Sr(1)-O(1)#1	2.5808(15)	Sr(1)-O(6)	2.6412(16)
Sr(1)-O(1W)	2.6017(16)	Sr(1)-O(4)	2.8067(16)
Sr(1)-O(5)	2.6156(17)	Sr(1)-O(7)	2.8702(17)
		3	
Sr(1)-O(3)	2.491(2)	Sr(2)-O(6)	2.549(2)
Sr(1)-O(1W)	2.515(3)	Sr(2)-O(2)#4	2.550(2)
Sr(1)-O(6)#1	2.541(2)	Sr(2)-O(2)	2.5685(19)
Sr(1)-O(1)	2.5516(19)	Sr(2)-O(3)#3	2.643(2)
Sr(1)-O(7)	2.616(2)	Sr(2)-O(7)	2.643(2)
Sr(1)-O(4)	2.650(2)	Sr(2)-O(4)#3	2.657(2)
Sr(1)-O(1)#1	2.722(2)	Sr(2)-O(1)#1	2.731(2)
Sr(1)-O(2)#2	2.774(2)	Sr(2)-N(1)	2.833(2)
		4	
Sr(1)-O(1)#1	2.544(3)	Sr(2)-O(2)#4	2.509(2)
Sr(1)-O(1)	2.641(3)	Sr(2)-O(5)	2.531(3)
Sr(1)-O(9)	2.668(2)	Sr(2)-O(3)	2.602(3)
Sr(1)-O(3)#2	2.695(3)	Sr(2)-O(8)	2.609(3)
Sr(1)-O(4)#3	2.705(3)	Sr(2)-O(9)#5	2.652(3)
Sr(1)-O(3)#3	2.780(3)	Sr(2)-O(11)	2.685(3)
Sr(1)-O(6)	2.830(3)	Sr(2)-O(7)#6	2.688(3)
Sr(1)-O(5)	2.831(3)	Sr(2)-O(1)	2.822(3)
Sr(1)-O(2)	2.870(3)	Sr(2)-O(9)#4	3.163(3)
Sr(1)-O(2)#2	2.946(3)		
		5	
Ba(1)-O(1)#1	2.702(2)	Ba(2)-O(2)#4	2.679(2)
Ba(1)-O(1)	2.745(2)	Ba(2)-O(5)	2.712(3)
Ba(1)-O(3)#2	2.785(2)	Ba(2)-O(8)	2.768(3)
Ba(1)-O(3)#3	2.813(2)	Ba(2)-O(3)	2.765(2)
Ba(1)-O(9)	2.869(2)	Ba(2)-O(11)	2.839(3)

Ba(1)-O(5)	2.887(3)	Ba(2)-O(9)#5	2.851(2)
Ba(1)-O(4)#3	2.904(3)	Ba(2)-O(7)#6	2.871(3)
Ba(1)-O(2)#2	3.010(3)	Ba(2)-O(1)	2.940(2)
Ba(1)-O(6)	3.025(3)	Ba(2)-O(9)#4	3.191(3)
Ba(1)-O(2)	3.026(3)		

6

Ba(1)-O(1)#1	2.6914(17)	Ba(1)-O(1)	2.8799(18)
Ba(1)-O(6)	2.7255(18)	Ba(1)-O(7)	2.918(2)
Ba(1)-O(2)	2.7585(18)	Ba(1)-O(8)	2.9736(4)
Ba(1)-O(4)	2.7911(18)	Ba(1)-O(6)#2	3.0088(18)
Ba(1)-O(3)	2.8167(17)		

Table S2. Hydrogen bonding distances (Å) and angles (°) for **1**, **2**, **3**, **4**, and **6**.

D — H ··· A	d(H···A)	d(D···A)	∠DHA	Symmetry Code
1				
O(2)-H(2C)···O(6)	1.94	2.751	168.1	[-x-1/2,y-1/2,-z+1/2]
O(7)-H(7A)···O(4)	1.97	2.674	138.9	[x+1,y,z]
O(7)-H(7B)···O(5)	2.18	2.957	152.5	
N(1)-H(1A)···O(2)	2.49	2.996	115.1	[-x,-y+1,-z+1]
2				
O3-H3C···O4	1.767	2.564	163.66	[x+1/2, -y+3/2, -z+1]
N1-H1A···O6	2.240	3.136	173.21	[x+1/2, -y+3/2, -z+1]
O1W-H1WB···O7	2.159	2.973	160.21	[x-1/2, -y+3/2, -z+1]
O1W-H1WA···O6	1.960	2.797	167.86	[x+1/2, -y+3/2, -z+1]
3				
O1W-H1WA···O5	1.985	2.774	164.81	[x, y+1, z+1]
O1W-H1WB···O5	1.704	2.697	167.82	[-x+1, -y+1, -z]
O1W-H1WB···O4	2.611	3.107	110.29	
4				
O4-H4A···O6	1.781	2.601	177.20	[-x, y+1/2, -z+1/2]
O7-H7A···O11	1.918	2.705	160.58	
4Eu				
N1-H1A···O10	2.155	2.610	110.04	[x-1/2, -y+1/2, -z]
O4-H4A···O6	1.764	2.583	176.72	[-x, y+1/2, -z+1/2]
O7-H7A···O11	1.964	2.746	159.12	
4Tb				
O4-H4A···O6	1.764	2.583	176.72	[-x, y+1/2, -z+1/2]
O7-H7A···O11	1.964	2.746	159.12	
6				
O3-H1···O4	1.656	2.520	162.40	[x, y-1, z]
O8-H2···O2	2.069	2.878	134.93	[-x+2, y, -z+1/2]
O8-H2···O7	2.585	3.162	115.82	
N1-H3···O7	2.172	2.652	110.04	[x, -y+1, z+1/2]