Supporting Information

Tuning the Structure, dimensionality and Luminescent properties of Lanthanide Metal-Organic Frameworks under Ancillary Ligand Influence. †

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Supporting Information.

Section S1. Experimental X-ray powder patterns for [Ln(3-OHNDS)(H_2O)$_2$, [Ln(3-OHNDS)(phen)(H_2O)]·3H_2O and [La(3-OHNDS)(3,4,7,8-TMphen)(H_2O)] compounds.

Section S2. TG analysis for the [Ln(3-OHNDS)(H_2O)$_2$, [Ln(3-OHNDS)(phen)(H_2O)]·3H_2O and [La(3-OHNDS)(3,4,7,8-TMphen)(H_2O)] compounds.

Section S3. IR spectra of [Ln(3-OHNDS)(H_2O)$_2$, [Ln(3-OHNDS)(phen)(H_2O)]·3H_2O and [La(3-OHNDS)(3,4,7,8-TMphen)(H_2O)] compounds.

Section S4. Excitation spectrum of the compounds [Ln(3-OHNDS)(H_2O)$_2$where Ln= La (1), Pr(2), Nd(3) and Sm(4); and [Ln(3-OHNDS)(phen)(H_2O)]·3H_2O, where Ln= La(5), Pr(6), Nd(7) and Sm(8).

Section S5. Assignment of the transitions in the excitation and emission spectra of 3-OHNDS and compounds (1)-(8).

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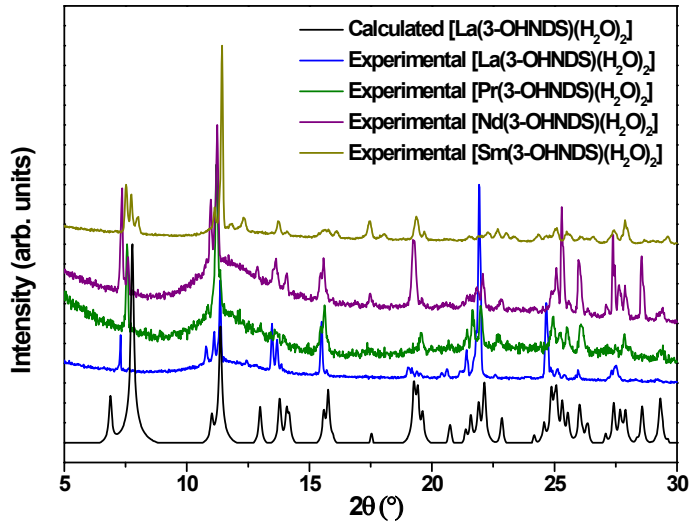
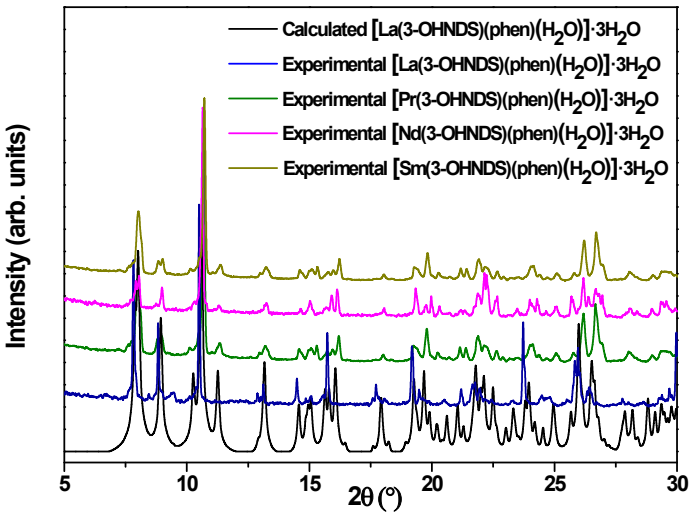
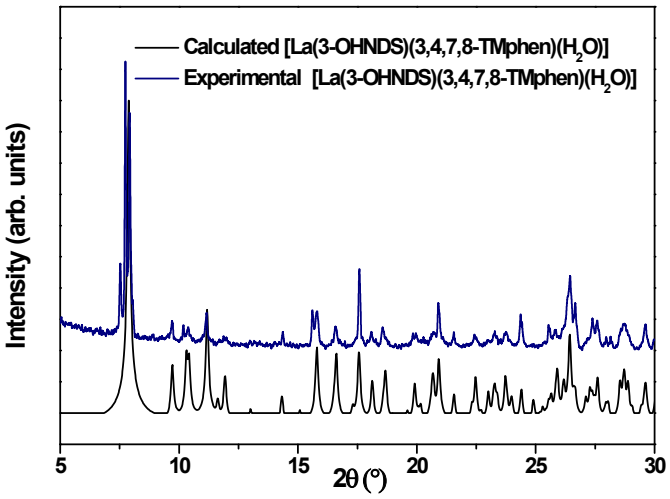
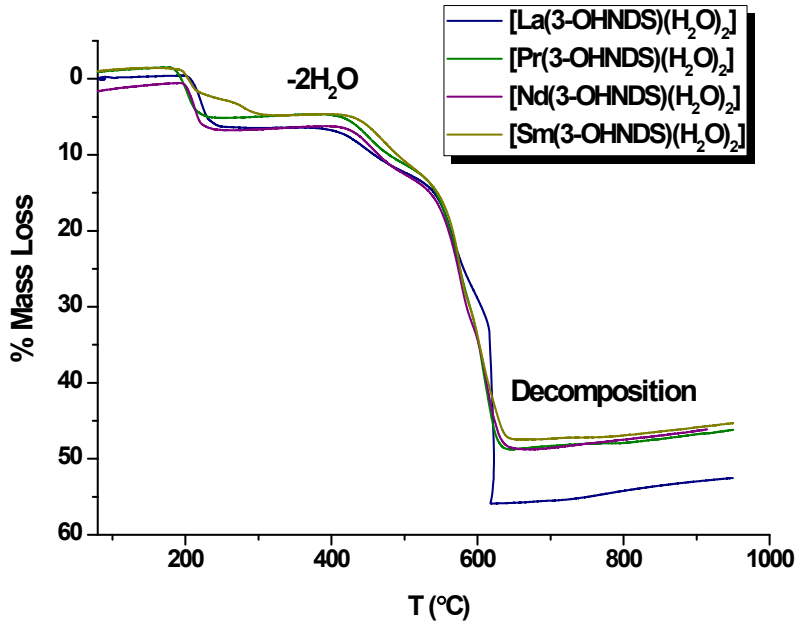
Section S1. Experimental X-ray powder patterns for [Ln(3-OHNDS)(H_2O)$_2$, [Ln(3-OHNDS)(phen)(H_2O)]·3H_2O and [La(3-OHNDS)(3,4,7,8-TMphen)(H_2O)] compounds.

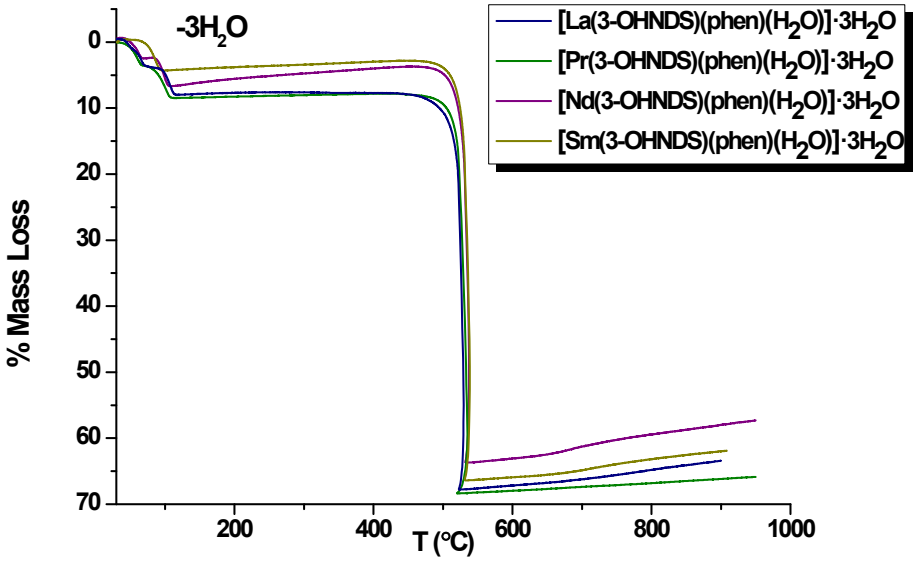


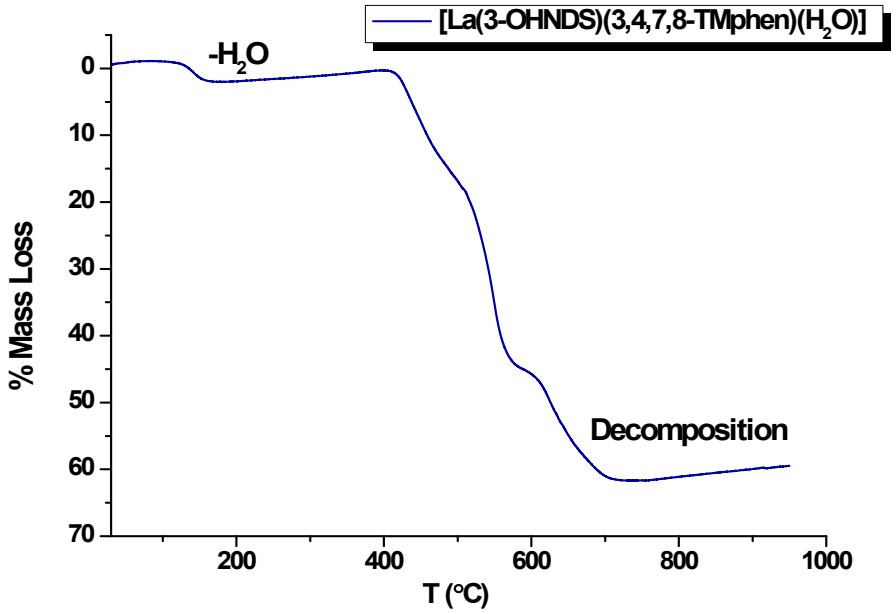



Calculated [La(3-OHNDS)(3,4,7,8-TMphen)(H2O)]
Experimental [La(3-OHNDS)(3,4,7,8-TMphen)(H2O)]
Intensity (arb. units)
5
10
15
20
25
30
2θ (°)

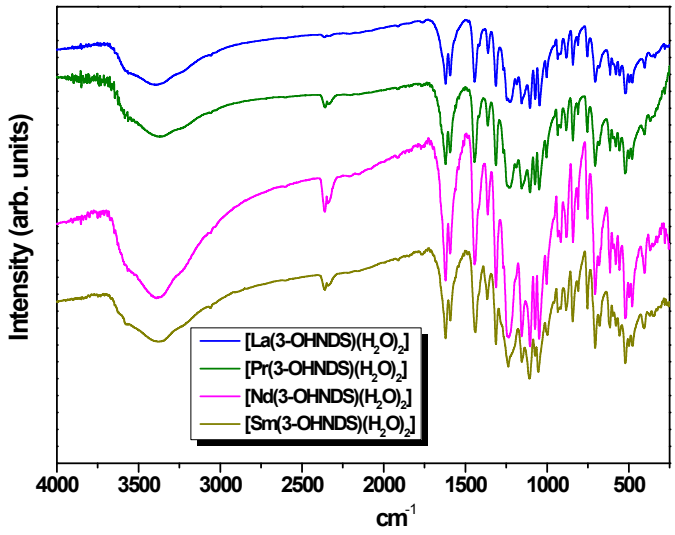
Section S2. TG analysis for the [Ln(3-OHNDS)(H_2O)$_2$, [Ln(3-OHNDS)(phen)(H_2O)]·3H_2O and [La(3-OHNDS)(3,4,7,8-TMphen)(H_2O)] compounds.

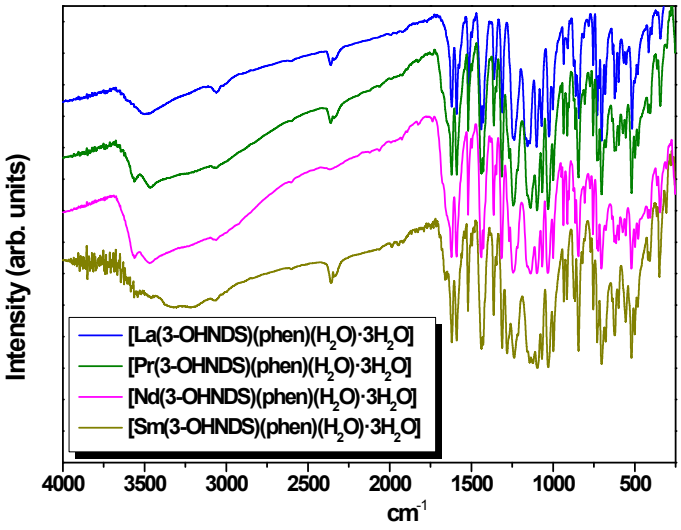


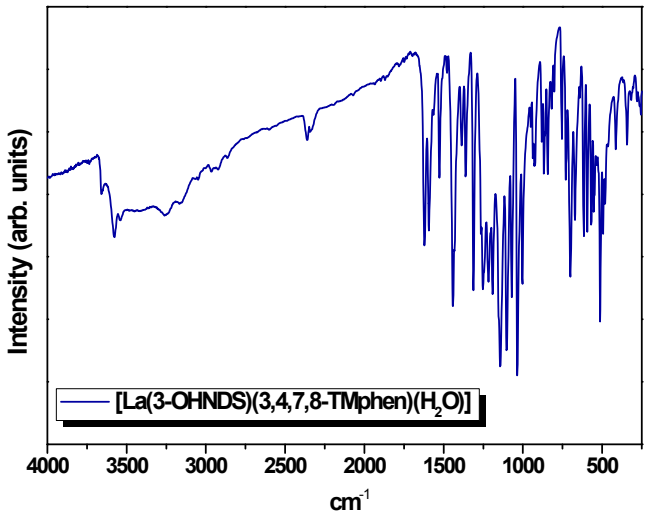



[La(3-OHNDS)(3,4,7,8-TMphen)(H2O)]
-H2O
Decomposition
% Mass Loss
T (°C)
0
10
20
30
40
50
60
70
200
400
600
800
1000

Section S3. IR spectra of [Ln(3-OHNDS)(H_2O)$_2$, [Ln(3-OHNDS)(phen)(H_2O)]·3H_2O and [La(3-OHNDS)(3,4,7,8-TMphen)(H_2O)] compounds.






Intensity (arb. units)
[La(3-OHNDS)(3,4,7,8-TMphen)(H2O)]
4000
3500
3000
2500
2000
1500
1000
500
cm-1

Section S4. Excitation spectrum of the compounds [Ln(3-OHNDS)(H_2O)$_2$where Ln= La (1), Pr(2), Nd(3) and Sm(4); and [Ln(3-OHNDS)(phen)(H_2O)]·3H_2O, where Ln= La(5), Pr(6), Nd(7) and Sm(8).

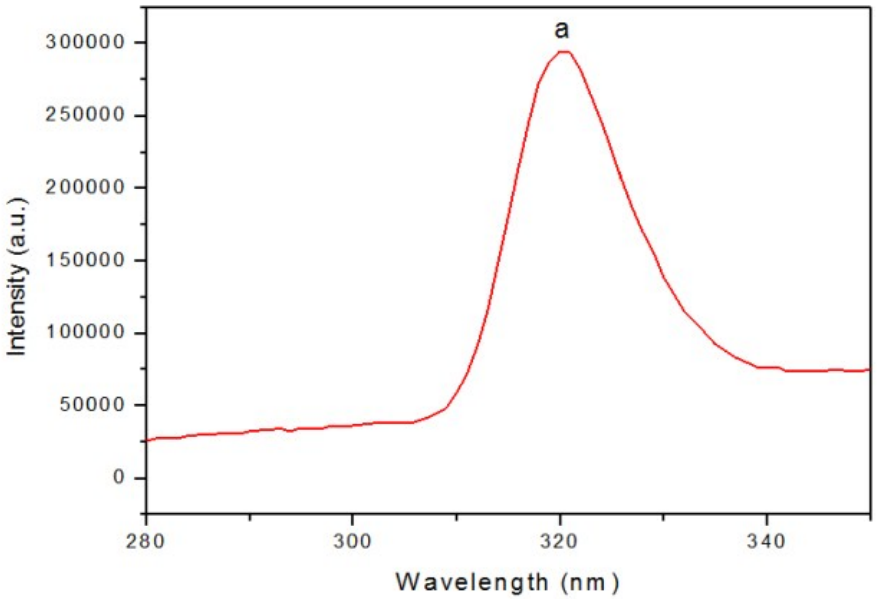


Figure S4.1. Excitation spectrum of compound (1) monitored at 430 nm.

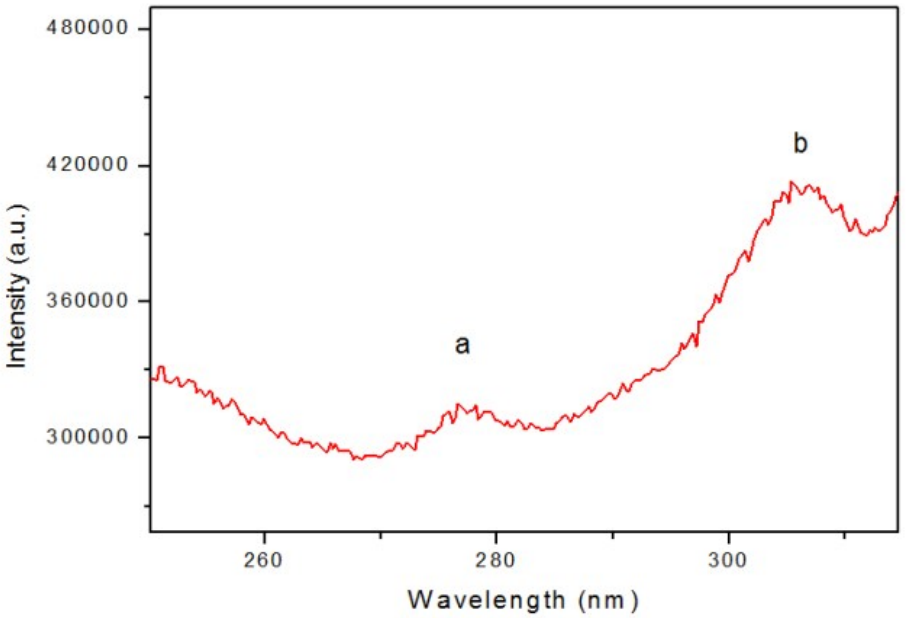


Figure S4.2. Excitation spectrum of compound (5) monitored at 430 nm.

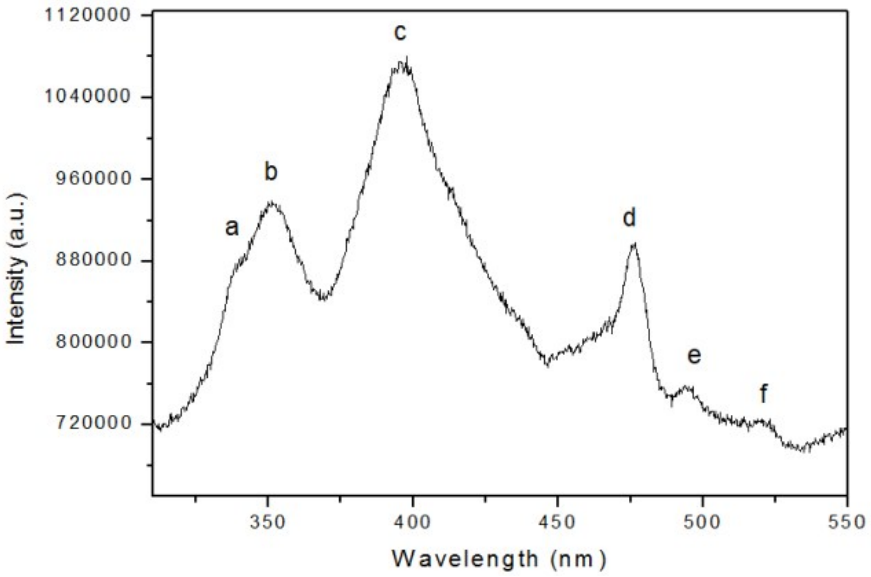


Figure S4.3. Excitation spectrum of compound (2) monitored at 610 nm.

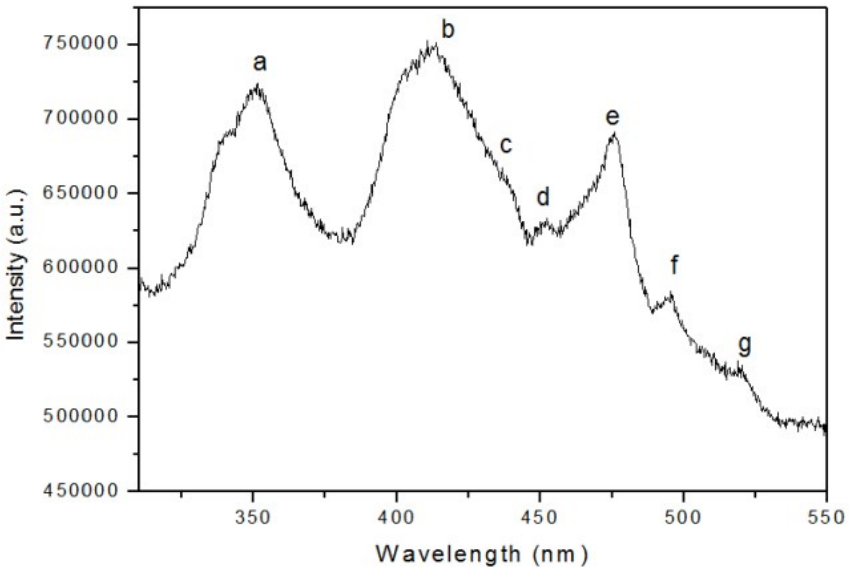


Figure S4.4. Excitation spectrum of compound (6) monitored at 610 nm.

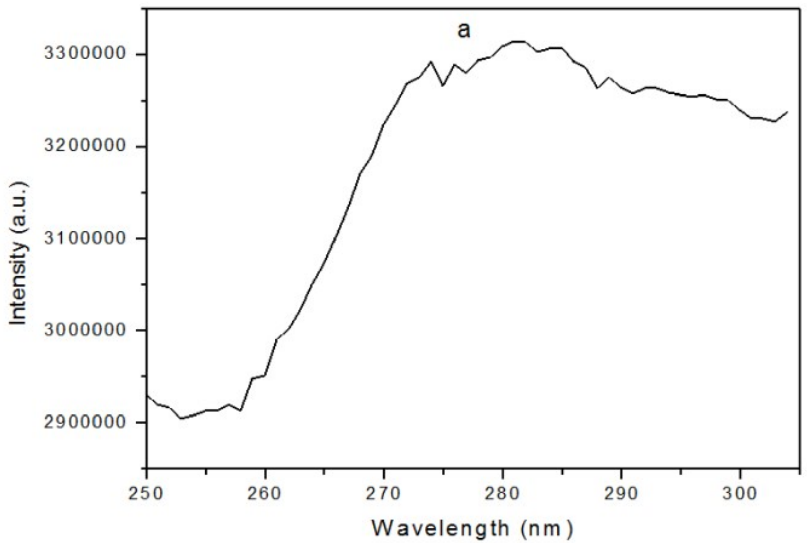


Figure S4.5. Excitation spectrum of compound (3) monitored at 464 nm.

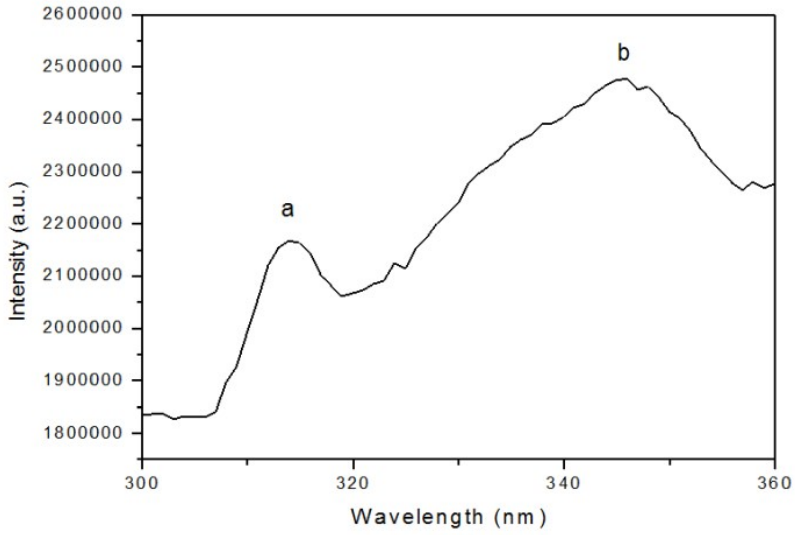


Figure S4.6. Excitation spectrum of compound (7) monitored at 464 nm.

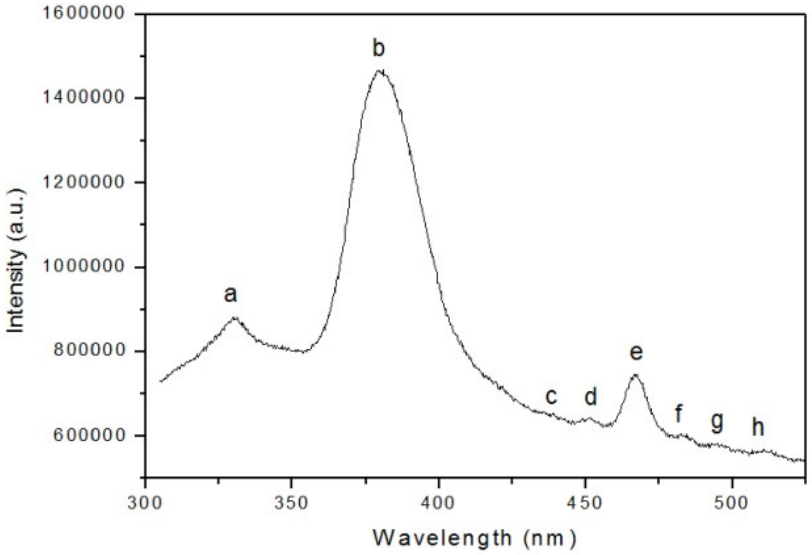


Figure S4.7. Excitation spectrum of compound (4) monitored at 594 nm.

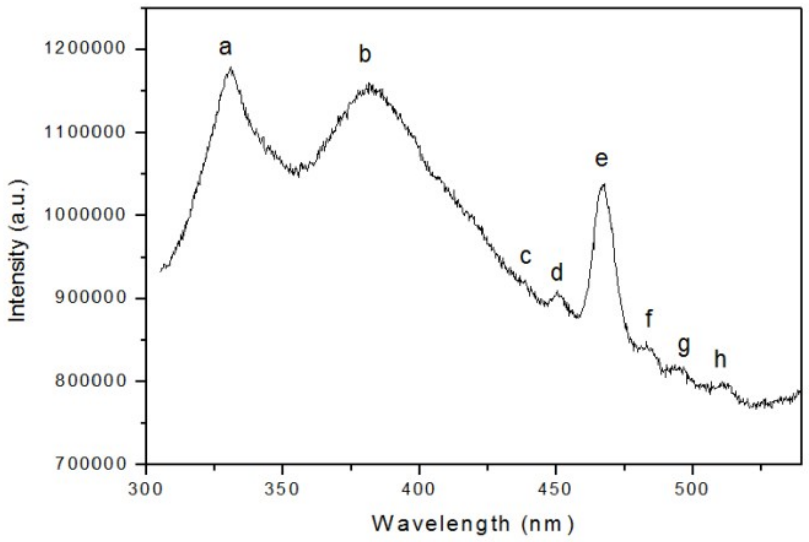


Figure S4.8. Excitation spectrum of compound (8) monitored at 594 nm.

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Section S5. Assignment of the transitions in the excitation and emission spectra of 3-OHNDS and compounds (1)-(8).

Table S1. Assignment of the transitions in the excitation and emission spectra of 3-OHNDS and compounds (1)-(9).

3-OHNDS							
Excitation				Emission			
Label	λ (nm)	Energy (cm^{-1})	Transition	Label	λ (nm)	Energy (cm^{-1})	Transition
a	279.9	35727	π→π* or n→π*	c	379.1	26378	π*→π or π*→n
b	308	32468	π→π* or n→π*	d	415.9	24044	π*→π or π*→n
(1)							
Excitation				Emission			
Label	λ (nm)	Energy (cm^{-1})	Transition	Label	λ (nm)	Energy (cm^{-1})	Transition
a	319.9	31260	π→π* or n→π*	b	431.9	23154	π*→π or π*→n
(2)							
Excitation				Emission			
Label	λ (nm)	Energy (cm^{-1})	Transition	Label	λ (nm)	Energy (cm^{-1})	Transition
a	340.9	29334	π→π* or n→π*	g	449.1	22267	π*→π or π*→n
b	351.4	28458	π→π* or n→π*	h	466	21459	π*→π or π*→n
c	394.9	25323	π→π* or n→π*	i	488.9	20454	$^3P_0 \rightarrow {}^3H_4$
d	476.65	20980	$^3P_1 \leftarrow {}^3H_4$	j	502.4	19904	$^3P_0 \rightarrow {}^3H_5$
e	494.9	20206	$^3P_0 \leftarrow {}^3H_4$	k	529.1	18900	π*→π or π*→n
f	520.9	19198	not assignable	l	586.4	17053	$^1D_2 \rightarrow {}^3H_4$
				m	611.8	16345	$^3P_0 \rightarrow {}^3H_6$
				n	634.3	15765	$^3P_0 \rightarrow {}^3F_2$
				o	684.4	14611	$^1D_2 \rightarrow {}^3H_5$
				p	711	14065	$^3P_0 \rightarrow {}^3F_3$
					728	13736	
(3)							
Excitation				Emission			
Label	λ (nm)	Energy (cm^{-1})	Transition	Label	λ (nm)	Energy (cm^{-1})	Transition
a	280.9	35600	π→π* or n→π*	b	410.7	24349	$^2P_{3/2} \rightarrow {}^4I_{9/2}$
				c	435.9	22941	$^2P_{3/2} \rightarrow {}^4I_{11/2}$
				d	447.9	22326	π*→π or π*→n
				e	464.9	21510	π*→π or π*→n
				f	479.3	20864	π*→π or π*→n
				g	488.4	20475	π*→π or π*→n
				h	507.3	19712	π*→π or π*→n

				i	533.8	18734	$^2G_{7/2}+^4G_{5/2}\rightarrow{}^4I_{9/2}$
				j	559.8	17864	$^2G_{7/2}+^4G_{5/2}\rightarrow{}^4I_{9/2}$
				k	569.3	17565	$^2G_{7/2}+^4G_{5/2}\rightarrow{}^4I_{9/2}$
				l	584.6	17106	$^2G_{7/2}+^4G_{5/2}\rightarrow{}^4I_{9/2}$

(4)

Excitation				Emission			
Label	λ (nm)	Energy (cm^{-1})	Transition	Label	λ (nm)	Energy (cm^{-1})	Transition
a	329.6	30340	π→π* or n→π*	i	449.6	22242	π*→π or π*→n
b	380.6	26274	π→π* or n→π*	j	464.2	21542	π*→π or π*→n
c	434.9	22994	$^4G_{9/2}\leftarrow{}^6H_{5/2}$	k	483.7	20674	π*→π or π*→n
d	450.9	22178	$^4M_{17/2}, {}^4F_{5/2}\leftarrow{}^6H_{5/2}$	l	496.4	20145	π*→π or π*→n
e	466.6	21432	$^4I_{13/2}\leftarrow{}^6H_{5/2}$	m	530.7	18843	π*→π or π*→n
f	483.4	20687	$^4I_{11/2}, {}^4M_{15/2}\leftarrow{}^6H_{5/2}$	n	559	17889	$^4G_{5/2}\rightarrow{}^6H_{5/2}$
g	494.9	20206	$^4I_{9/2}, {}^4G_{7/2}\leftarrow{}^6H_{5/2}$	o	593.9	16838	$^4G_{5/2}\rightarrow{}^6H_{7/3}$
h	511.1	19566	$^4I_{11/2}, \leftarrow{}^6H_{5/2}$	p	639.9	15627	$^4G_{5/2}\rightarrow{}^6H_{9/4}$
				q	687.8	14539	$^4G_{5/2}\rightarrow{}^6H_{11/5}$
				r	708.6	14112	$^4G_{5/2}\rightarrow{}^6H_{11/5}$

(5)

Excitation				Emission			
Label	λ (nm)	Energy (cm^{-1})	Transition	Label	λ (nm)	Energy (cm^{-1})	Transition
a	277.5	36036	π→π* or n→π*	c	430.2	23245	π*→π or π*→n
b	306	32680	π→π* or n→π*				

(6)

Excitation				Emission			
Label	λ (nm)	Energy (cm^{-1})	Transition	Label	λ (nm)	Energy (cm^{-1})	Transition
a	351.4	28458	π→π* or n→π*	h	451.9	22129	π*→π or π*→n
b	413.6	24178	π→π* or n→π*	i	463.8	21561	π*→π or π*→n
c	435.9	22941	π→π* or n→π*	j	476.4	20991	π*→π or π*→n
d	452.4	22104	$^3P_2\leftarrow{}^3H_4$	k	489.7	20421	$^3P_0\rightarrow{}^3H_4$
e	475.6	21026	$^3P_1\leftarrow{}^3H_4$	l	525.9	19015	π*→π or π*→n
f	495.4	20186	$^3P_0\leftarrow{}^3H_4$	m	605.1	16526	$^3P_0\rightarrow{}^3H_6$
g	520.4	19216	not assignable	n	644.4	15518	$^3P_0\rightarrow{}^3F_2$
				o	682.8	14646	$^1D_2\rightarrow{}^3H_5$
				p	714	14006	$^3P_0\rightarrow{}^3F_3$
				q	725	13793	$^3P_0\rightarrow{}^3F_3$

(7)

Excitation				Emission			
Label	λ (nm)	Energy (cm^{-1})	Transition	Label	λ (nm)	Energy (cm^{-1})	Transition
a	313.9	31857	π→π* or n→π*	c	404.9	24697	$^2P_{3/2}\rightarrow{}^4I_{9/2}$

b	345.9	28910	π→π* or n→π*	d	416	24038	$^2P_{3/2}\rightarrow{}^4I_{9/2}$
				e	434.5	23015	$^2P_{3/2}\rightarrow{}^4I_{11/2}$
				f	447	22371	π*→π or π*→n
				g	463.7	21566	π*→π or π*→n
				h	479.3	20864	π*→π or π*→n
				i	488.9	20454	π*→π or π*→n
				j	512.9	19497	π*→π or π*→n
				k	551.2	18142	$^2G_{7/2}+{}^4G_{5/2}\rightarrow{}^4I_{9/2}$
				l	588.9	16981	$^2G_{7/2}+{}^4G_{5/2}\rightarrow{}^4I_{9/2}$

(8)

Excitation

Label	λ (nm)	Energy (cm^{-1})	Transition	Label	λ (nm)	Energy (cm^{-1})	Transition
a	330.9	30221	π→π* or n→π*	i	436.2	22925	π*→π or π*→n
b	382.6	26137	π→π* or n→π*	j	447.3	22356	π*→π or π*→n
c	436.9	22889	$^4G_{9/2}\leftarrow{}^6H_{5/2}$	k	465.4	21487	π*→π or π*→n
d	450.4	22202	$^4M_{17/2}, {}^4F_{5/2}\leftarrow{}^6H_{5/2}$	l	486.4	20559	π*→π or π*→n
e	467.4	21395	$^4I_{13/2}\leftarrow{}^6H_{5/2}$	m	532.7	18772	π*→π or π*→n
f	484.6	20636	$^4I_{11/2}, {}^4M_{15/2}\leftarrow{}^6H_{5/2}$	n	558	17921	$^4G_{5/2}\rightarrow{}^6H_{5/2}$
g	496.9	20125	$^4I_{9/2}, {}^4G_{7/2}\leftarrow{}^6H_{5/2}$	o	594.9	16810	$^4G_{5/2}\rightarrow{}^6H_{7/3}$
h	511.6	19547	$^4I_{11/2}, \leftarrow{}^6H_{5/2}$	p	639.7	15632	$^4G_{5/2}\rightarrow{}^6H_{9/4}$
				q	685.6	14586	$^4G_{5/2}\rightarrow{}^6H_{11/5}$
				r	708	14124	$^4G_{5/2}\rightarrow{}^6H_{11/5}$

Section S6. Luminescence decay traces for compounds (1)-(8).

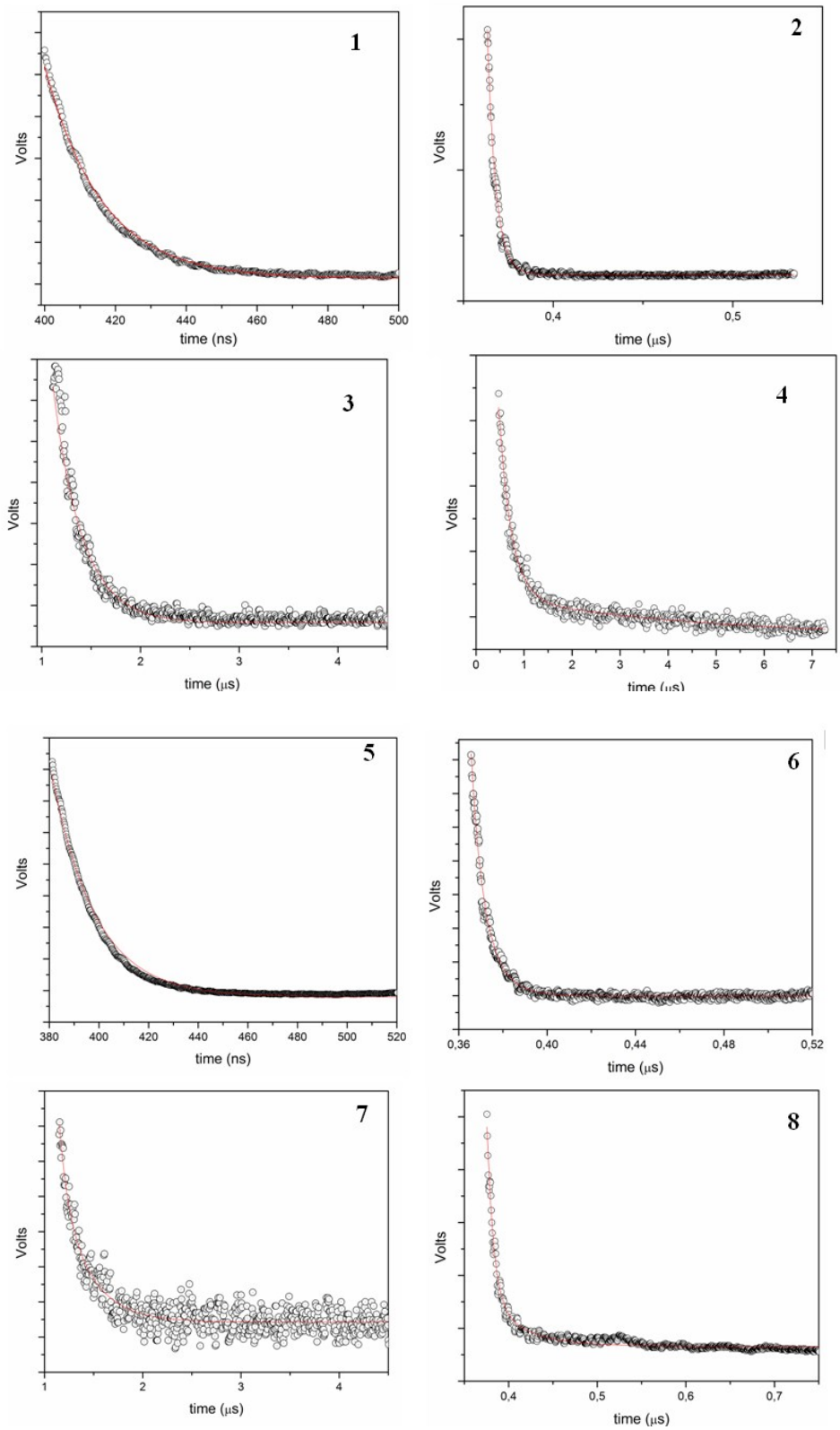

Figure S6.1. Luminescence decay traces for compounds 1-8. The red line is an exponential fit to the data.

Section S7. CIE coordinates and color emission of 3-OHNDS y (1)-(8) compounds.

Table S2. (x,y) CIE coordinates and color emission of 3-OHNDS y (1)-(8) compounds.

	CIE coordinates		Color emission
	x	y	
3-OHNDS	0.14	0.1	blue
1	0.15	0.06	bluish purple
2	0.18	0.26	greenish blue
3	0.26	0.36	bluegreen
4	0.33	0.28	purplish pink
5	0.17	0.11	blue
6	0.27	0.36	bluish green
7	0.22	0.30	bluegreen
8	0.31	0.32	white

Section S8. Squeeze results.

A disordered solvent molecule was identified in the final stages of refinement for the compounds (1)-(4) and (9). This highly disordered region of the asymmetric unit was treated by application of the of the program Squeeze as implemented in Platon which allows for the mathematical compensation of the electron contribution of disordered solvent contained in the voids to the calculated diffraction intensities. The disordered solvent (water molecules) was treated as a diffuse contribution to the scattering without specific atomic coordinates by PLATON/SQUEEZE as is shown in the Table S3.

Table S3. Squeeze located voids, coordinates, volume and content for compounds (1)-(4) and (9).

Compound	**Coordinates x,y,z**	**Volume**	**Electrons**	**No. Water molecules**
(1)	0.000,0.500, -0.013	131	26	3.25
	0.000,0.500, -0.013	131	26	3.25
(2)	0.000, 0.500,-0.015	130	24	3
	0.500, 0.000, 0.001	130	24	3
(3)	0.000, 0.500, -0.015	130	20	2.5
	0.500, 1.000, 0.009	130	20	2.5
(4)	0.000, 0.500, -0.017	149	15	1.9
	0.500, 1.000, 0.036	149	15	1.9
(9)	0.000, 0.000, 0.500	120	30	3.8
	0.500, 0.500, 0.000	120	30	3.8