

SUPPORTING INFORMATION

High brightness and easy color modulation in lanthanide-based coordination polymers with 5-methoxyisophthalate as ligand: Toward emission colors additive strategy

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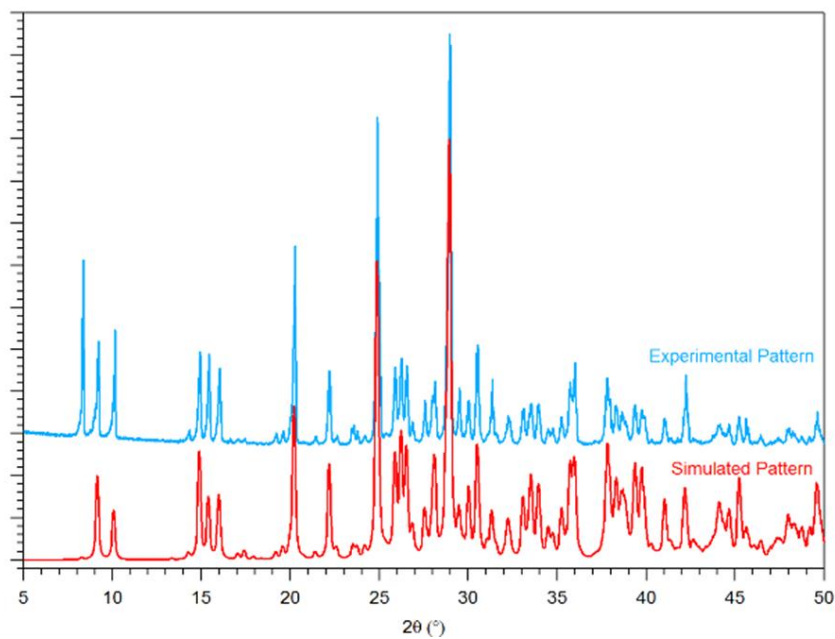
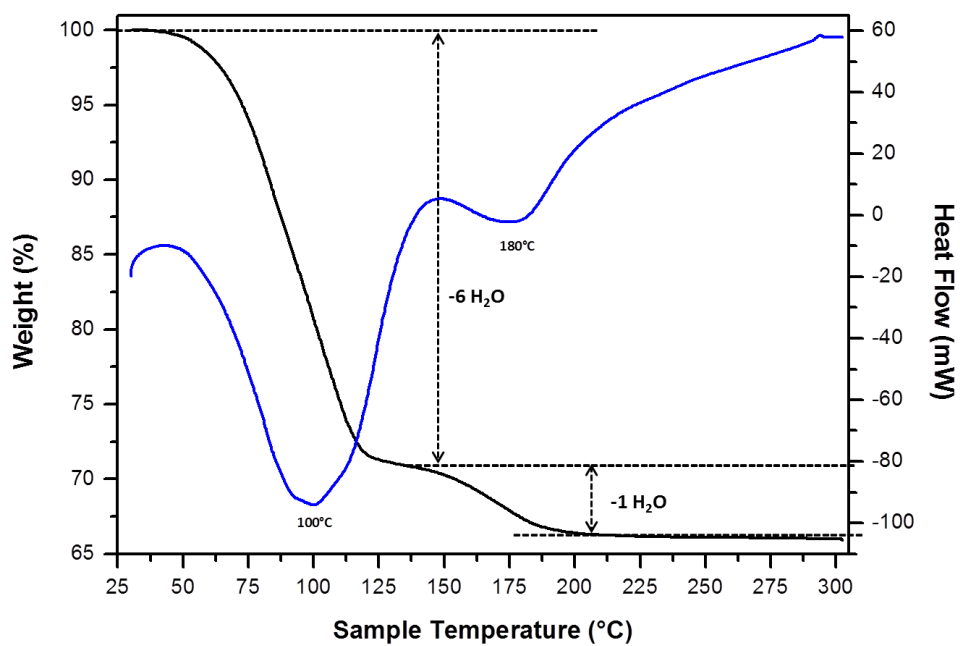


Figure S1. Experimental and simulated (on the basis of the crystal structure) powder X-ray diffraction patterns of $\text{Na}_2(\text{mip}) \cdot 7\text{H}_2\text{O}$.



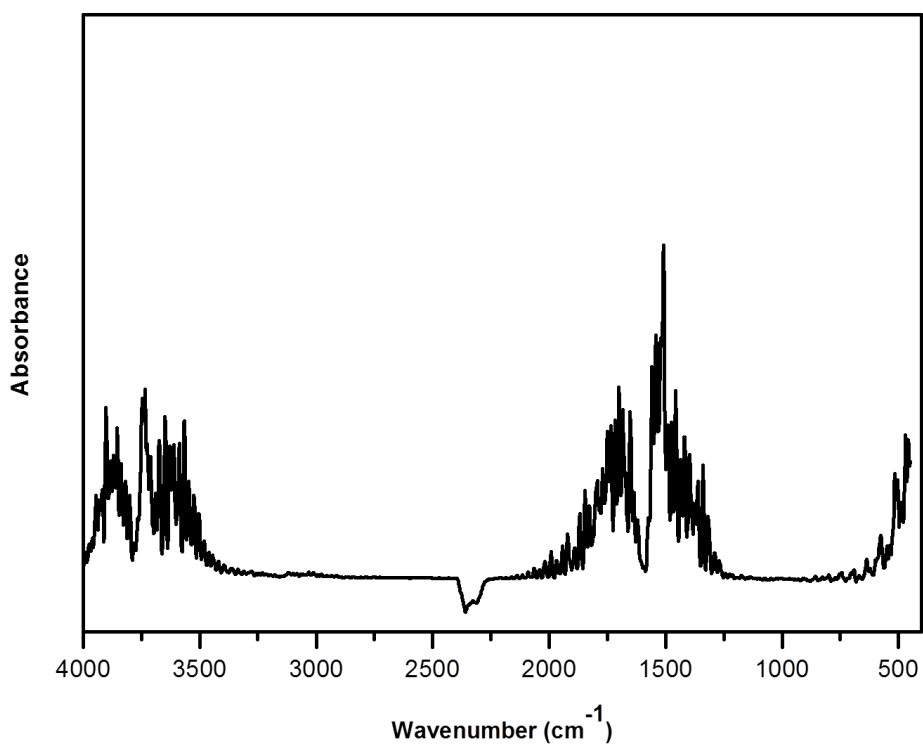
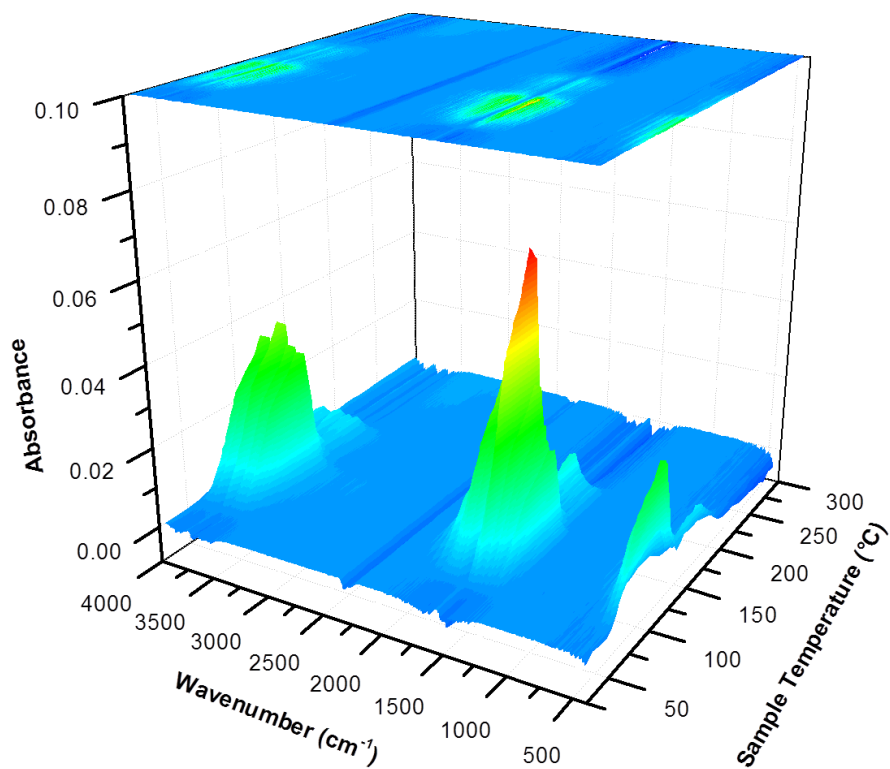


Figure S2. Top: ATG/DSC of Na₂(mip)·7H₂O between room temperature and 300°C under N₂ flux. Middle: IR spectra of the exhausted gas during thermal analyses versus temperature. Bottom: IR spectrum recorded at T=90°C.

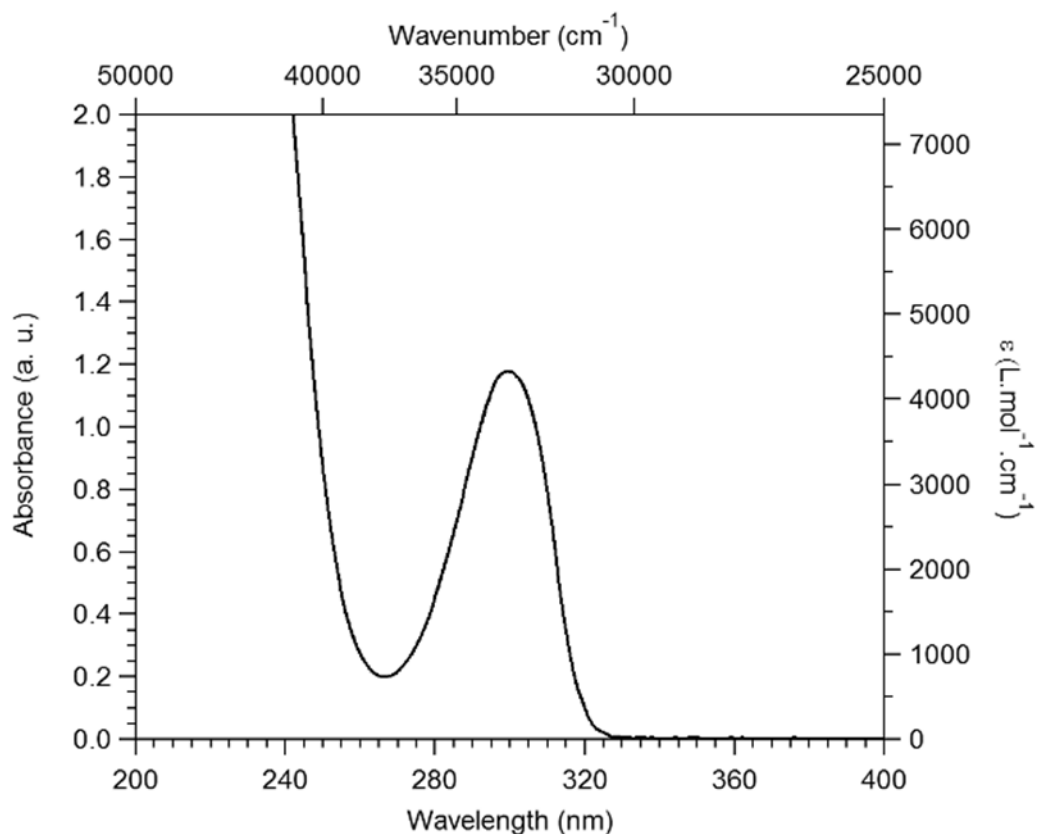


Figure S3. Liquid state UV-visible absorption spectrum of a diluted ($2.73 \cdot 10^{-4} \text{ mol.L}^{-1}$) aqueous solution of $\text{Na}_2(\text{mip}) \cdot 7\text{H}_2\text{O}$

Table S1. Chemical analyzes for compounds that constitute families (1) and (2).

Chemical formula	MW (g.mol^{-1})	%C		%H		%O		%Ln	
		calc.	(found)	calc.	(found)	calc.	(found)	calc.	(found)
$[\text{La}(\text{mip})(\text{Hmip})(\text{H}_2\text{O})_5 \cdot \text{H}_2\text{O}]_\infty$	635.9	34.0	(34.2)	3.9	(4.1)	40.3	(40.1)	21.8	(21.6)
$[\text{Ce}(\text{mip})(\text{Hmip})(\text{H}_2\text{O})_5 \cdot \text{H}_2\text{O}]_\infty$	637.1	33.9	(33.9)	3.9	(3.8)	40.2	(40.3)	22.0	(22.0)
$[\text{Sm}_2(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	1098.8	29.5	(29.4)	3.8	(3.6)	39.3	(39.5)	27.4	(27.5)
$[\text{Eu}_2(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	1102.0	29.4	(29.6)	3.8	(3.4)	39.2	(39.4)	27.6	(27.6)
$[\text{Gd}_2(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	1112.6	29.1	(29.4)	3.8	(3.5)	38.8	(38.4)	28.3	(28.7)
$[\text{Tb}_2(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	1115.8	29.0	(29.1)	3.8	(3.5)	38.7	(38.4)	28.5	(29.0)
$[\text{Dy}_2(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	1123.0	28.9	(28.9)	3.7	(3.3)	38.5	(39.0)	28.9	(28.8)
$[\text{Ho}_2(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	1127.8	28.7	(28.9)	3.7	(3.4)	38.3	(38.3)	29.2	(29.4)
$[\text{Er}_2(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	1132.6	28.6	(28.5)	3.7	(3.4)	38.1	(38.2)	29.5	(29.9)
$[\text{Y}_2(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	975.8	33.2	(33.1)	4.3	(4.4)	44.3	(44.2)	18.2	(18.3)

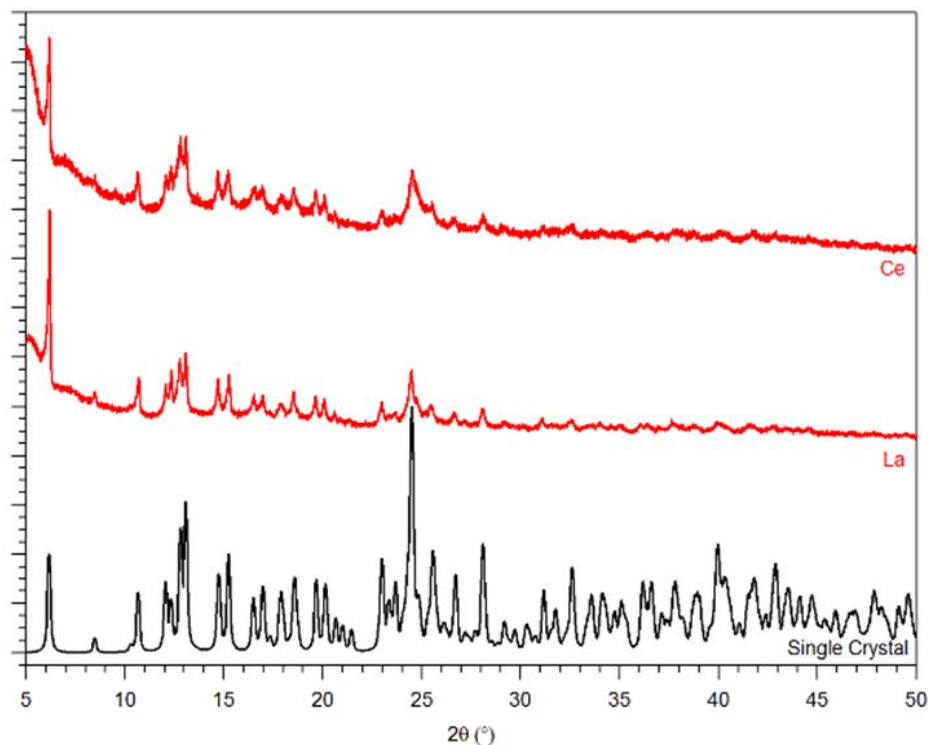


Figure S4. Experimental and simulated powder X-ray diffraction patterns of compounds with general chemical formula $[\text{Ln}(\text{mip})(\text{Hmip})(\text{H}_2\text{O})_5 \cdot \text{H}_2\text{O}]_\infty$ with Ln = La or Ce. Simulated diagram has been drawn on the basis of the corresponding crystal structure.

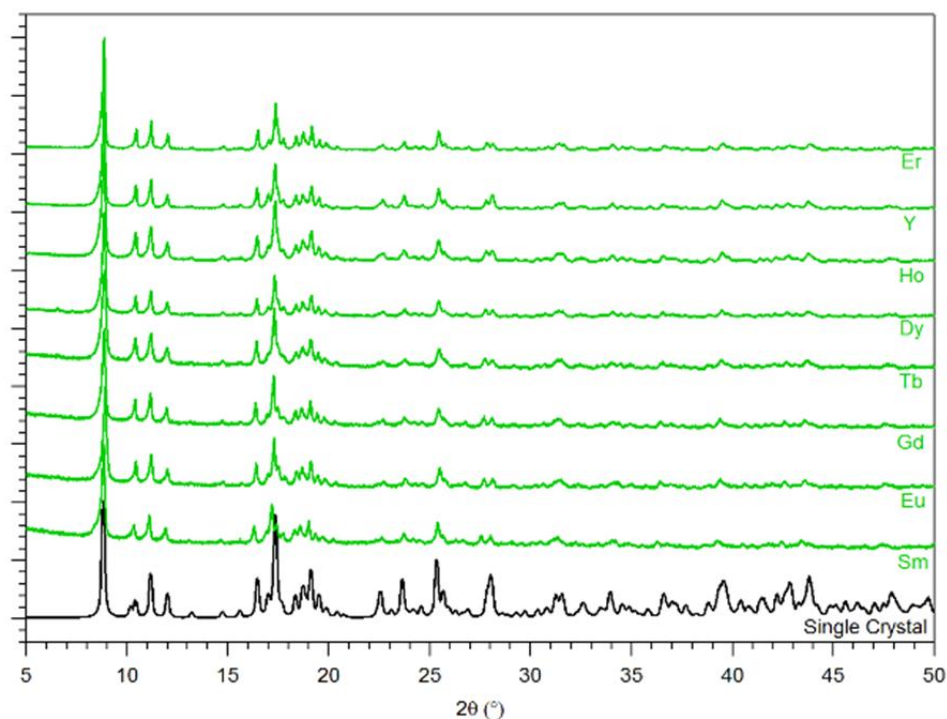


Figure S5. Experimental and simulated powder X-ray diffraction patterns of compounds that have general chemical formula $[\text{Ln}_2(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$ with Ln = Sm-Er plus Y. Simulated diagram has been drawn on the basis of the corresponding crystal structure.

Table S2. Continuous Shape Measurements (CSM) performed on the Ce center of $[\text{Ce}(\text{mip})_{3/2}(\text{H}_2\text{O})_5 \cdot 2\text{H}_2\text{O}]_\infty$.

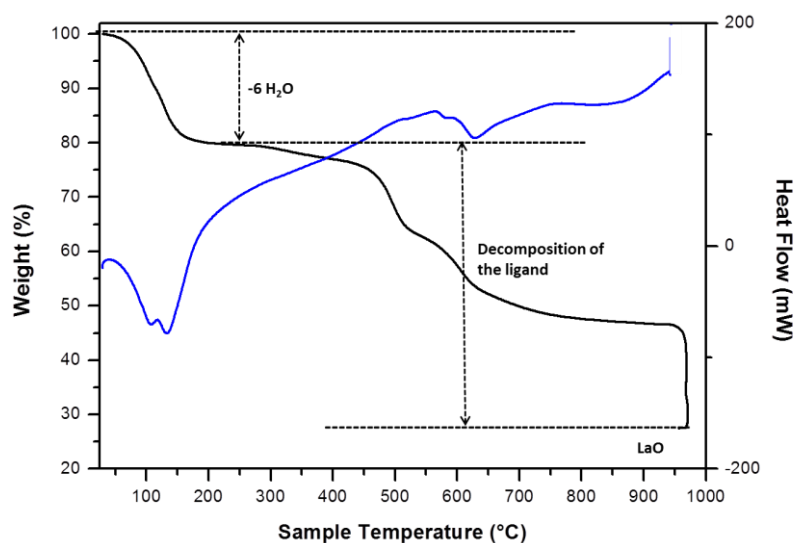
Atom label	Ce1
Lowest CSM value	1.709
Associated polyhedron, site symmetry	Muffin, C_s
2 nd lowest CSM value	2.605
Associated polyhedron, site symmetry	Capped square antiprism, C_{4v}
3 rd lowest CSM value	2.765
Associated polyhedron, site symmetry	Tricapped trigonal prism, D_{3h}

Lowest values indicates best agreement to theoretical coordination polyhedra symmetry (whose CSM = 0.000).

Table S3. Continuous Shape Measurements (CSM) performed on the Gd center of $[\text{Gd}(\text{mip})(\text{Hmip})(\text{H}_2\text{O})_5 \cdot \text{H}_2\text{O}]_\infty$.

Atom label	Gd
Lowest CSM value	0.644
Associated polyhedron, site symmetry	Capped square antiprism, C_{4v}
2 nd lowest CSM value	1.134
Associated polyhedron, site symmetry	Muffin, C_s
3 rd lowest CSM value	1.604
Associated polyhedron, site symmetry	Tricapped trigonal prism, D_{3h}

Lowest values indicates best agreement to theoretical coordination polyhedra symmetry (whose CSM = 0.000).



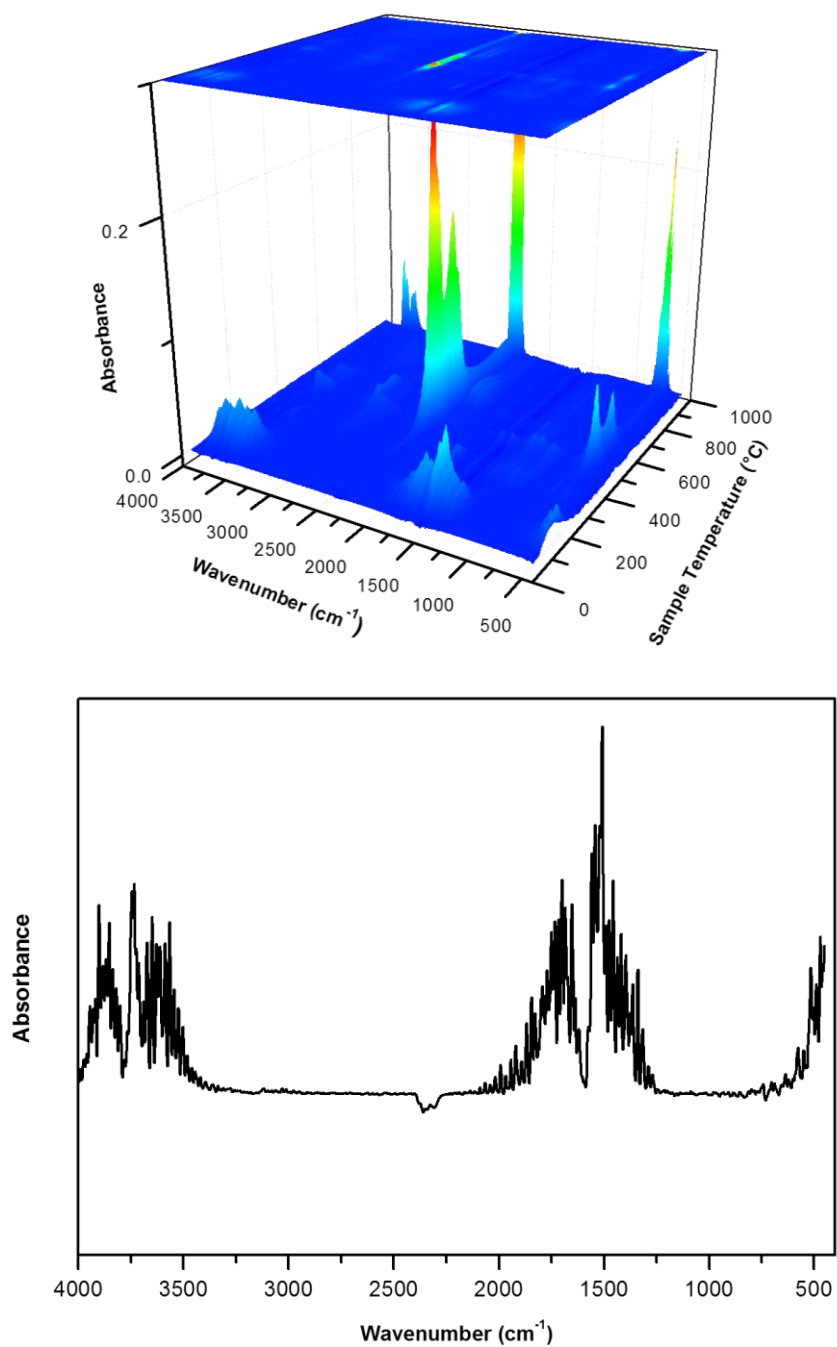


Figure S6. Top: ATG/DSC of $[\text{La}(\text{mip})(\text{Hmip})(\text{H}_2\text{O})_5]\cdot\text{H}_2\text{O}]_\infty$. Middle: IR spectra versus temperature of the exhausted gas during thermal analysis. Bottom: IR spectrum recorded at 90°C.

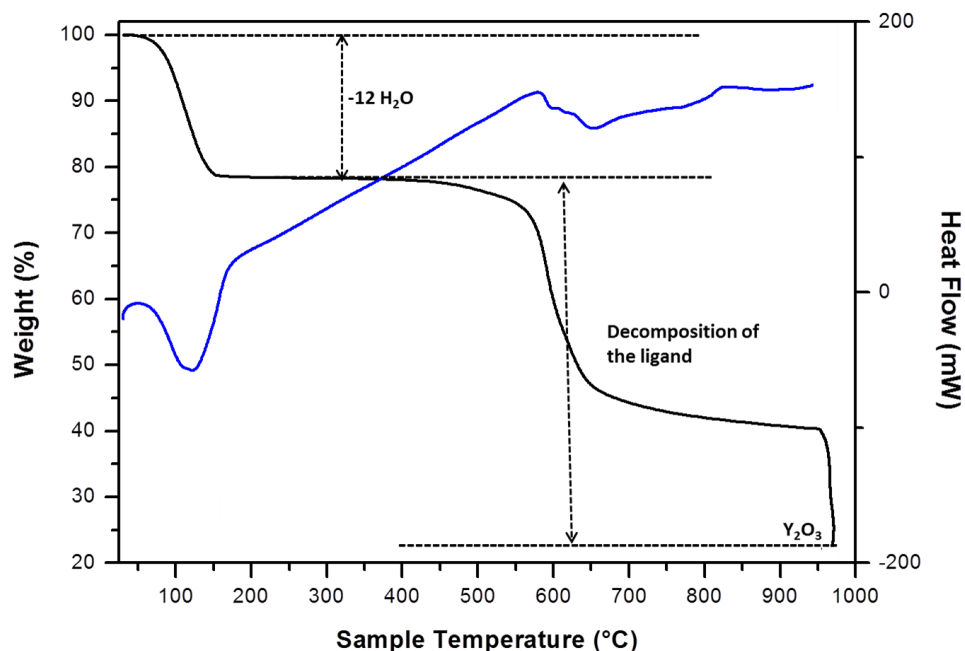
Table S4. Continuous Shape Measurements (CSM) performed on the Y centers of $[\text{Ln}_2(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$

Atom label	Y1	Y2
Lowest CSM value	2.099	2.034
Associated polyhedron, site symmetry	Capped square antiprism, C_{4v}	Capped square antiprism, C_{4v}
2 nd lowest CSM value	2.130	2.042
Associated polyhedron, site symmetry	Muffin, C_s	Muffin, C_s
3 rd lowest CSM value	2.815	2.675
Associated polyhedron, site symmetry	Tricapped trigonal prism, D_{3h}	Tricapped trigonal prism, D_{3h}

Lowest values indicates best agreement to theoretical coordination polyhedra symmetry (whose CSM = 0.000).

Table S5. Selected hydrogen-bond distances in $[\text{Y}_2(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$.

Atom 1	Atom2	Symmetry	Distance (Å)
O027	O032	2-x, 1-y, 1-z	2.7077(2)
O006	O015	x, y, z	2.7519(1)
O005	O015	x, y, z	2.7683(1)
O007	O026	2-x, 1-y, 1-z	2.7930(2)
O007	O011	x, y, z	2.8049(1)
O023	O032	2.5-x, -0.5+y, 1.5-z	2.8355(1)
O006	O018	x, y, z	2.8877(2)
O007	O021	x, y, z	2.9090(2)
O027	O027	2-x, 1-y, 1-z	2.9118(2)
O021	O028	2.5-x, -0.5+y, 1.5-z	3.0292(2)
O015	O032	2.5-x, -0.5+y, 0.5-z	3.4510(2)
O023	O028	2.5-x, -0.5+y, 1.5-z	3.5923(2)



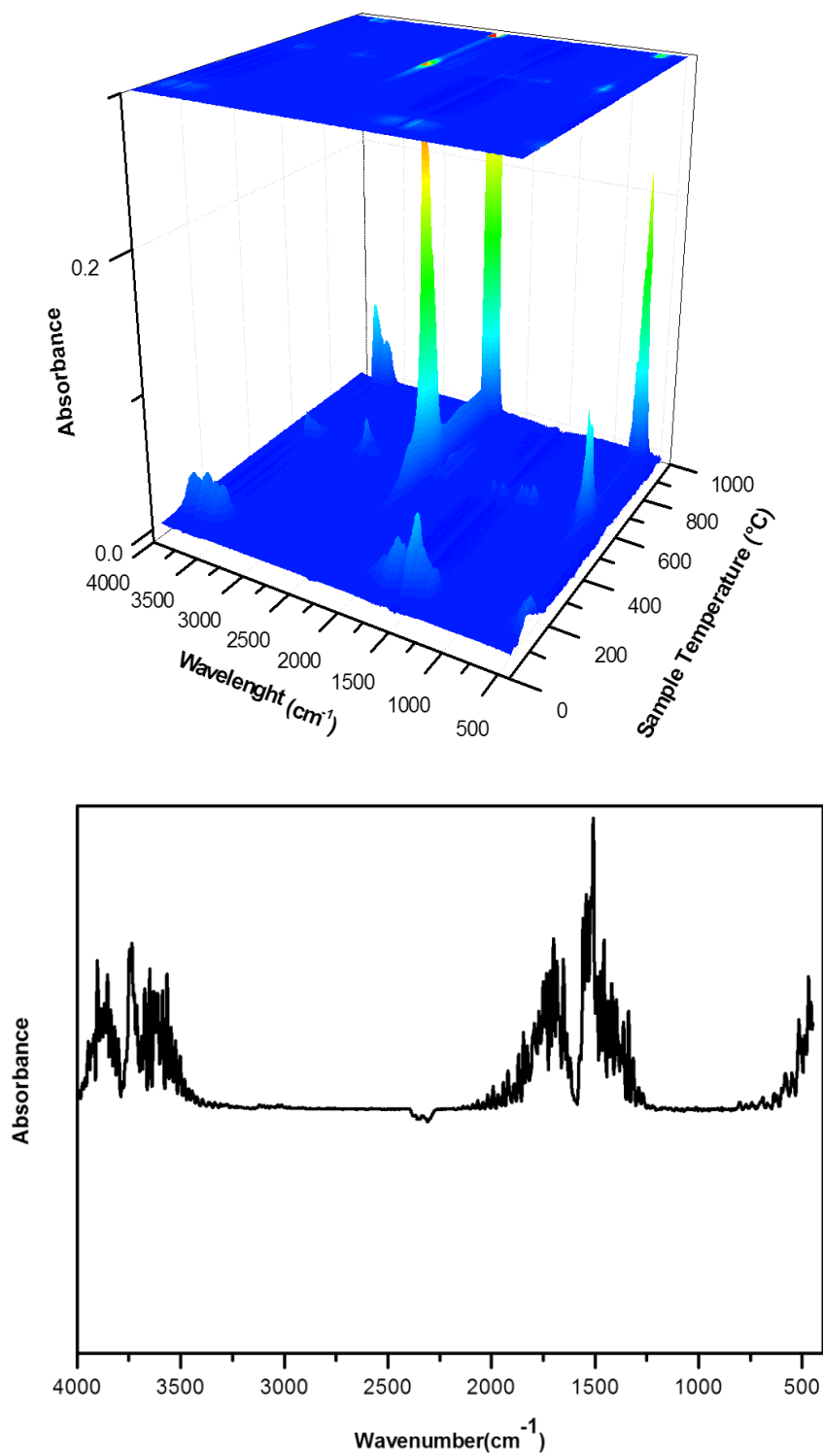


Figure S7. Top: ATG/DSC of $[\text{Y}_2(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$. Middle: IR spectra versus temperature of the exhausted gas during thermal analysis. Bottom: IR spectrum recorded at 90°C.

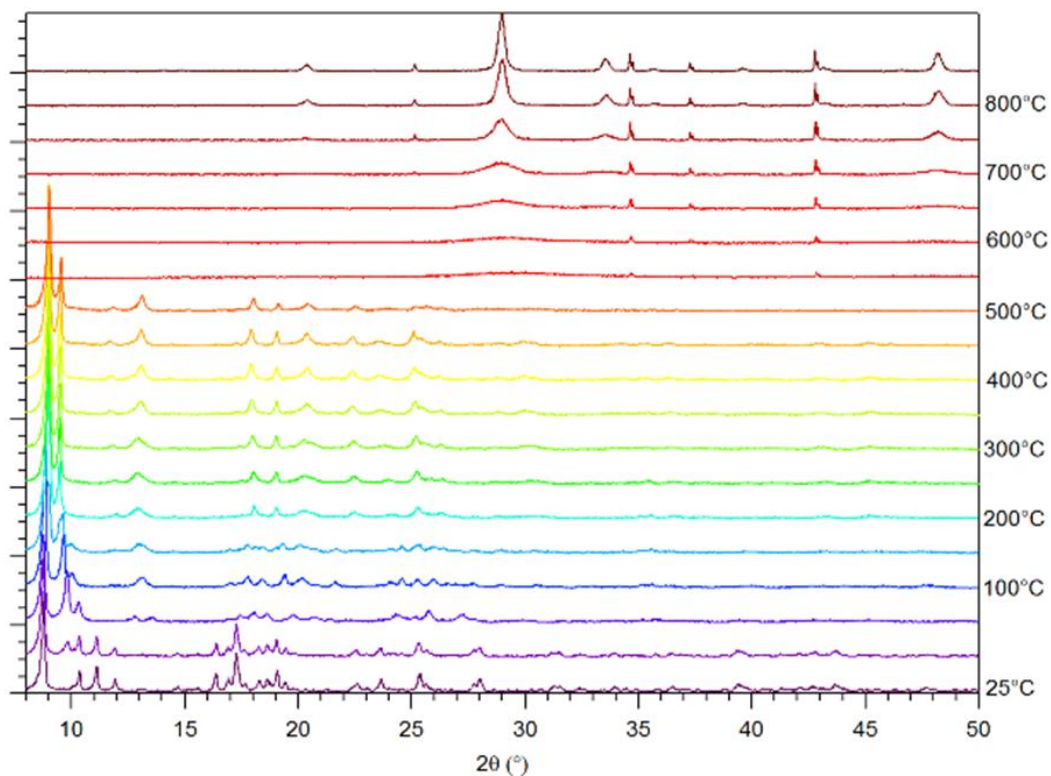


Figure S8. Thermo-dependent powder X-ray diffraction patterns of $[\text{Y}_2(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$.

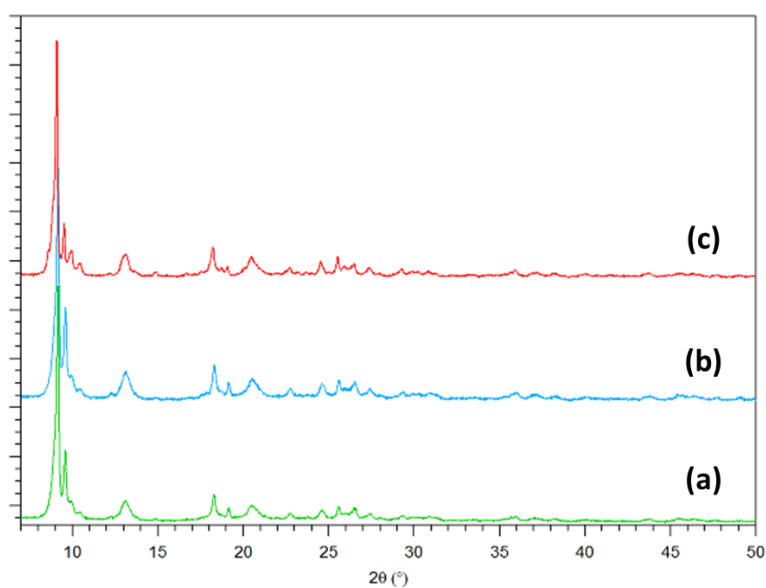


Figure S9. Powder X-ray diffraction patterns of $[\text{Y}_2(\text{mip})_3]_\infty$: (a) as obtained by dehydration at 200°C ; (b) after exposure to ambient air ; (c) after immersion in water.

Table S6. Numerical values for colorimetric coordinates and luminance of $\text{Na}_2(\text{mip})\cdot 7\text{H}_2\text{O}$ and $[\text{Ln}_2(\text{mip})_3(\text{H}_2\text{O})_8\cdot 4\text{H}_2\text{O}]_\infty$ with Ln = Sm-Dy under UV excitation ($\lambda_{\text{exc}} = 312 \text{ nm}$).

	Colorimetric coordinates		Luminance ($\text{Cd}\cdot\text{m}^{-2}$)
	x	y	
$\text{Na}_2(\text{mip})\cdot 7\text{H}_2\text{O}$	0.200(5)	0.144(5)	-
$[\text{Sm}_2(\text{mip})_3(\text{H}_2\text{O})_8\cdot 4\text{H}_2\text{O}]_\infty$	0.430(5)	0.264(5)	0.35(5)
$[\text{Eu}_2(\text{mip})_3(\text{H}_2\text{O})_8\cdot 4\text{H}_2\text{O}]_\infty$	0.681(5)	0.319(5)	3.3(1)
$[\text{Gd}_2(\text{mip})_3(\text{H}_2\text{O})_8\cdot 4\text{H}_2\text{O}]_\infty$	0.221(5)	0.140(5)	0.62(5)
$[\text{Tb}_2(\text{mip})_3(\text{H}_2\text{O})_8\cdot 4\text{H}_2\text{O}]_\infty$	0.321(5)	0.616(5)	107(5)
$[\text{Dy}_2(\text{mip})_3(\text{H}_2\text{O})_8\cdot 4\text{H}_2\text{O}]_\infty$	0.371(5)	0.387(5)	1.7(2)

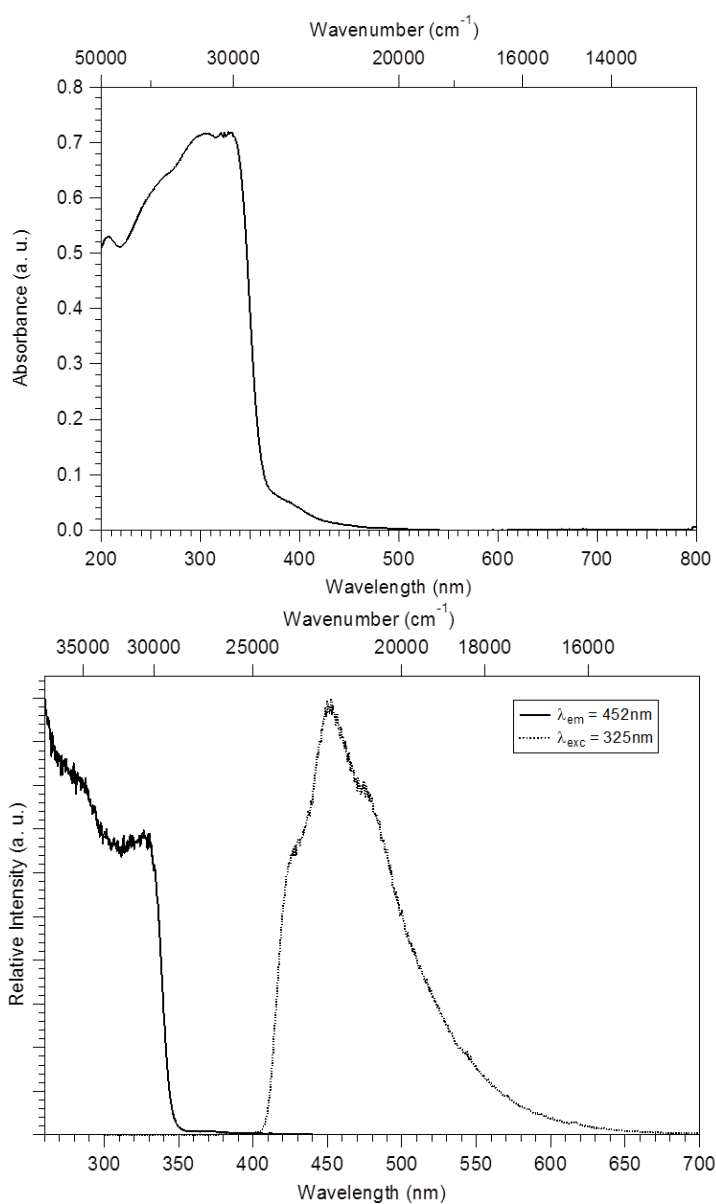


Figure S10. Top: Solid state UV-vis absorption spectrum of $[\text{Gd}_2(\text{mip})_3(\text{H}_2\text{O})_8\cdot 4\text{H}_2\text{O}]_\infty$. Bottom: Solid state excitation and emission spectra recorded at 77K of $[\text{Gd}_2(\text{mip})_3(\text{H}_2\text{O})_8\cdot 4\text{H}_2\text{O}]_\infty$.

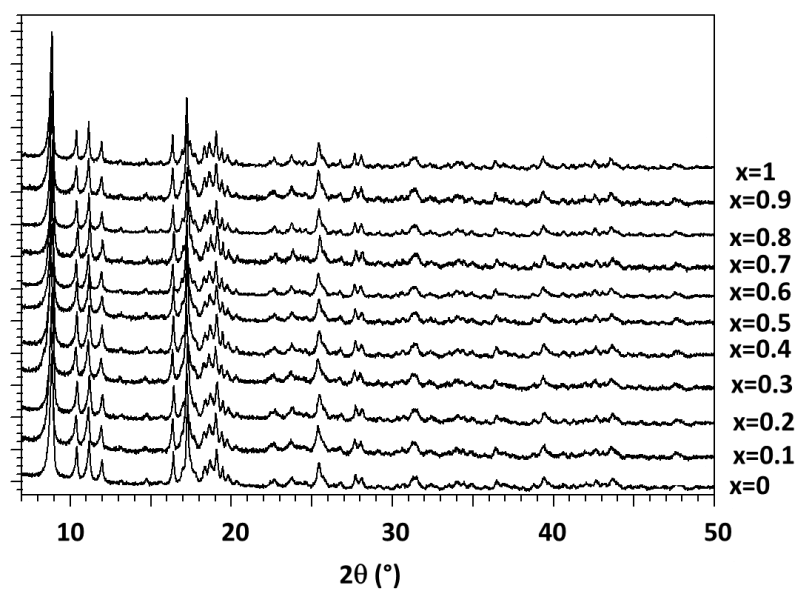


Figure S11. Powder diffraction diagrams of $[\text{Tb}_{2-2x}\text{Gd}_{2x}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_{\infty}$ with $0 \leq x \leq 1$.

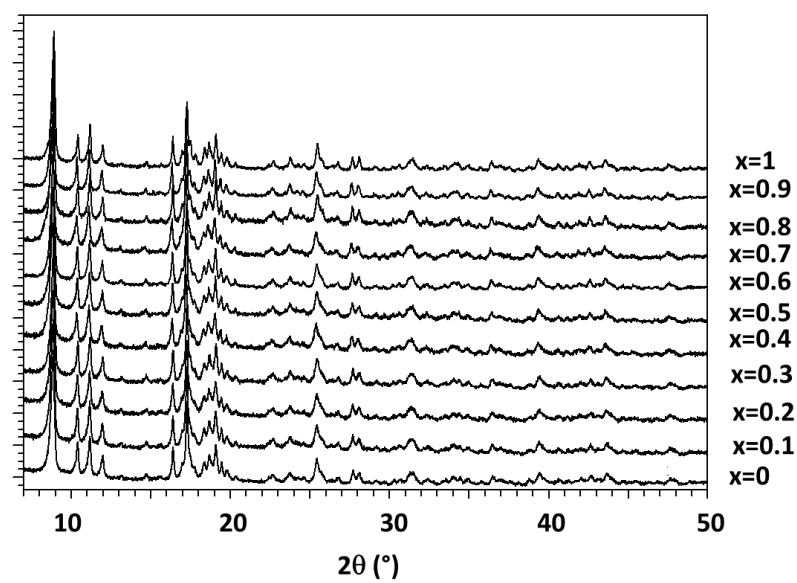


Figure S12. Powder diffraction diagrams of $[\text{Tb}_{2-2x}\text{Eu}_{2x}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_{\infty}$ with $0 \leq x \leq 1$.

Table S7. Metallic contents measured by EDS for $[\text{Tb}_{2-2x}\text{Gd}_{2x}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$ with $0 < x < 1$

	Expected ratios		Measured ratios	
	%Gd	%Tb	%Gd	%Tb
$[\text{Tb}_{1.8}\text{Gd}_{0.2}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	10	90	12(1)	88(1)
$[\text{Tb}_{1.6}\text{Gd}_{0.4}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	20	80	23(1)	77(1)
$[\text{Tb}_{1.4}\text{Gd}_{0.6}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	30	70	34(1)	66(1)
$[\text{Tb}_{1.2}\text{Gd}_{0.8}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	40	60	43(1)	57(1)
$[\text{Tb}_{1.0}\text{Gd}_{1.0}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	50	50	55(1)	45(1)
$[\text{Tb}_{0.8}\text{Gd}_{1.2}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	60	40	65(1)	35(1)
$[\text{Tb}_{0.6}\text{Gd}_{1.4}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	70	30	73(1)	27(1)
$[\text{Tb}_{0.4}\text{Gd}_{1.6}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	80	20	82(1)	18(1)
$[\text{Tb}_{0.2}\text{Gd}_{1.8}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	90	10	93(1)	7(1)

Table S8. Metallic contents measured by EDS for $[\text{Tb}_{2-2x}\text{Eu}_{2x}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$ with $0 < x < 1$

	Expected ratios		Measured ratios	
	%Eu	%Tb	%Eu	%Tb
$[\text{Tb}_{1.8}\text{Eu}_{0.2}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	10	90	10(1)	90(1)
$[\text{Tb}_{1.6}\text{Eu}_{0.4}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	20	80	22(1)	78(1)
$[\text{Tb}_{1.4}\text{Eu}_{0.6}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	30	70	33(1)	67(1)
$[\text{Tb}_{1.2}\text{Eu}_{0.8}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	40	60	44(1)	56(1)
$[\text{Tb}_{1.0}\text{Eu}_{1.0}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	50	50	54(1)	46(1)
$[\text{Tb}_{0.8}\text{Eu}_{1.2}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	60	40	64(1)	36(1)
$[\text{Tb}_{0.6}\text{Eu}_{1.4}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	70	30	74(1)	26(1)
$[\text{Tb}_{0.4}\text{Eu}_{1.6}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	80	20	82(1)	18(1)
$[\text{Tb}_{0.2}\text{Eu}_{1.8}(\text{mip})_3(\text{H}_2\text{O})_8 \cdot 4\text{H}_2\text{O}]_\infty$	90	10	91(1)	9(1)