Electronic Supplementary Material (ESI) for RSC Advances.

Lanthanide contraction effect and white-emitting luminescence in a series of metal-organic frameworks based on 2, 5-pyrazindicarboxylic acid

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Table S1. Crystal data and structure refinement for 1La and 2Y.

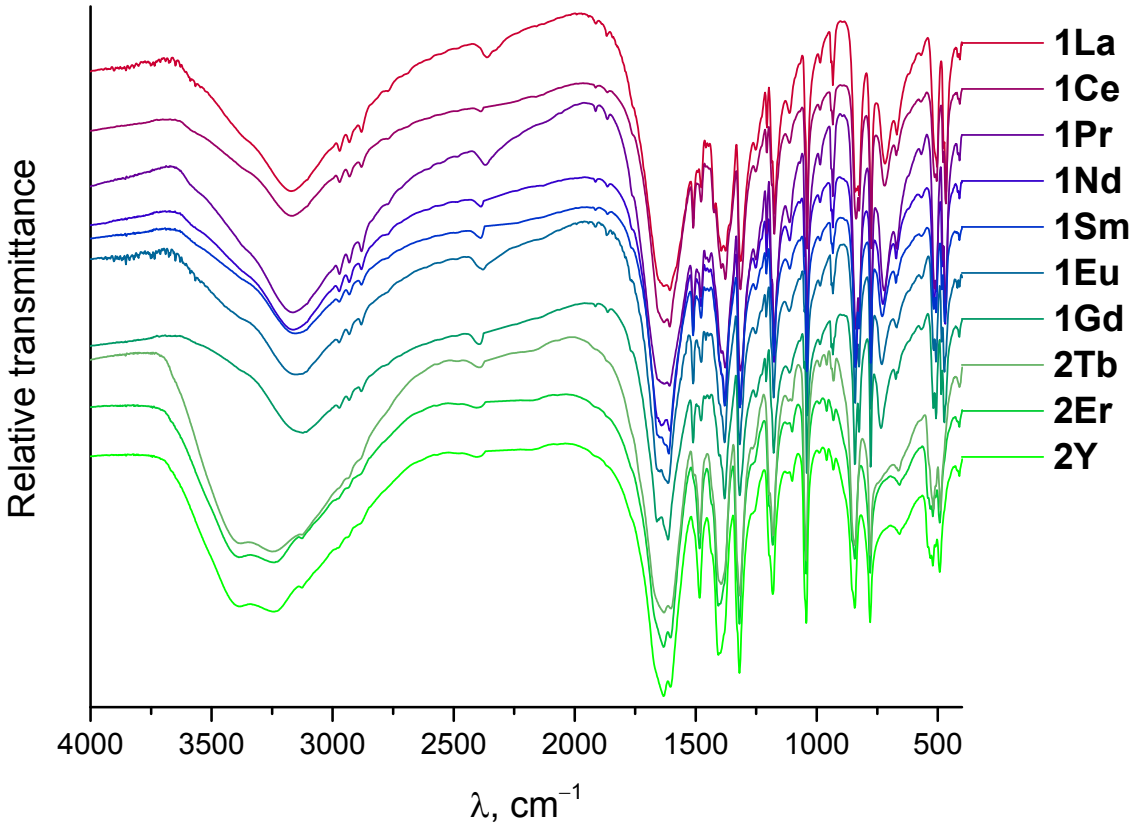
	1La	**2Y**
Formula	$C_{28}H_{28}La_2N_8O_{16}$	$C_{23}H_{33}N_7O_{22}Y_2$
Formula weight	1010.40	937.38
Crystal system	Monoclinic	Triclinic
Space group	$P\,2_1/c$	$P\,-1$
***a*, Å**	6.1241(2)	6.0453(2)
***b*, Å**	12.8424(3)	12.6860(5)
***c*, Å**	20.6476(4)	13.2051(5)
***α*, °**	90	62.174(4)
***β*, °**	90.852(2)	86.835(3)
***γ*, °**	90	87.582(3)
Z	2	1
***V*, Å^3**	1623.72(7)	894.09(6)
***θ* range, °**	3.72 − 29.47	3.64 − 29.33
Crystal size, mm	0.27 × 0.11 × 0.07	0.11 × 0.10 × 0.06
***D*$_c$, g cm^{-3}**	2.067	1.741
***μ*, mm^{-1}**	2.687	3.326
Reflections collected/ unique	7395 / 2963	7032 / 4170
Reflections with $I > 2\sigma(I)$	2724	3683
R_{int}	0.0239	0.0296
GOF on F^2	1.097	1.065
R_1, wR_1 [$I > 2\sigma(I)$]	0.0285, 0.0685	0.0378, 0.0871
R_2, wR_2 (all data)	0.0322, 0.0700	0.0449, 0.0896
$\Delta\rho_{max}$/ $\Delta\rho_{min}$,eÅ^{-3}	2.496 / −0.731	1.041 / −0.521

Table S2. List of selected bond distances and bond angles for 1La and 2Y.

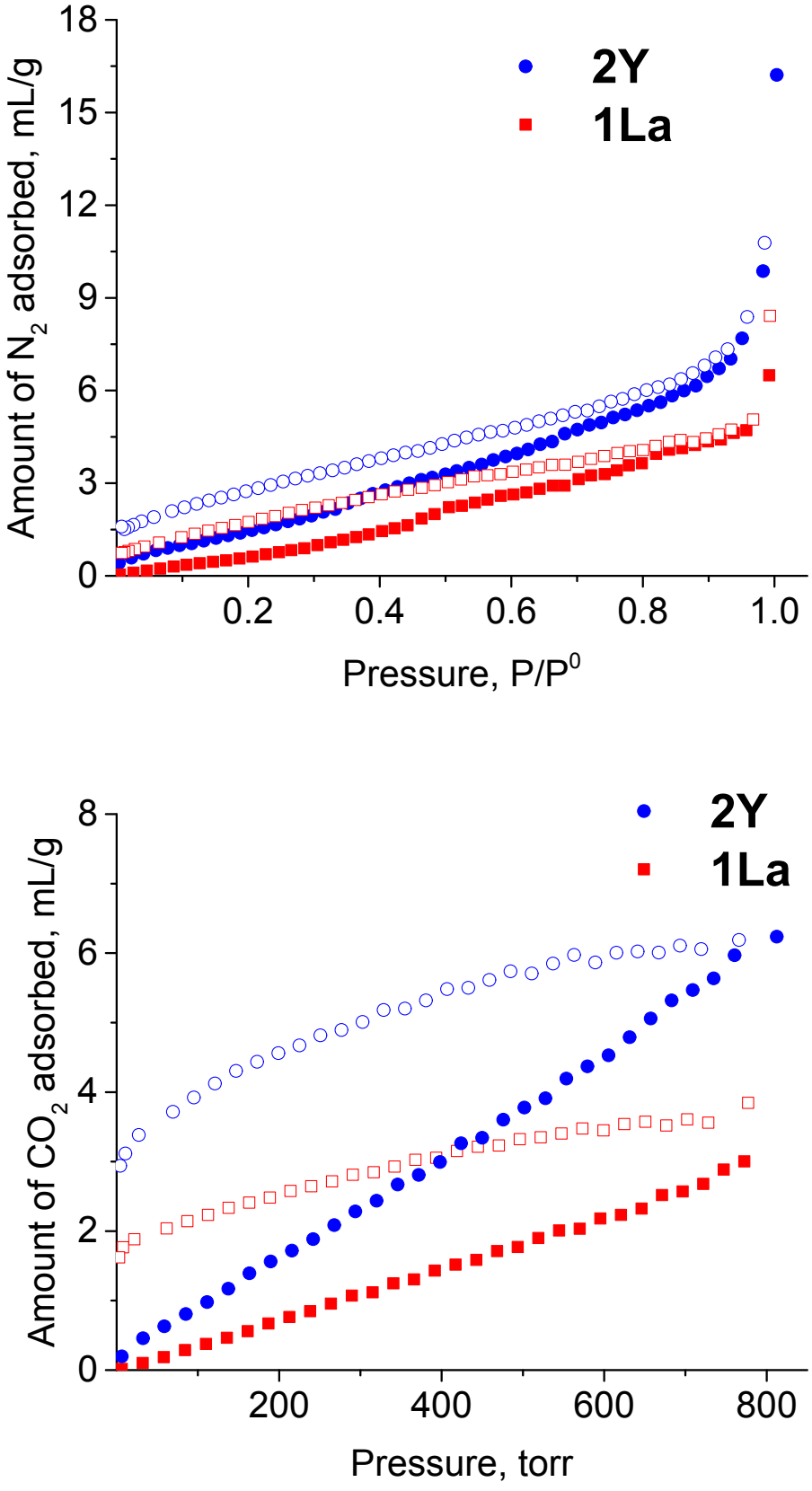
Bond distance, Å		Bond angle, °	
1La			
La(1) – O(11)	2.456(3)	O(1M) – La(1) – O(21)	110.83(10)
La(1) – O(14)	2.487(3)	O(11) – La(1) – O(1M)	73.84(9)
La(1) – O(21)	2.520(3)	O(11) – La(1) – O(21)	78.23(9)
La(1) – O(22)	2.528(3)	O(11) – La(1) – O(1N)	74.22(10)
La(1) – O(1M)	2.490(3)	O(1N) – La(1) – O(1M)	145.48(10)
La(1) – O(1N)	2.487(3)	O(1N) – La(1) – O(21)	74.73(9)
La(1) – N(11)	2.783(3)	O(1M) – La(1) – N(11)	71.10(9)
La(1) – N(12)	2.833(3)	O(11) – La(1) – N(11)	60.59(9)
La(1) – N(21)	2.746(3)	O(21) – La(1) – N(11)	136.93(9)
		O(1N) – La(1) – N(11)	82.04(10)
2Y			
Y(1) – O(11)	2.3602(19)	O(11) – Y(1) – O(1M)	81.23(7)
Y(1) – O(12)	2.377(2)	O(21) – Y(1) – O(11)	75.36(7)
Y(1) – O(21)	2.310(2)	O(21) – Y(1) – O(1M)	76.40(8)
Y(1) – O(32)	2.294(2)	O(21) – Y(1) – O(2M)	135.60(7)
Y(1) – O(1M)	2.371(2)	O(32) – Y(1) – O(11)	140.42(7)
Y(1) – O(2M)	2.360(2)	O(32) – Y(1) – O(21)	136.48(7)
Y(1) – N(11)	2.638(2)	O(32) – Y(1) – O(1M)	85.12(8)
Y(1) – N(21)	2.604(2)	O(32) – Y(1) – O(2M)	84.02(7)
Y(1) – N(31)	2.740(2)	O(2M) – Y(1) – O(11)	80.27(7)
		O(2M) – Y(1) – O(1M)	135.46(7)
		O(11) – Y(1) – N(21)	135.03(8)
		O(11) – Y(1) – N(31)	78.20(7)
		O(21) – Y(1) – N(21)	65.14(7)
		O(21) – Y(1) – N(31)	138.17(8)
		O(32) – Y(1) – N(21)	71.56(7)
		O(32) – Y(1) – N(31)	62.25(7)
		O(1M) – Y(1) – N(21)	69.68(7)
		O(1M) – Y(1) – N(31)	67.94(7)
		O(2M) – Y(1) – N(21)	143.93(8)
		O(2M) – Y(1) – N(31)	68.78(7)
		N(21) – Y(1) – N(31)	118.33(7)

Table S3. Comparison of unit cell parameters for 1La, 1Pr, 1Eu, 1Gd, 2Tb and 2Y.

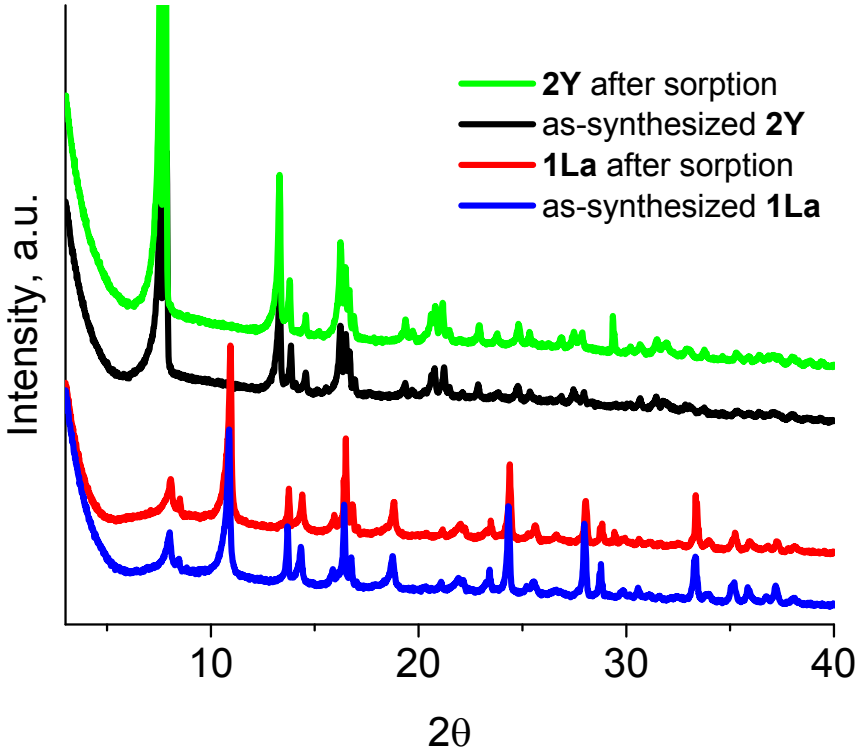
	Space group	***a*, Å**	***b*, Å**	***c*, Å**	***α*, °**	***β*, °**	***γ*, °**
1La	$P\,2_1/c$	6.1241(2)	12.8424(3)	20.6476(4)	90	90.852(2)	90
1Pr	$P\,2_1/c$	6.12230(10)	12.7498(2)	20.5400(4)	90	90.579(2)	90
1Eu	$P\,2_1/c$	6.07080(10)	12.5768(3)	20.3957(5)	90	90.053(2)	90
1Gd	$P\,2_1/c$	6.0560(3)	12.5462(4)	20.3789(8)	90	90.097(4)	90
2Tb	$P\,\bar{1}$	6.0521(4)	12.7395(8)	13.3541(2)	62.547(5)	87.095(7)	87.743(9)
2Y	$P\,\bar{1}$	6.0453(2)	12.6860(5)	13.2051(5)	62.174(4)	86.835(3)	87.582(3)



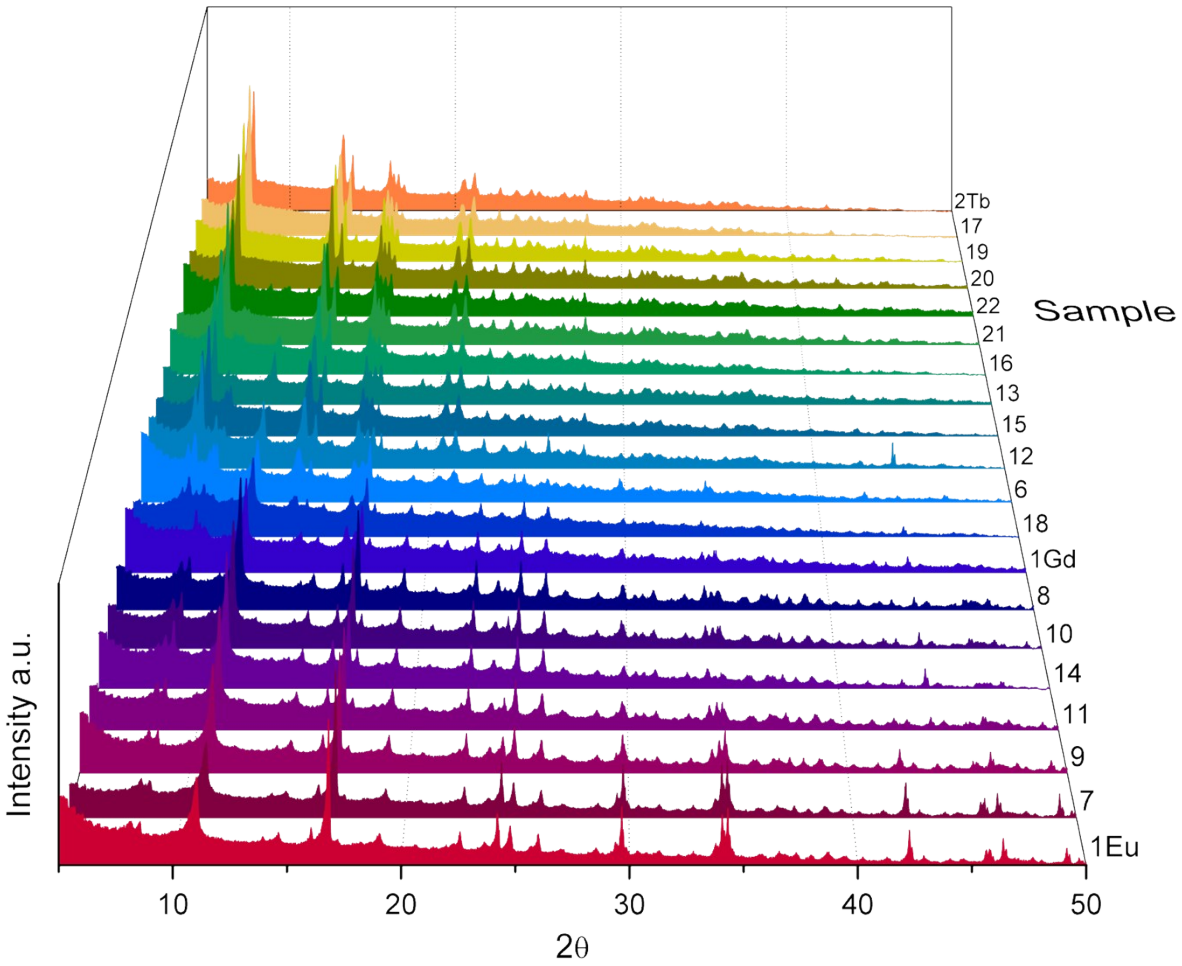
S1. IR spectra for obtained compounds 1La, 1Ce, 1Pr, 1Nd, 1Sm, 1Eu, 1Gd, 2Tb, 2Er and 2Y.



S2. Adsorption isotherms of N_2 at 77 K (upper) and CO_2 at 195K (bottom) for activated 1La and 2Y



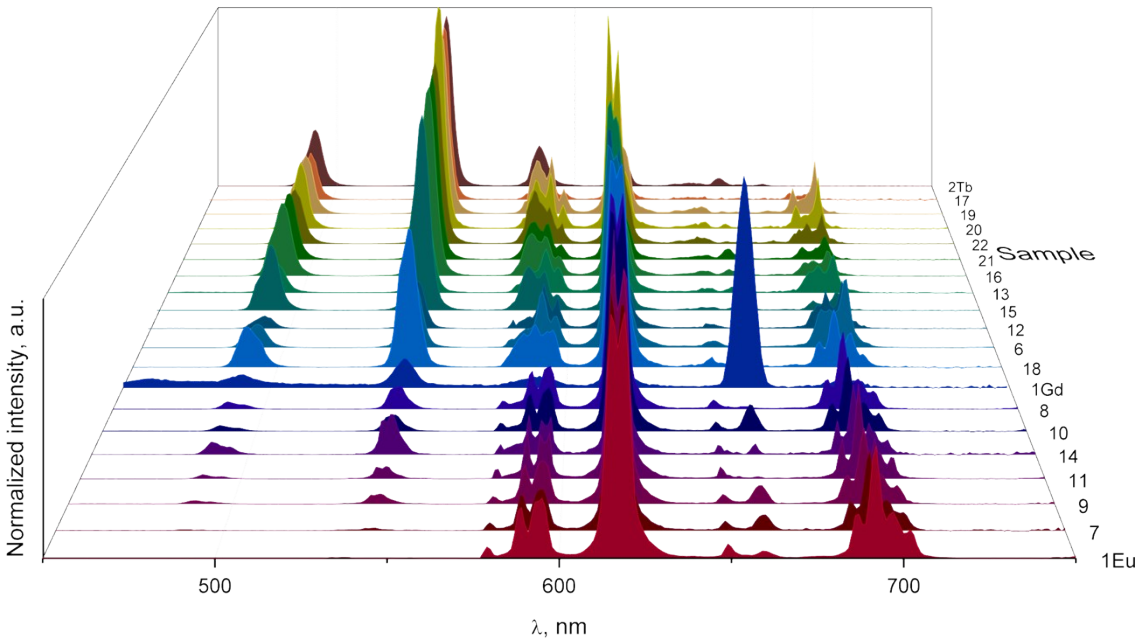
S3. PXRD patterns of as-synthesized 1La and 2Y and after sorption ones.



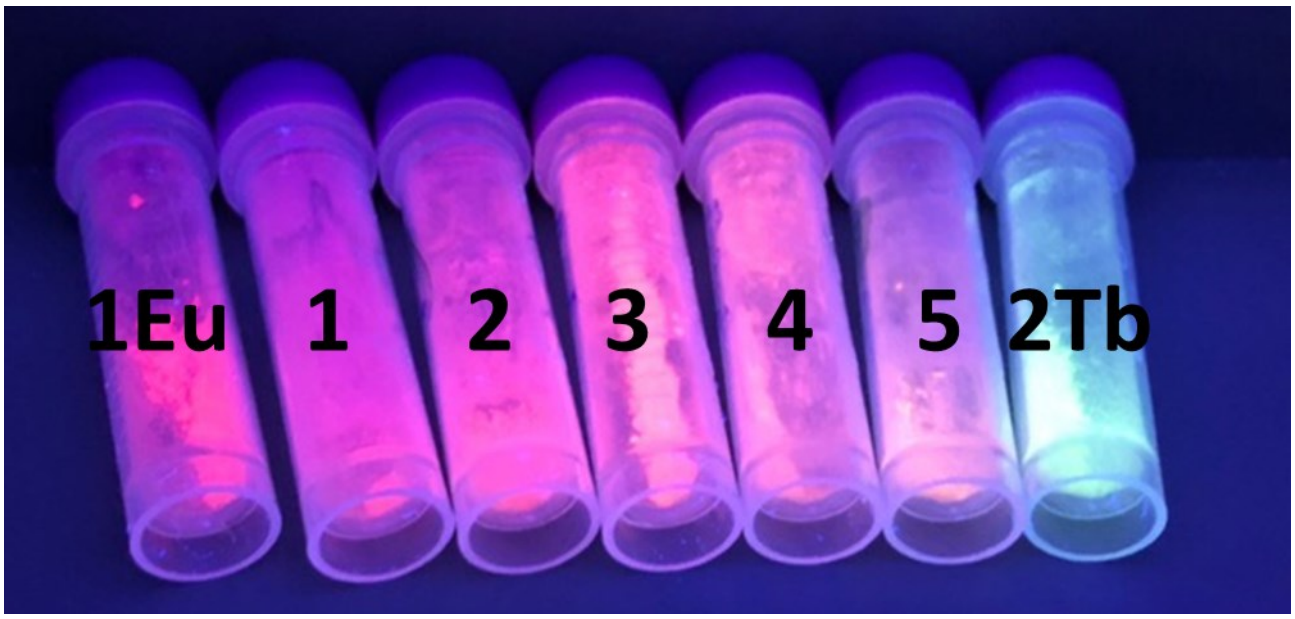
S4. PXRD patterns for samples 6 – 22 in comparison with 1Eu, 1Gd and 2Tb.

Table S4. "Mirror" samples, where mole fractions of Eu and Gd have "mirror" values relative to the mole fraction of Tb, which value is the same for both samples in pair.

Mole fraction	"Mirror" samples		"Mirror" samples		"Mirror" samples		"Mirror" samples	
	7	**18**	**8**	**16**	**9**	**11**	**10**	**14**
Eu	0.90	0.05	0.50	0.10	0.50	0.40	0.50	0.25
Tb	0.05	0.05	0.40	0.40	0.10	0.10	0.25	0.25
Gd	0.05	0.90	0.10	0.50	0.40	0.50	0.25	0.50



S5. Luminescence spectra for mixed metal samples 6 – 22 in comparison with 1Eu, 1Gd and 2Tb ones, λEx = 330 nm.



S6. Photo of samples Eu/Tb (1 – 5) mixed metal series and 1Eu, 2Tb under UV light, λ_{Ex} = 365 nm.