Supplementary Information (SI) for Physical Chemistry Chemical Physics.
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Supporting information

Multicolour luminescence of supramolecular compounds based on Dy-mixed lanthanide complexes and cucurbit[6]uril for logic gate operation and WLED application

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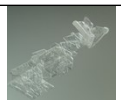
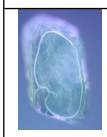
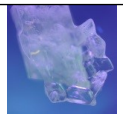
DyPr (1)	DyNd (2)	DySm (3)	DyGd (4)	DyTb (5)	DyHo (6)	DyEr (7)	DyYb (8)
							
							

Figure S1 .Photographs of the 365 nm ultraviolet LED lighting the crystals of heterolanthanide compounds **1-8** when the LED is turned off and turned on.

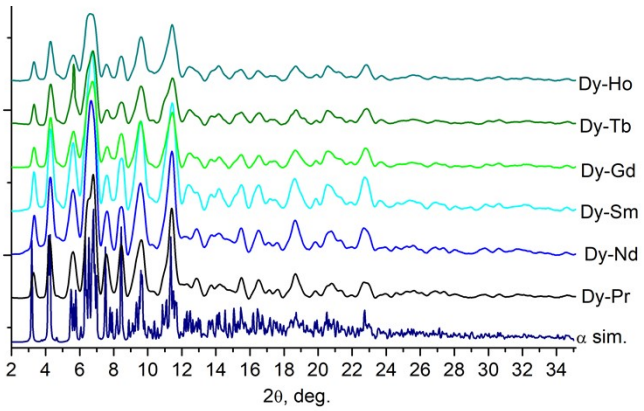


Figure S2. Simulated and experimental (Mo Kα radiation, 150 K) powder XRD patterns for type α bicomponent compounds **1**–**6**.

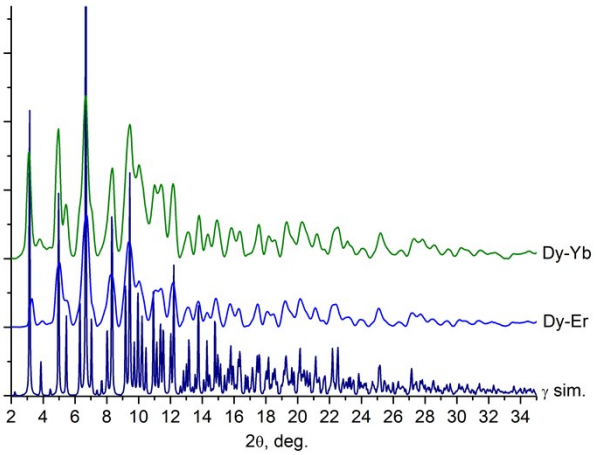


Figure S3. Simulated and experimental (Mo Kα radiation, 150 K) powder XRD patterns for type γ bicomponent compounds **7**–**8**.

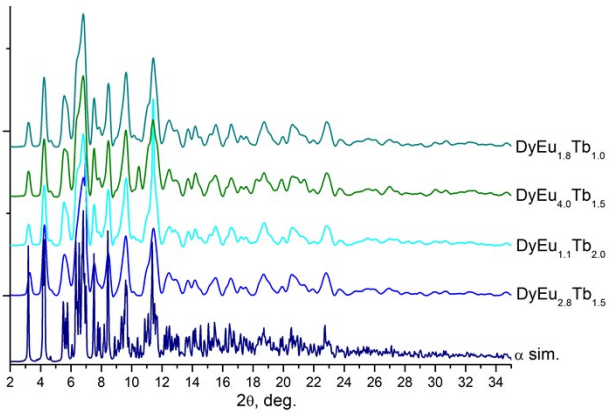


Figure S4a. Simulated and experimental (Mo Kα radiation, 150 K) powder XRD patterns for type α tricomponent compounds **9**–**12**.

Fig. S4b. The TGA curves of compounds Dy-Pr (1) left and Dy-Nd (2) right.

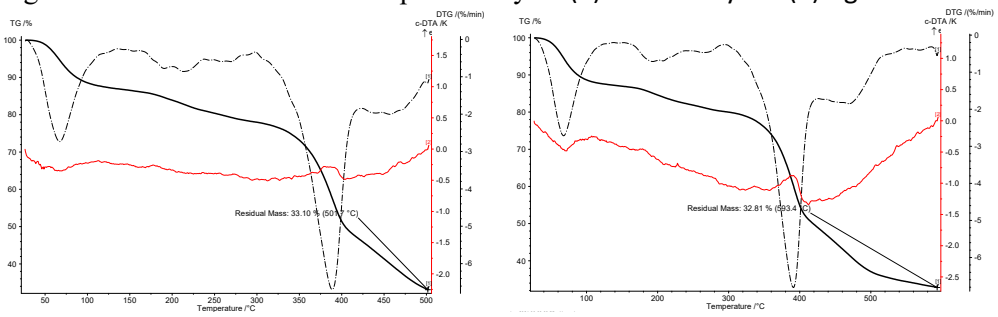


Fig. S4c. The TGA curves of compounds Dy-Gd (4) left and Dy-Tb(5) right.

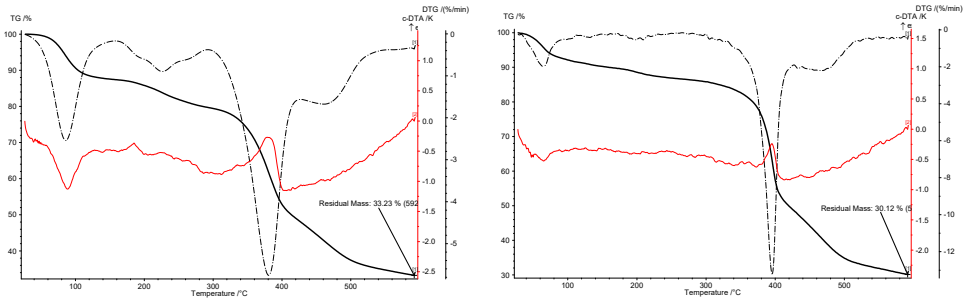


Fig. S4d. The TGA curves of compounds Dy-Ho (6) left and Dy-Er(7) right.

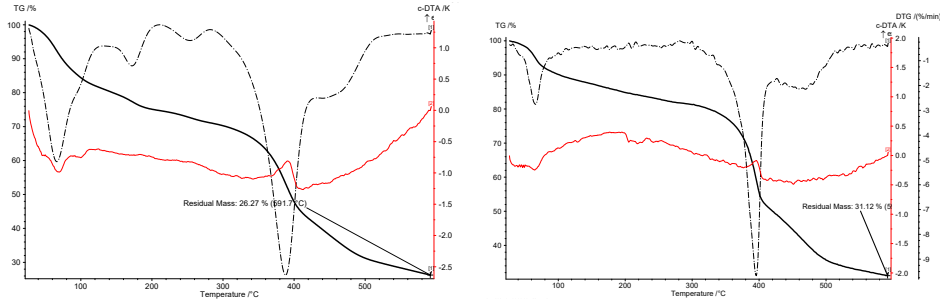
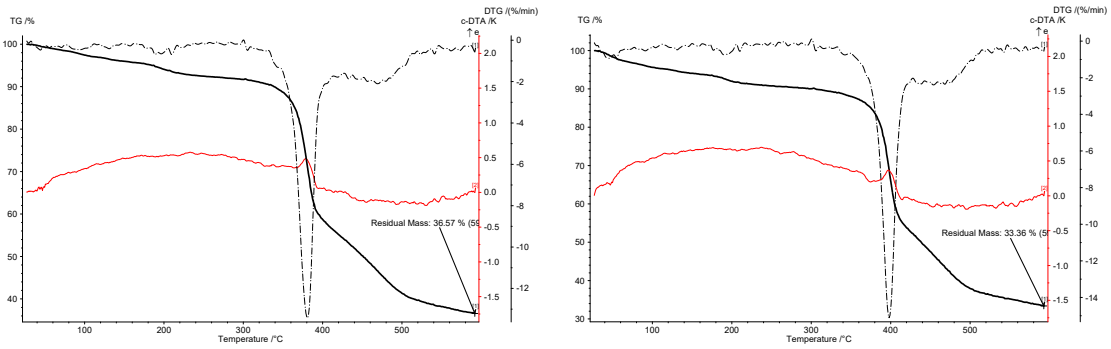


Fig. S4e. The TGA curves of compounds (10) left and (11) right.



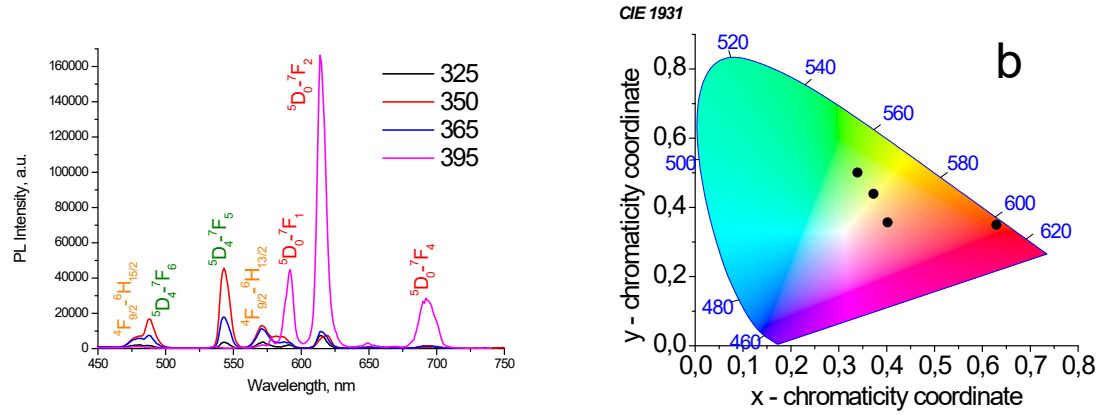


Fig. S5 a - Emission spectra of the compound **9** with different excitation wavelengths; b - CIE 1931 chromaticity coordinate diagram in the solid state under different excitation at room temperature.

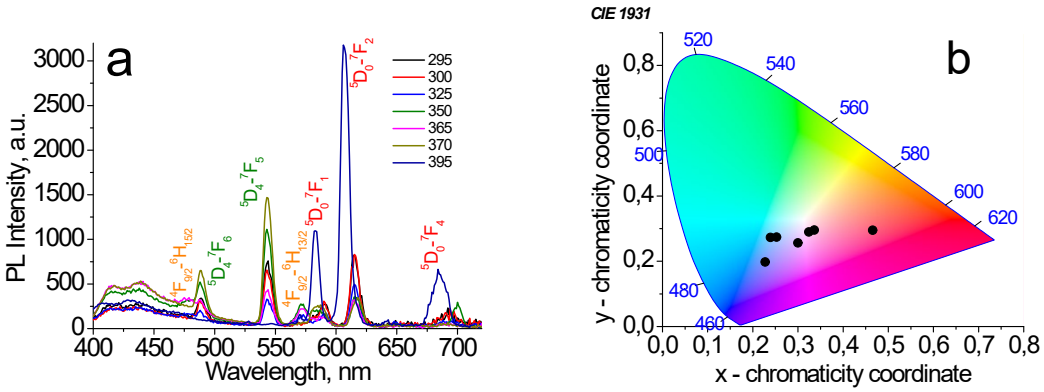


Fig. S6. a - Emission spectra of the compound **10** with different excitation wavelengths; b - CIE 1931 chromaticity coordinate diagram in the solid state under different excitation at room temperature.

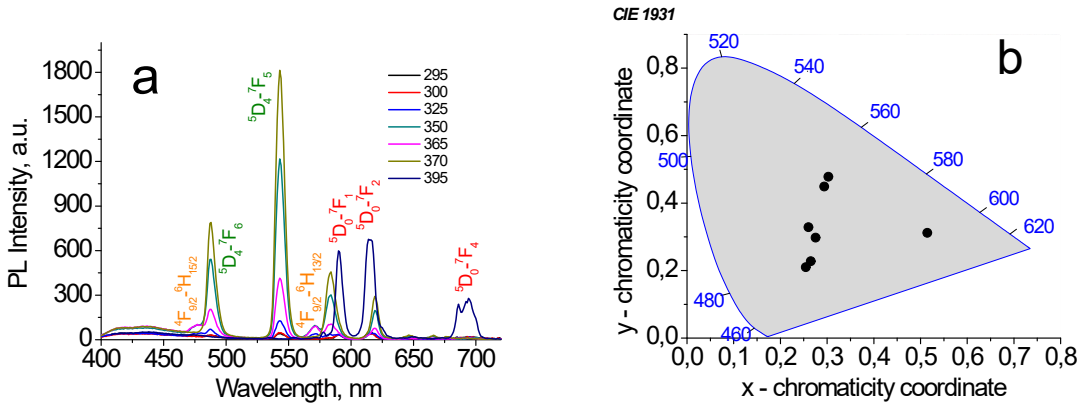


Fig. S7. a - Emission spectra of the compound **12** with different excitation wavelengths; b - CIE 1931 chromaticity coordinate diagram in the solid state under different excitation at room temperature.

Table S1. Crystal data and structure refinement for the compounds **1-12**.

Identification code	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
Empirical formula		$C_{36}H_{68}Dy_{0.67}N_{31}Nd_{1.33}O_{49}$					$C_{36}H_{80}Dy_{1.44}Er_{0.56}N_{32}O_{63}$		$C_{36}H_{68}Dy_{0.38}Eu_{1.06}N_{31}O_{49}Tb_{0.56}$			
Formula weight		2019.83					2306.98		2031.03			
Temperature/K	150(2)	150(2)	150(2)	150(2)	150(2)	150(2)	150(2)	150(2)	150(2)	150(2)	150(2)	150(2)
Space group	*P*–1	*P*–1	*P*–1	*P*–1	*P*–1	*P*–1	*R*–3	*R*–3	*P*–1	*P*–1	*P*–1	*P*–1
a/Å	13.471(3)	13.4485(3)	13.428(2)	13.423(2)	13.393(2)	13.399(2)	25.8207(7)	25.8087(6)	13.4119(3)	13.431(4)	13.426(3)	13.4308(13)
b/Å	14.485(2)	14.4739(4)	14.4919(15)	14.482(2)	14.497(3)	14.494(2)	25.8207(7)	25.8087(6)	14.4765(2)	14.512(3)	14.481(2)	14.5109(8)
c/Å	18.269(2)	18.2996(5)	18.284(2)	18.230(2)	18.198(1)	18.176(2)	31.7971(7)	31.7815(7)	18.2272(4)	18.159(3)	18.227(2)	18.2376(12)
α/°	73.768(9)	73.7510(10)	73.81(1)	73.81(1)	73.87(1)	73.93(1)	90	90	73.8275(6)	73.65(1)	73.833(8)	73.780(5)
β/°	87.44(1)	87.3320(10)	87.35(1)	87.36(1)	87.14(1)	87.22(1)	90	90	87.2830(7)	87.377(9)	87.367(9)	87.273(7)
γ/°	87.84(1)	87.8130(10)	87.88(1)	87.72(1)	87.72(1)	87.74(1)	120	120	87.7342(6)	87.878(9)	87.727(8)	87.929(7)
Volume/Å^3	3417.9(8)	3414.89(15)	3412.3(6)	3398.4(4)	3388.8(4)	3386.6(4)	18359.2(11)	18333.1(9)	3393.80(12)	3393.7(7)	3398.6(7)	3408.1(4)
Z		2					9		2			
ρ_{calc}g/cm^3		1.964					1.870		1.988			
μ/mm^{-1}		1.865					2.021		2.105			
F(000)		2034.0					10414.0		2043.0			
Crystal size/mm^3		0.17 × 0.16 × 0.05					0.17 × 0.10 × 0.10		0.14 × 0.09 × 0.08			
Radiation		MoKα (λ = 0.71073)					MoKα (λ = 0.71073)		MoKα (λ = 0.71073)			
2Θ range for data collection/°		2.932 to 57.45					3.154 to 57.416		2.93 to 59.146			
Index ranges		-18 ≤ h ≤ 16, -18 ≤ k ≤ 19, -24 ≤ l ≤ 24					-34 ≤ h ≤ 34, -34 ≤ k ≤ 34, -42 ≤ l ≤ 42		-18 ≤ h ≤ 18, -20 ≤ k ≤ 18, -23 ≤ l ≤ 25			
Reflections collected		51389					10539		53733			
Independent reflections		17453 [R_{int} = 0.0406, R_{sigma} = 0.0506]					10539 [R_{int} = 0.0691, R_{sigma} = 0.0563]		18606 [R_{int} = 0.0618, R_{sigma} = 0.0812]			
Restraints/parameters		229/1209					403/780		231/1209			
Goodness-of-fit on F^2		1.039					1.183		0.991			
Final *R* indexes [*I*>=2σ (*I*)]		R_1 = 0.0371, wR_2 = 0.0713					R_1 = 0.0418, wR_2 = 0.1200		R_1 = 0.0402, wR_2 = 0.0692			
Final *R* indexes [all data]		R_1 = 0.0542, wR_2 = 0.0762					R_1 = 0.0528, wR_2 = 0.1303		R_1 = 0.0697, wR_2 = 0.0767			
Largest diff. peak/hole / e Å^{-3}		1.18/-1.30					1.55/-0.99		1.25/-0.82			

Table S2. Ln–O bond distances in the β structures with color coding for each distance from green (large) through yellow (medium) to red (small).

Ln*	Dy-Nd (**2**)	Eu-Sm**	Eu**	Eu-Gd**	Eu-Tb**	Eu-Dy**	Eu-Dy-Tb (**9**)	Eu-Ho**
Ln1–O11M	2.514(2)	2.503(3)	2.4950(18)	2.491(3)	2.485(2)	2.482(5)	2.477(2)	2.479(5)
Ln1–O12M	2.438(2)	2.418(3)	2.4084(18)	2.412(3)	2.3970(18)	2.401(5)	2.393(2)	2.389(5)
Ln1–O13M	2.454(3)	2.443(3)	2.4310(18)	2.427(3)	2.4153(18)	2.419(5)	2.413(3)	2.405(5)
Ln1–O14M	2.458(2)	2.445(3)	2.4337(18)	2.430(3)	2.4242(18)	2.428(5)	2.420(2)	2.413(5)
Ln1–O15M	2.415(3)	2.409(3)	2.3899(19)	2.390(3)	2.3774(19)	2.379(5)	2.374(3)	2.376(5)
Ln1–O11N	2.501(2)	2.489(3)	2.4795(17)	2.481(3)	2.467(2)	2.471(5)	2.469(2)	2.467(5)
Ln1–O12N	2.563(2)	2.550(3)	2.5434(18)	2.541(3)	2.533(2)	2.527(5)	2.531(2)	2.526(5)
Ln1–O11	2.400(2)	2.381(3)	2.3764(16)	2.377(3)	2.3665(19)	2.376(5)	2.366(2)	2.363(4)
Ln1–O21	2.493(2)	2.480(3)	2.4753(17)	2.474(3)	2.4700(17)	2.479(5)	2.470(2)	2.469(4)
Ln2–O21M	2.442(3)	2.436(3)	2.4309(18)	2.430(3)	2.414(2)	2.416(5)	2.414(3)	2.408(5)
Ln2–O22M	2.430(2)	2.428(3)	2.4111(18)	2.412(3)	2.4016(18)	2.404(5)	2.401(2)	2.392(5)
Ln2–O23M	2.518(2)	2.517(3)	2.5023(17)	2.500(3)	2.4891(19)	2.488(5)	2.489(2)	2.479(5)
Ln2–O24M	2.411(3)	2.407(3)	2.3946(18)	2.391(3)	2.380(2)	2.376(5)	2.378(2)	2.368(5)
Ln2–O25M	2.433(3)	2.429(3)	2.4188(18)	2.414(3)	2.4045(19)	2.410(5)	2.407(2)	2.398(5)
Ln2–O21N	2.528(2)	2.521(3)	2.5152(18)	2.516(3)	2.5067(18)	2.507(5)	2.509(2)	2.495(5)
Ln2–O22N	2.511(2)	2.505(3)	2.4945(17)	2.494(3)	2.4859(17)	2.483(5)	2.482(2)	2.475(5)
Ln2–O41	2.475(2)	2.473(3)	2.4664(17)	2.461(3)	2.4578(17)	2.462(5)	2.461(2)	2.458(5)
Ln2–O51	2.373(2)	2.363(3)	2.3572(17)	2.350(3)	2.3461(17)	2.342(5)	2.342(2)	2.334(5)
Ln1-Ln1	7.9405(7)	7.9386(7)	7.9377(7)	7.9274(7)	7.9188(7)	7.9068(8)	7.9267(7)	7.9203(8)
Ln2-Ln2	7.6607(7)	7.6551(8)	7.6405(7)	7.6478(7)	7.6310(7)	7.6514(8)	7.6449(2)	7.6443(8)

* – Ln1 and Ln2 are two crystallographically independent atoms;

** – data from ref. ***CrystEngComm***, 2024, **26**, 3954-3963. DOI: 10.1039/D4CE00375F

Table S3. Quantum yields (QY,%) and lifetime (t, μs) of compounds **1-12**.

	QY,%	t, μs
1	<1 (λex=350nm)	15
2	< 1 (λex=350nm)	17
3	2 (λex=350nm)	22
4	2 (λex=350nm)	18
5	< 1 (λex=350nm)	18 (572 nm) Dy 691(543 nm) Tb
6	<1 (λex=350nm)	18
7	1 (λex=350nm)	17
8	<1 (λex=350nm)	14
9	7 (λex=395nm)	20 (572 nm) Dy 707 (543 nm) Tb 175 (615 nm) Eu
10	6 (λex=395nm)	18 (572 nm)Dy 658 (543 nm) Tb 212 (615 nm) Eu
11	5 (λex=370nm)	21 (572 nm) Dy 664 (543 nm) Tb 182 (615 nm) Eu
12	4 (λex=370nm)	20 (572 nm) Dy 641 (543 nm) Tb 174 (615 nm) Eu