Supplementary Information

Luminescent Thermochromism in Novel Mixed Eu(II)-Cu(I) Iodide

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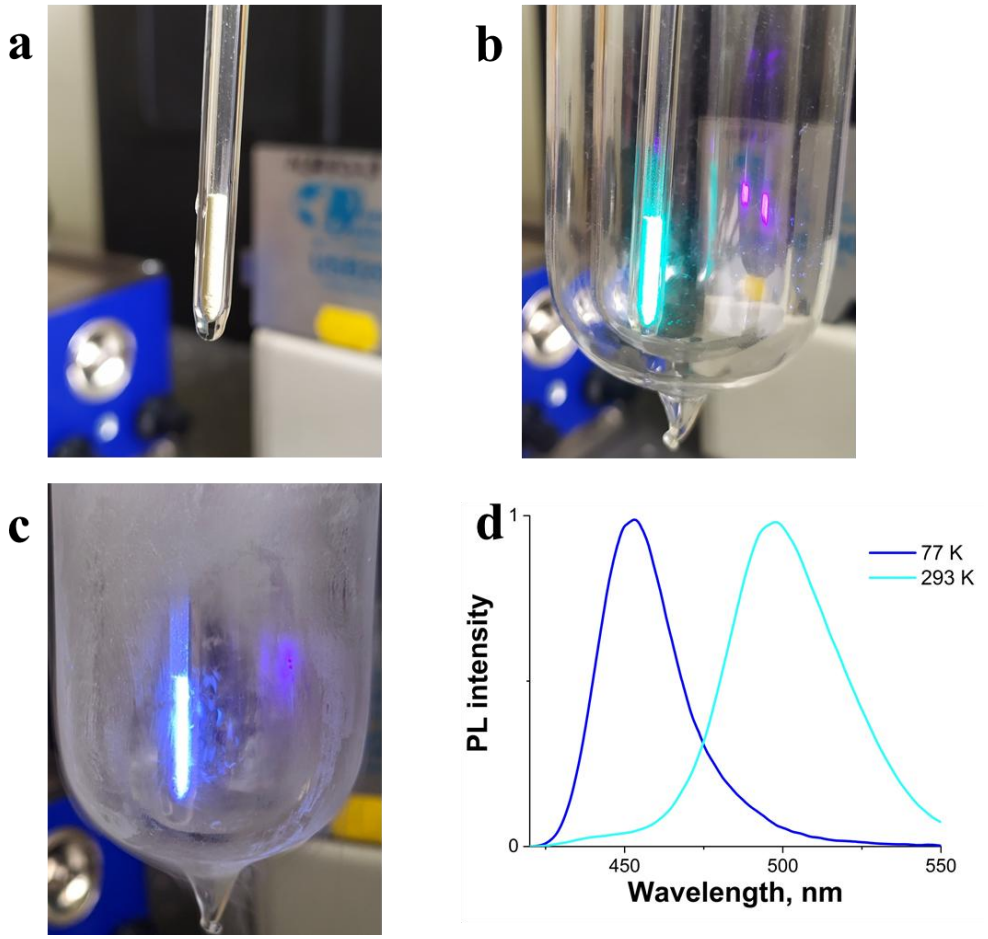


Figure 1S. Photo of **1** in evacuated quartz tube (a), under irradiation by 365 nm UV LED at 293 (b) and 77 K (c); PL spectra of **1** at 293 and 77 K (d).

Table 1S. Details of crystallographic, collection and refinement data for complex **1** at 100 and 280 K.

	1	
Empirical formula	$C_{16}H_{40}Cu_2EuI_4O_8$	
M	1147.12	
T/K	100(2)	280(2)
Crystal system	Orthorhombic	
Space group	*Pna2₁*	
a (Å)	15.8800(4)	16.0747(8)
b (Å)	12.7849(3)	12.9699(6)
c (Å)	16.1773(4)	16.3759(10)
V (Å)^3	3284.40(14)	3414.2(3)
Z	4	
d_{calc} (*g* cm^{-3})	2.320	2.232
M (mm^{-1})	6.960	6.695
F(000)	2132	2132
Crystal size (mm)	0.56 × 0.39 × 0.35	
θ (deg)	3.020–30.034	2.982–25.026
Limiting indices *h*, *k*, *l*	$-22 \le h \le 22$ $-18 \le k \le 18$ $-22 \le l \le 22$	$-18 \le h \le 19$ $-15 \le k \le 15$ $-19 \le l \le 19$
Reflections collected / unique	62458 / 9595	27338 / 5843
R(int)	0.0420	0.0691
S	1.034	1.048
R_1/wR_2 ($I > 2\sigma(I)$)	0.0475 / 0.1151	0.0480 / 0.1052
R_1/wR_2 (all data)	0.0515 / 0.1180	0.0655 / 0.1153
Absolute structure parameter	–0.01(3)	–0.03(2)
Largest diff. peak / hole (e·Å^{-3})	1.855 / –1.176	1.147 / –1.196

Table 2S. Selected Bond Distances (Å) and Angles (deg) for compound **1** at 100 and 280 K.

Lengths (Å) / Angles (deg)	**1**	
	100 K	280 K
Eu(1)-O(1)	2.64(2)	2.63(3)
Eu(1)-O(2)	2.59(4)	2.58(3)
Eu(1)-O(3)	2.567(7)	2.599(11)
Eu(1)-O(4)	2.608(8)	2.609(11)
Eu(1)-O(5)	2.549(7)	2.579(11)
Eu(1)-O(6)	2.577(7)	2.582(11)
Eu(1)-O(7)	2.57(7)	2.61(3)
Eu(1)-O(8)	2.63(4)	2.63(3)
Cu(1)-I(1)	2.494(2)	2.495(4)
Cu(1)-I(2)	2.608(2)	2.610(3)
Cu(1)-I(3)	2.580(2)	2.596(4)
Cu(1)···Cu(2)	2.617(2)	2.653(4)
Cu(2)-I(2)	2.568(2)	2.583(3)
Cu(2)-I(3)	2.569(2)	2.563(3)
Cu(2)-I(4)	2.489(2)	2.485(4)
O(2)-Eu(1)-O(1)	62.2(7)	64.0(8)
O(3)-Eu(1)-O(1)	107.3(5)	106.9(7)
O(4)-Eu(1)-O(1)	163.0(6)	162.5(7)
O(5)-Eu(1)-O(1)	74.5(5)	74.6(6)
O(6)-Eu(1)-O(1)	101.4(5)	100.5(7)
O(7)-Eu(1)-O(1)	75.8(15)	73.3(11)
O(8)-Eu(1)-O(1)	119.1(9)	120.6(9)
O(3)-Eu(1)-O(2)	73.5(8)	73.1(8)
O(2)-Eu(1)-O(4)	122.7(7)	121.4(7)
O(5)-Eu(1)-O(2)	116.3(7)	118.4(8)
O(6)-Eu(1)-O(2)	161.1(7)	160.9(8)
O(7)-Eu(1)-O(2)	91.0(16)	90.8(11)
O(2)-Eu(1)-O(8)	76.3(10)	76.7(11)
O(3)-Eu(1)-O(4)	62.7(2)	62.8(3)
O(5)-Eu(1)-O(3)	78.0(3)	78.2(4)
O(3)-Eu(1)-O(6)	123.0(3)	124.2(4)
O(3)-Eu(1)-O(7)	159.3(12)	161.1(7)
O(3)-Eu(1)-O(8)	100.5(7)	101.7(7)
O(5)-Eu(1)-O(4)	89.5(3)	89.0(4)
O(6)-Eu(1)-O(4)	75.8(3)	76.9(4)
O(7)-Eu(1)-O(4)	118.6(14)	121.3(9)
O(4)-Eu(1)-O(8)	77.4(7)	76.5(7)
O(5)-Eu(1)-O(6)	63.7(2)	63.5(4)
O(5)-Eu(1)-O(7)	121.9(11)	119.1(6)
O(5)-Eu(1)-O(8)	165.7(7)	163.4(8)
O(7)-Eu(1)-O(6)	75.0(13)	73.3(8)
O(6)-Eu(1)-O(8)	106.9(7)	104.6(8)
O(7)-Eu(1)-O(8)	61.8(13)	64.2(8)
I(1)-Cu(1)-I(2)	122.82(8)	122.64(15)
I(1)-Cu(1)-I(3)	123.38(7)	124.09(13)
I(3)-Cu(1)-I(2)	113.76(7)	113.26(13)

I(1)-Cu(1)-Cu(2)	161.98(8)	162.30(13)
I(2)-Cu(1)-Cu(2)	58.88(5)	58.77(10)
I(3)-Cu(1)-Cu(2)	59.24(6)	58.46(10)
I(2)-Cu(2)-I(3)	115.51(7)	115.29(13)
I(4)-Cu(2)-I(2)	125.27(7)	124.37(12)
I(4)-Cu(2)-I(3)	119.18(7)	120.31(14)
I(2)-Cu(2)-Cu(1)	60.38(6)	59.78(10)
I(3)-Cu(2)-Cu(1)	59.65(6)	59.65(11)
I(4)-Cu(2)-Cu(1)	160.92(8)	161.79(12)
Cu(2)-I(2)-Cu(1)	60.75(6)	61.45(11)
Cu(2)-I(3)-Cu(1)	61.10(5)	61.90(10)

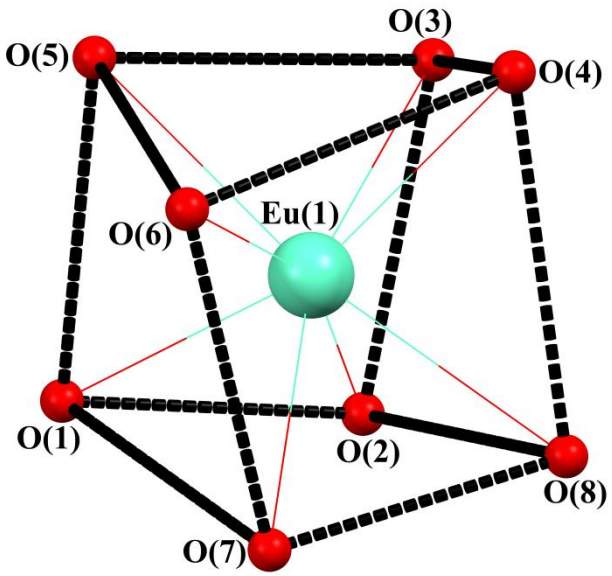


Figure 2S. The coordination environment of europium atom in complex **1** at 100 K.

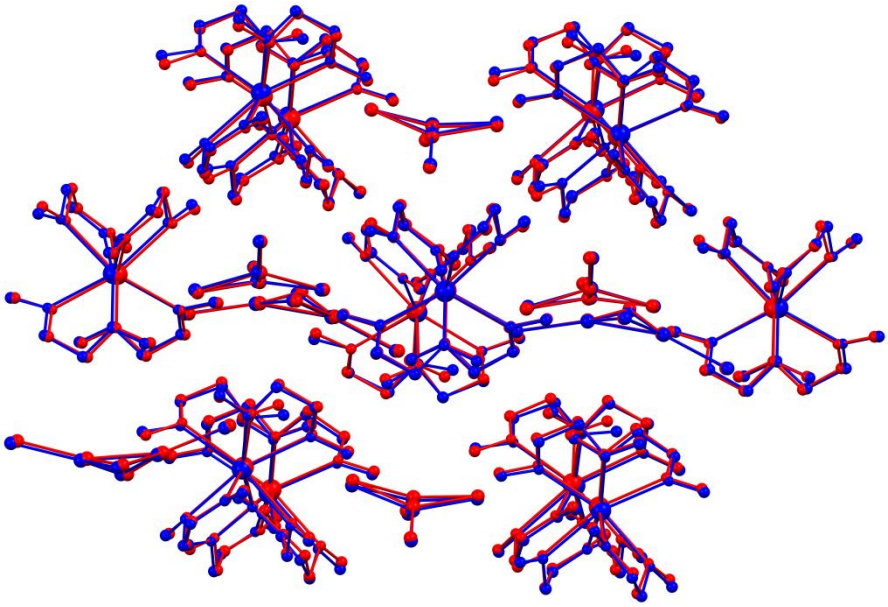
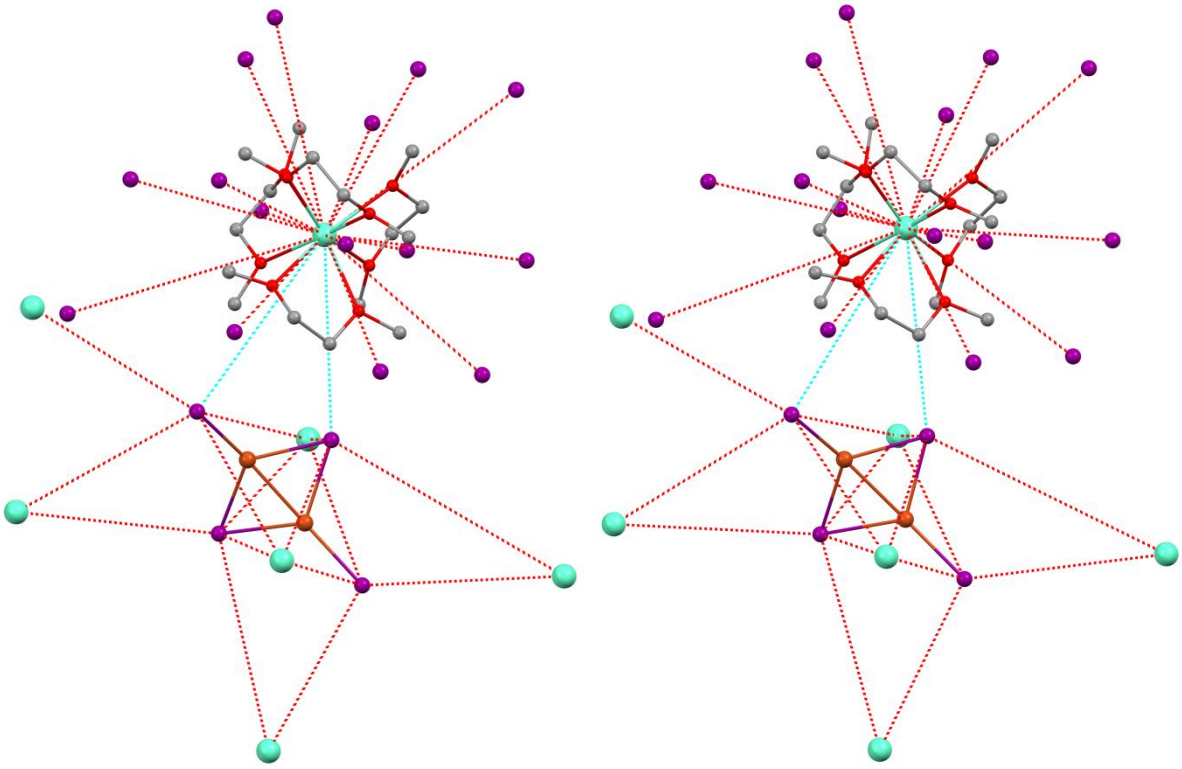


Figure 3S. The comparison of crystal packing of complex **1** at 100 (red) and 280 K (blue).



a **b**

Figure 4S. Intermolecular Eu···I distances in complex **1** at 100 (a) and 280 K (b).

Table 3S. Intermolecular Eu···I and H···I distances in complex **1** at 100 and 280 K.

Lengths (Å)	100 K	280 K
Eu(1)···I(1)	6.408	6.501
Eu(1)···I(1A)	6.486	6.564
Eu(1)···I(1B)	6.618	6.668
Eu(1)···I(1C)	7.597	7.781
Eu(1)···I(1D)	8.823	8.877
Eu(1)···I(2A)	5.974	6.121
Eu(1)···I(2B)	6.728	6.774
Eu(1)···I(2C)	6.958	7.037
Eu(1)···I(2D)	7.003	7.102
Eu(1)···I(3)	6.192	6.326
Eu(1)···I(3A)	6.257	6.406
Eu(1)···I(3B)	7.145	7.183
Eu(1)···I(3C)	7.910	7.903
Eu(1)···I(4A)	5.928	6.021
Eu(1)···I(4B)	6.275	6.307
Eu(1)···I(4C)	6.691	6.819
Eu(1)···I(4D)	7.568	7.666
H(2A)···I(4)	2.999	3.249
H(5C)···I(4)	3.166	3.197
H(15A)···I(2)	3.132	3.265
H(6A)···I(1)	3.163	3.210
H(4B)···I(3)	3.153	3.269

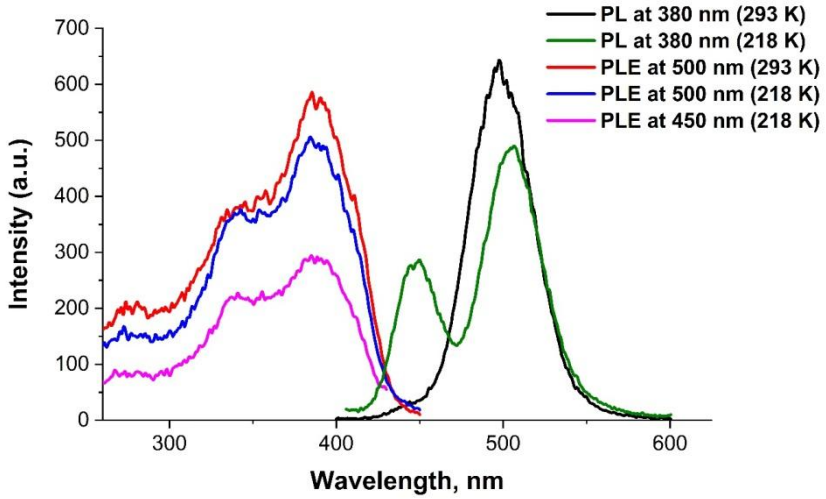


Figure 5S. PL and PLE spectra of **1** at various emission wavelengths and temperatures.

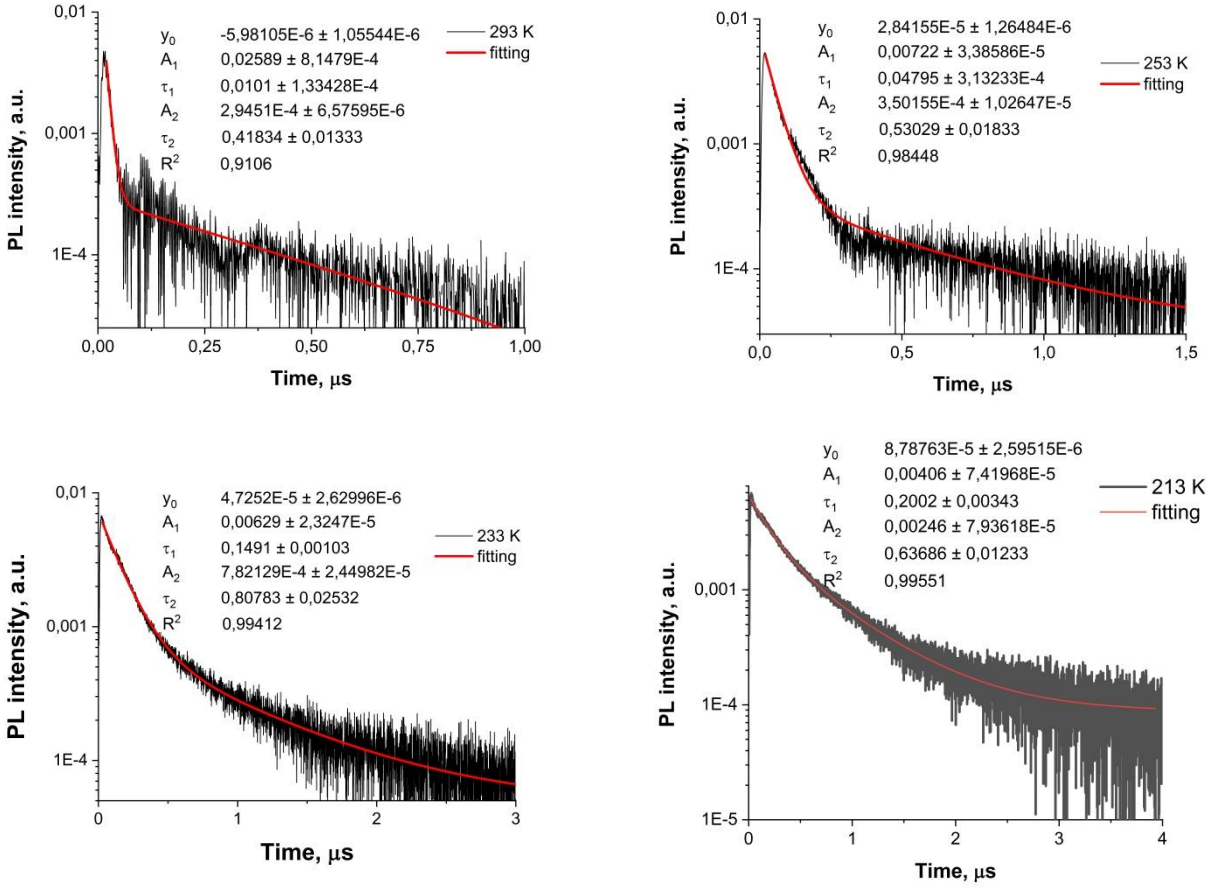


Figure 6S. PL kinetics of **1** at 445 nm at various temperatures and their fittings by equation $y(t) = A_1*\exp(-t/\tau_1) + A_2*\exp(-t/\tau_2) + y_0$.

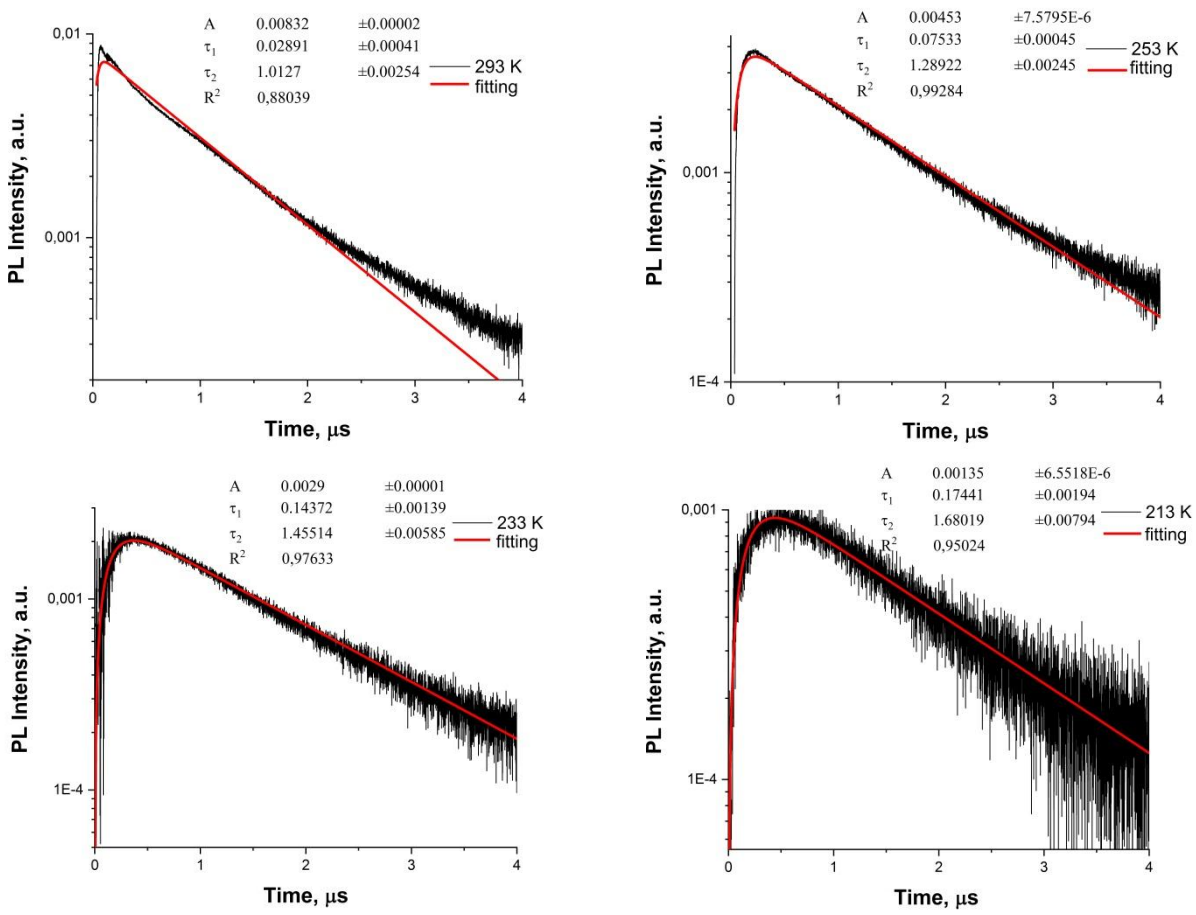


Figure 7S. PL kinetics of **1** at 500 nm at various temperatures and their fittings by equation $y(t) = A*(\exp(-t/\tau_2) - \exp(-t/\tau_1))$

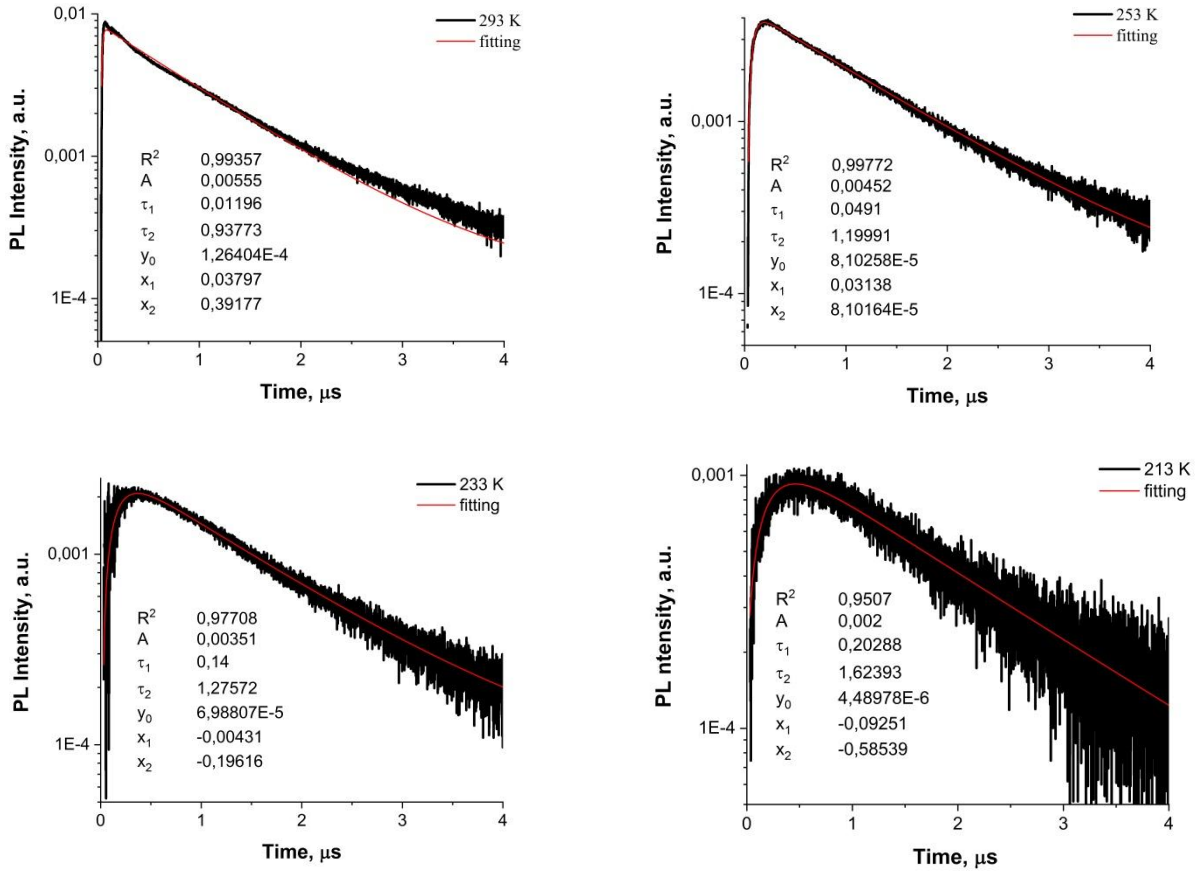


Figure 8S. PL kinetics of **1** at 500 nm at various temperatures and their fittings by equation $y(t) = A*(\exp(-(t-x_2)/\tau_2) - \exp(-(t-x_1)/\tau_1)) + y_0$.

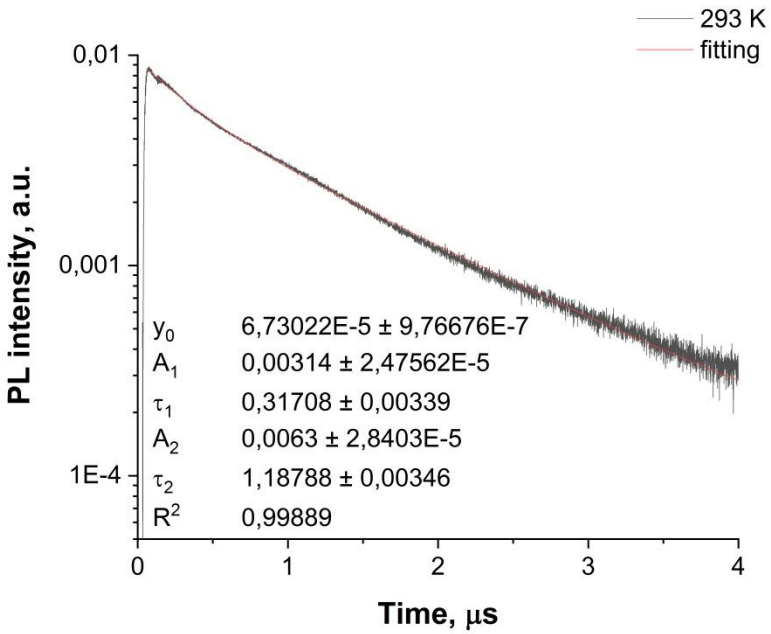


Figure 9S. PL kinetic of **1** at 500 nm at 293 K and its fitting by equation $y(t) = A_1*\exp(-t/\tau_1) + A_2*\exp(-t/\tau_2) + y_0$.