Electronic Supplementary Information

Table 1S. The fitting parameters for equation 4, determined from the spectra of the $^5D_0 \rightarrow {}^7F_0$ transition of Eu–EDTA system in aqueous solution.

Table 2S. Parameter values for equation 5 used to generate the simulated spectra of the $^5D_0 \rightarrow {}^7F_2$ and $^5D_0 \rightarrow {}^7F_4$ transitions.

Figure 1S. Luminescence spectra of solution (276-363K) and crystals **I** and **II** at RT.
Figure 2S. Luminescence lifetimes of crystals **I** and **II** as well as solution (λ_{ex} = 394 nm, λ_{ex} = 612 nm).
Figure 3S. IR spectra of **I** and **II**.
Figure 4S. Scanning electron microscope spectrum of **II**.
Figure 5S. UV-vis absorption spectrum of crystals **I** and **II**.
Figure 6S. Species distribution diagram for LnEDTA compex (T = 25^{0}C, μ = 1M) derived from Y. P. Galactinov, K. V. Astakhov, *Zh. Neorg. Khim.,* 1963, **8**, 896.

Table 1S. The fitting parameters for equation (4), determined from the spectra of the $^5D_0 \rightarrow {}^7F_0$ transition for Eu–EDTA system in aqueous solution

T / K	I_{sim}			II_{sim}		
	J_{max}	λ_{max}	$\Delta\lambda$	J_{max}	λ_{max}	$\Delta\lambda$
273	0.064671	579.62	0.270797	0.237907	579.14	0.270797
283	0.077146	579.60	0.270046	0.213398	579.11	0.270046
293	0.105476	579.57	0.267380	0.205432	579.08	0.267380
303	0.122923	579.55	0.270342	0.188366	579.05	0.270342
313	0.145331	579.52	0.274050	0.170132	579.00	0.274050
323	0.159230	579.48	0.278874	0.151958	578.96	0.278874
333	0.178601	579.45	0.277388	0.137367	578.92	0.277388
343	0.199222	579.42	0.281269	0.125999	578.88	0.281269
353	0.207434	579.38	0.284510	0.113858	578.84	0.284510
363	0.225120	579.36	0.288506	0.107462	578.79	0.288506

Where

I_{sim} simulated spectrum of the 9-coordinate species

II_{sim} simulated spectrum of the 8-coordinate species

J_{max} is the maximum intensity of the peak;

λ_{max} is the wavelength of the peak maximum;

$\Delta\lambda$ is the half-width of a peak.

Table 2S. Parameter values for equation 5 used to generate the simulated spectra of the $^5D_0 \rightarrow {}^7F_2$ and $^5D_0 \rightarrow {}^7F_4$ transitions

		$\mathbf{I_{sim}}\ ^5D_0 \rightarrow {}^7F_2$		
A_9	I_{max}	λ_{max}	B_9	$\Delta\lambda$
1.092380	0.075000	612.50	1.569071	1.368137
1.092380	0.804283	614.20	1.569071	0.658269
1.092380	0.424743	615.09	1.569071	0.338460
1.092380	0.587493	615.95	1.569071	0.661347
1.092380	0.105879	617.90	1.569071	1.038688
1.092380	0.150087	620.70	1.569071	1.021581
1.092380	0.026076	625.20	1.569071	3.564338
		$\mathbf{II_{sim}}\ ^5D_0 \rightarrow {}^7F_2$		
A_8	I_{max}	λ_{max}	B_8	$\Delta\lambda$
0.474677	0.073640	611.70	3.625299	0.759000
0.474677	0.398300	613.10	3.625299	0.527062
0.474677	0.081980	614.40	3.625299	0.878480
0.474677	0.165600	616.30	3.625299	0.882320
0.474677	0.027700	618.25	3.625299	0.613007
0.474677	0.034570	620.20	3.625299	1.493333
0.474677	0.030290	623.75	3.625299	1.728942
0.474677	0.016389	627.95	3.625299	2.412105
		$\mathbf{I_{sim}}\ ^5D_0 \rightarrow {}^7F_4$		
A_9	I_{max}	λ_{max}	A_9	I_{max}
0.949790	0.012160	682.10	0.949790	0.012160
0.949790	0.093576	687.00	0.949790	0.093576
0.949790	0.127110	689.89	0.949790	0.127110
0.949790	0.268644	692.78	0.949790	0.268644
0.949790	0.183584	694.45	0.949790	0.183584
0.949790	0.153350	697.42	0.949790	0.153350
0.949790	0.029800	703.55	0.949790	0.029800
0.949790	0.027365	706.79	0.949790	0.027365
		$\mathbf{I_{sim}}\ ^5D_0 \rightarrow {}^7F_4$		
A_8	I_{max}	λ_{max}	B_8	$\Delta\lambda$
0.504703	0.123200	683.35	2.823059	0.979322
0.504703	0.042830	697.00	2.823059	1.981809
0.504703	0.364050	700.10	2.823059	0.742621
0.504703	0.035498	704.21	2.823059	1.031447
0.504703	0.033720	706.82	2.823059	0.644092
0.504703	0.020870	708.33	2.823059	0.639462

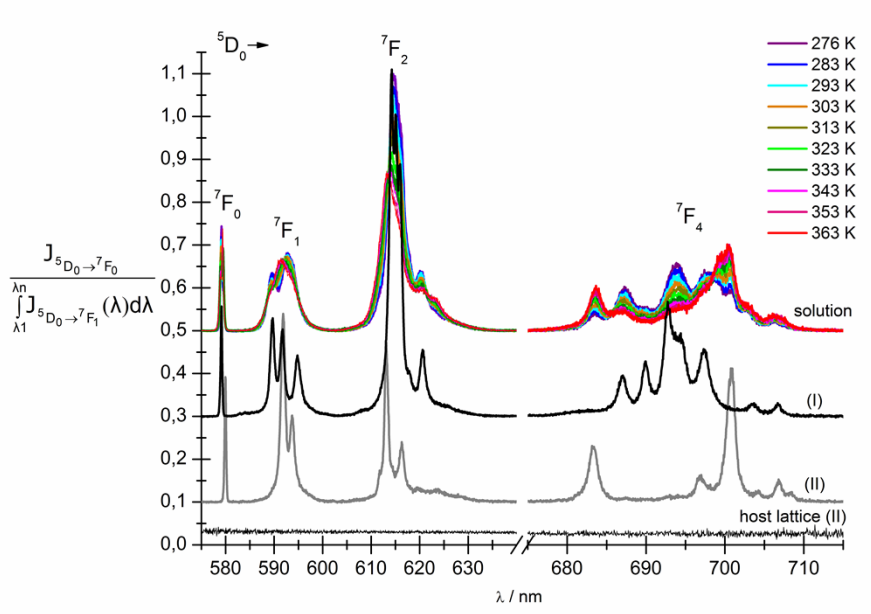


Figure 1S. Luminescence spectra of solution (276-363K) and crystals **I** and **II** at RT.

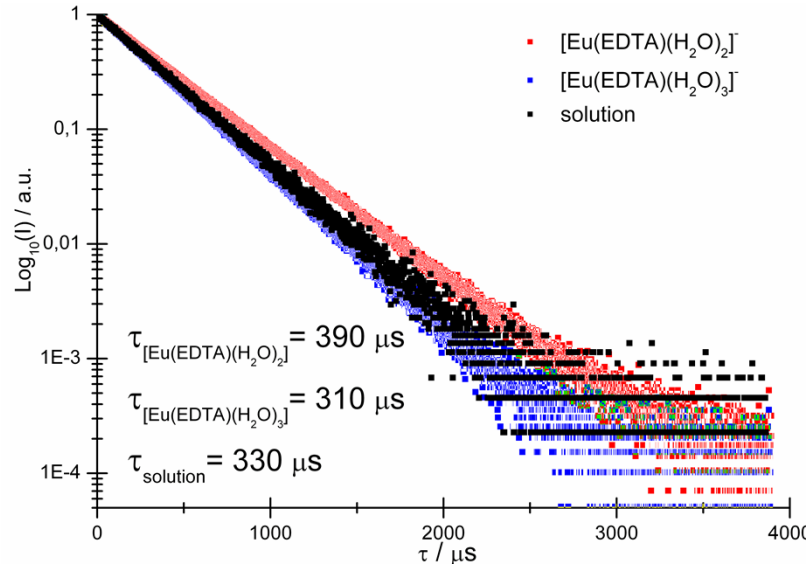


Figure 2S. Luminescence lifetimes of crystals **I** and **II** as well as solution (λ_{ex} = 394 nm, λ_{ex} = 612 nm).

Using the equation $q_{Eu^{3+}} = 1.05 \times \frac{1}{\tau_{H_2O}} - 0.7$ derived by P. P. Barthelemy and G. R. Choppin **(***Inorg. Chem.,* 1989, **28**, 3354) the average number of coordinated water molecules to Eu^{3+} was calculated for the systems under study. (1)

q_{H_2O} = 2.7 (for I), q_{H_2O} = 2.0 (for II) and q_{H_2O} = 2.5 (for solution T=293 K).

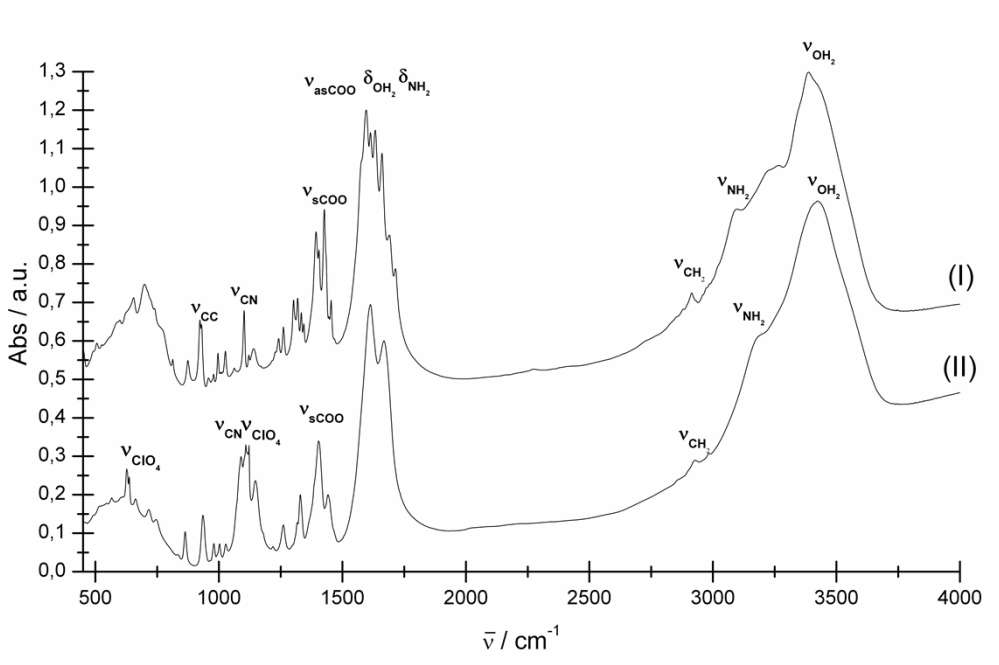


Figure 3S. IR spectra of **I** and **II**.

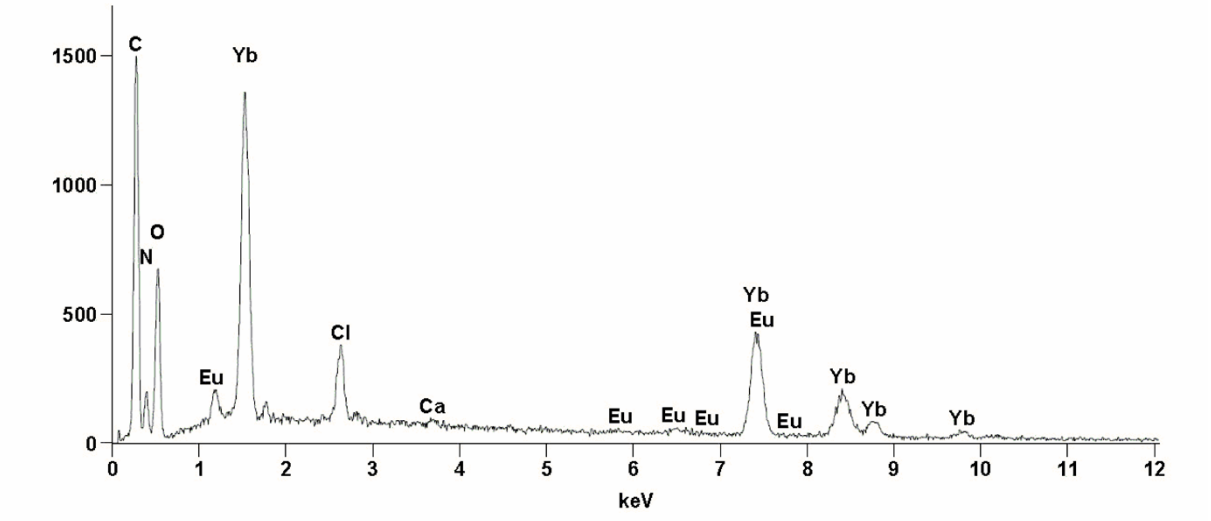


Figure 4S. Scanning electron microscope spectrum of **II**.

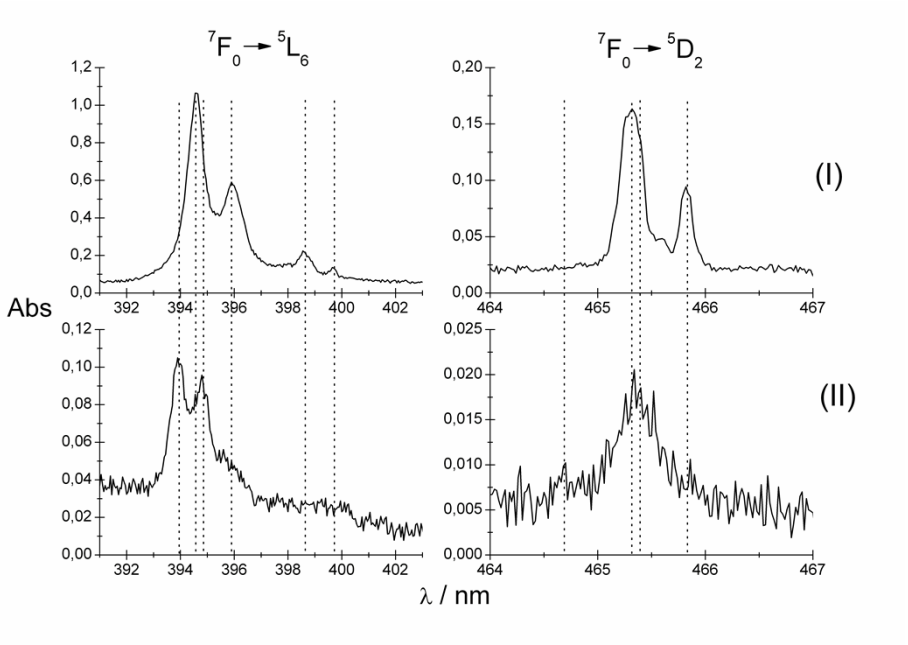
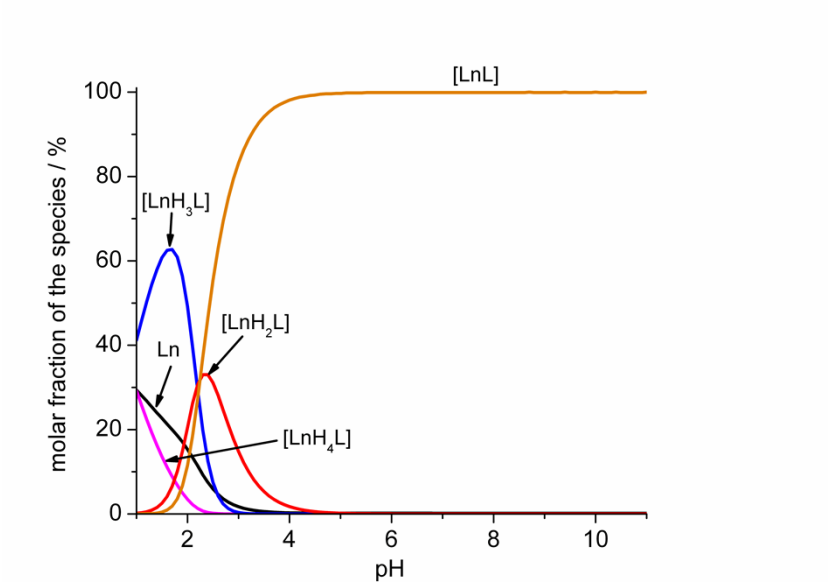


Figure 5S. UV-vis absorption spectrum of crystals **I** and **II**.



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