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# Lanthanide complexes with (4,7-dichloro-1,10-phenanthroline-2,9-diyl)-bis(pyrrolidin-1-ylmethanone): bifunctional materials for homogeneous catalysis and luminescent thermometry

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## Contents

## Experimental details

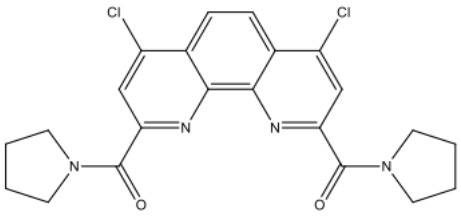

**Fig. S1** Structural formula of ligand

*The ligand* used in this work was synthesized according to the method presented in the work [S1].

*Lanthanide complexes* $LnLCl_3(H_2O)_2 \equiv$ **LnL** (Ln = Eu, Yb, Gd) were obtained by the dissolution of lanthanide chlorides and ligands (1:1 mol%) in ethanol. The solution was stirred for 24 hours and evaporated to dryness, the obtained powder was recrystallized from water.

The *IR spectra* were recorded on a Thermo ScientificTM NicoletTM iS50 FTIR Spectrometer as powdered at ATR.

*MALDI MS* spectra were carried out on a Bruker Autoflex II instrument (resolution FWHM 18000) equipped with a nitrogen laser with an operating wavelength of 337 nm and a time-of-flight mass analyzer operating in the reflectron mode. Accelerating voltage 20 kV. The samples were applied to a polished steel substrate. The spectra were recorded in the positive ion mode. The resulting spectrum was the sum of 50 spectra obtained at different points in the sample.

NMR spectra were recorded using standard 5 mm sample tubes on Agilent 400-MR spectrometer with operating frequencies of 400.1 MHz ($^1$H) and Bruker Avance-600 spectrometer with operating frequencies of 600.1 MHz ($^1$H). Deuterated solvent acetonitrile-$d_3$ for NMR spectra were purchased from commercial sources and used without further purification.

The study of *luminescent properties* was carried out in CC solutions in ethanol and acetonitrile (c=2mg/ml). Luminescence properties in visible range (emission and excitation spectra, lifetimes) at room temperature and upon heating were carried out on a FluoroMax-Plus spectrometer (HORIBA) with 1905-OFR 150-W Xenon Lamp as excitation source, excitation was performed through a ligand, and the absolute method in the integration sphere was used. Measurement of luminescence properties in NIR rage was performed by an Ocean Optics Maya 2000 detector with diode laser ($\lambda_{ex}$ = 365 nm) as an excitation source.

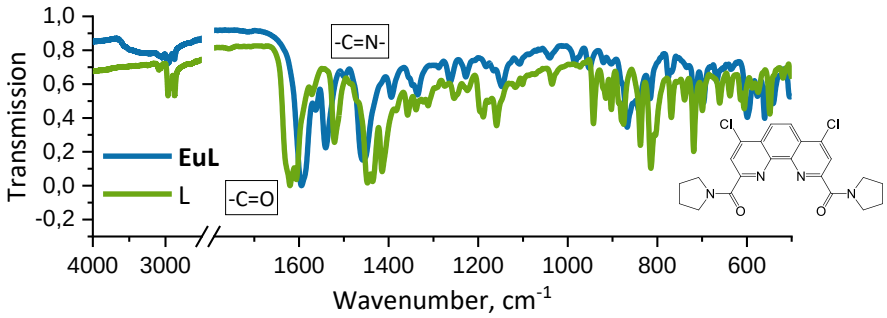


**Fig. S2** FTIR spectra of ligand and corresponding Eu-complex

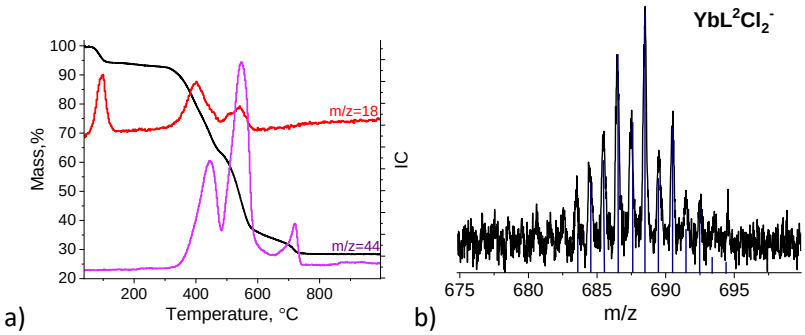


**Fig. S3 a)** TGA data and **b)** Fragment of MALDI mass-spectra with Yb isotopic distribution.

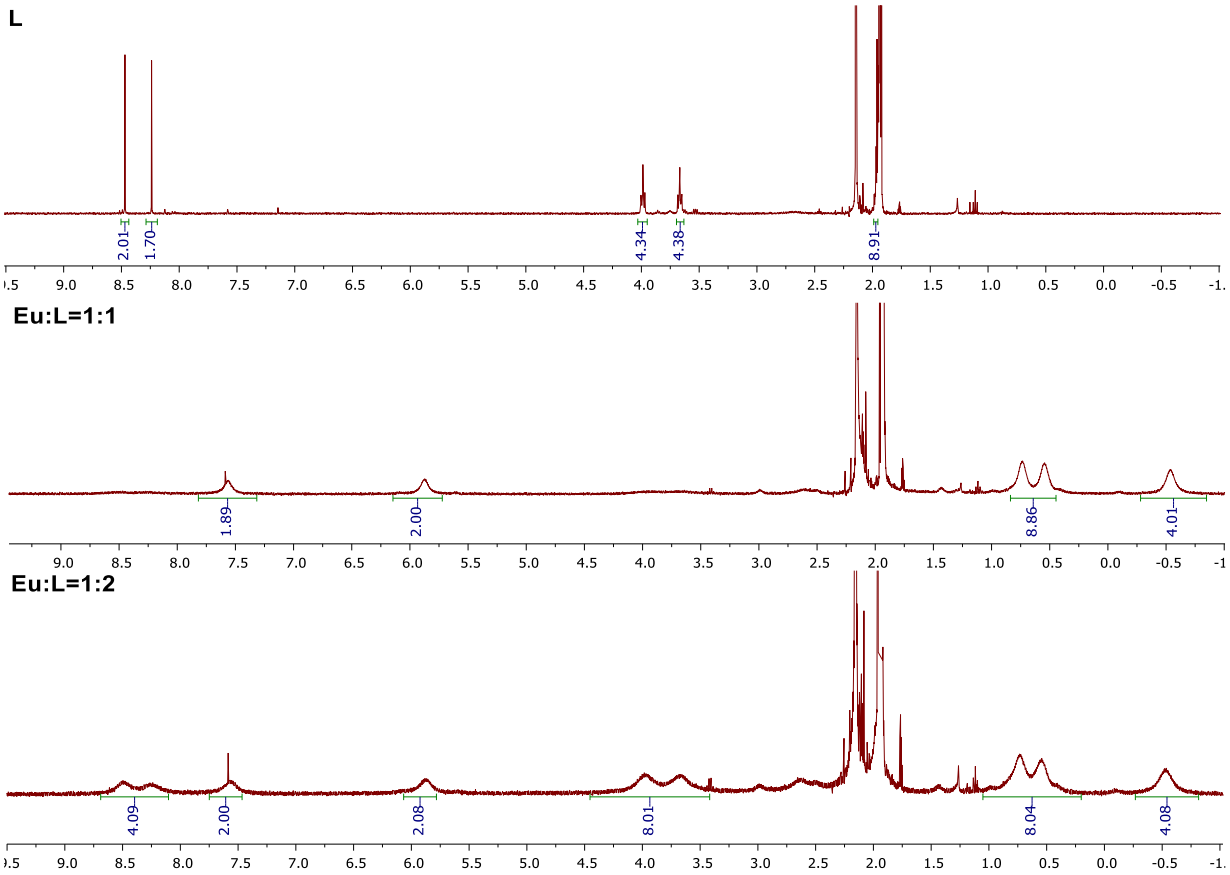


**Fig. S4** NMR spectra for $EuCl_3$ and ligand mixture in ratio 0:1, 1:1, 1:2

According to MALDI data complex exist in the form $LnL^{3+}$ in a solution of methanol and acetonitrile. From the NMR spectra for mixtures of $EuCl_3$ and L in a ratio of 1:2 (mol) and 1:1 (mol), we see that the ions bind in a ratio of 1:1, and a two-fold excess of the ligand leads to the existence of equimolar amounts of a europium-bound and unbound form in the solution.

## Photophysical properties

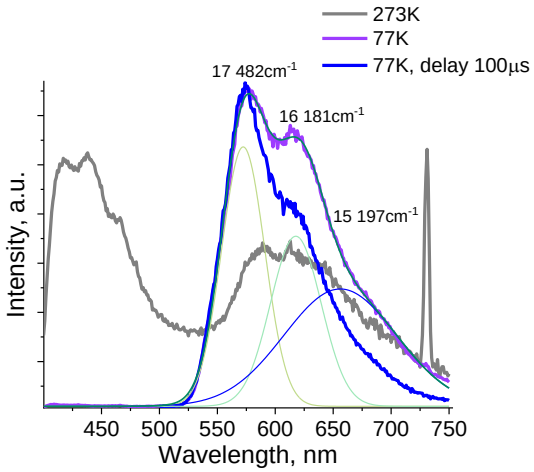


**Fig. S5** Luminescence spectrum for gadolinium complex at room temperature and 77K

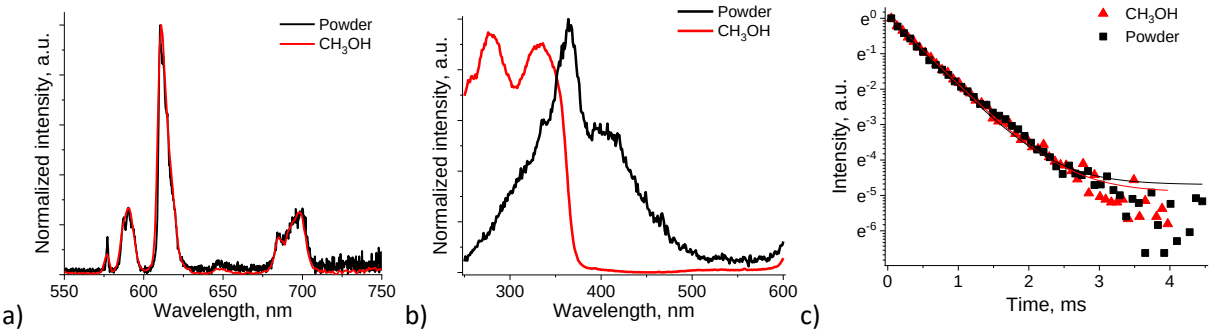


**Fig. S6** Luminescence characteristics of **EuL** $CH_3OH$ solutions and powders: emission (a) and excitation (b) spectra, lifetimes (c).

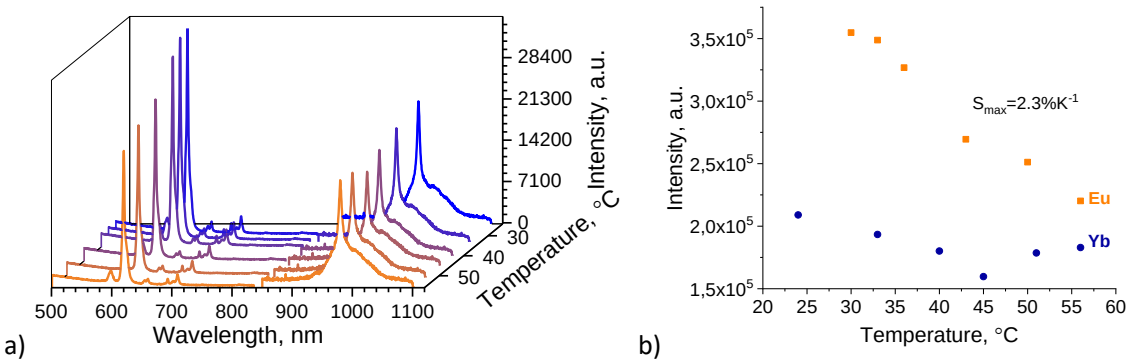


**Fig. S7** Luminescence spectra and intensities of **EuL** and **YbL** acetonitrile solutions during heating

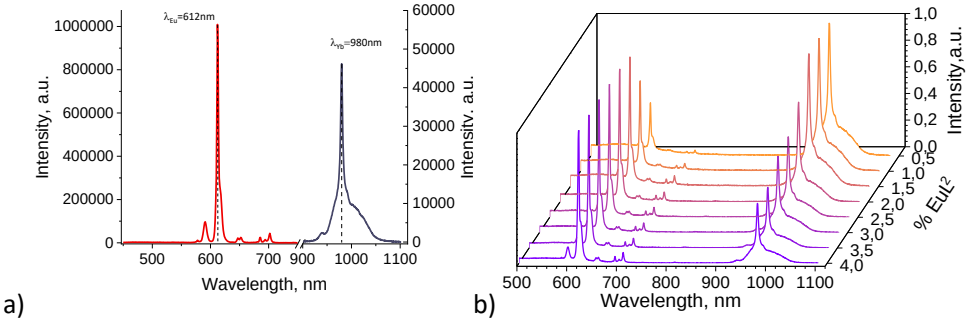


**Fig. S8** Luminescence spectra of **EuL** and **YbL** in $CH_3CN$ solutions (a) and luminescent titration to comparable intensities of both ions (b)

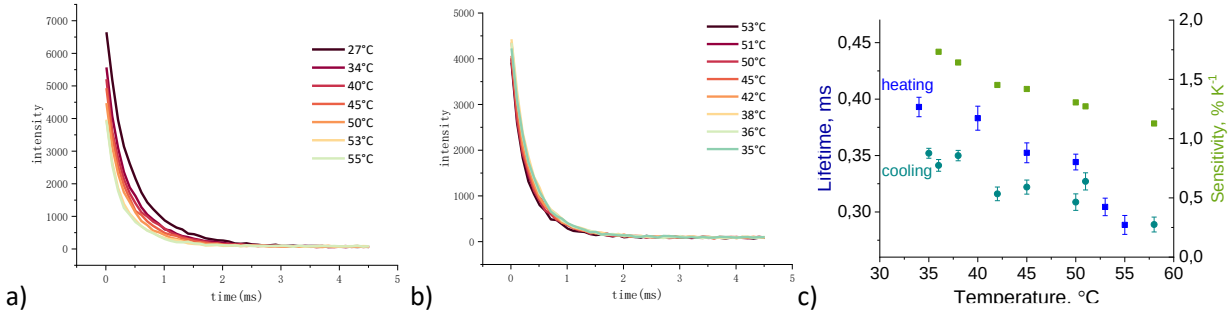


**Fig. S9** Decay curves (a,b), lifetime and temperature sensitivity dependence on temperature (c) for a solution of **EuL** in methanol (heating up to 55°C and further cooling)

## CC luminescence in the reaction mixture

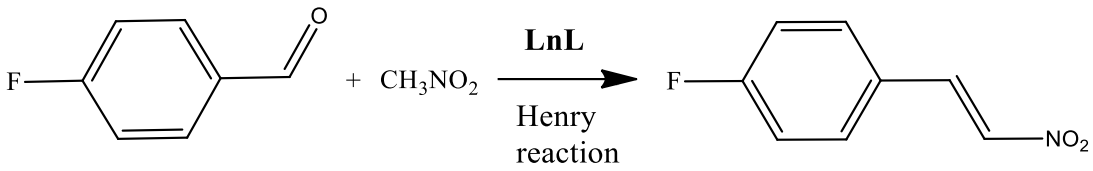


**Fig. S10.** Henri's reaction scheme

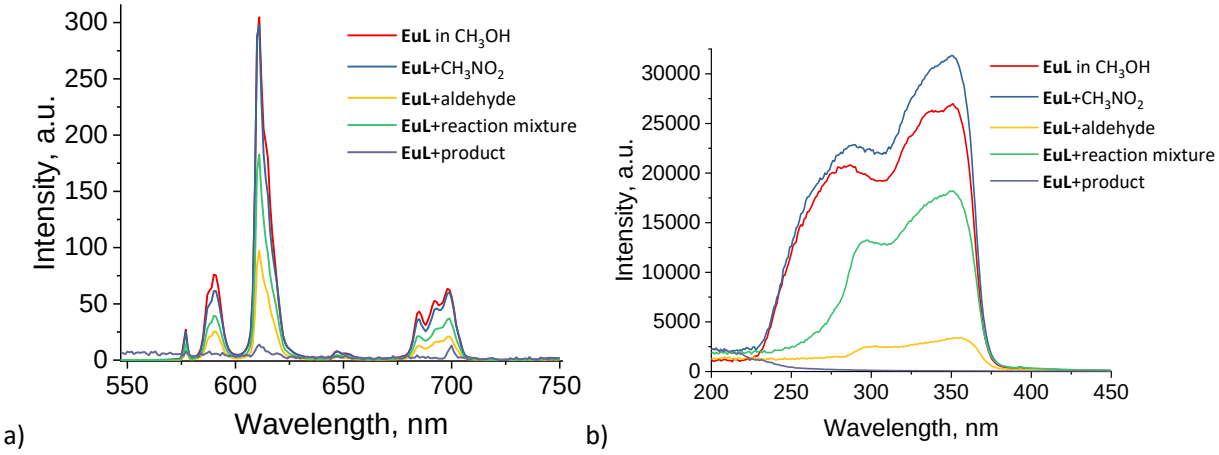


**Fig. S11** a) Emission and b) excitation spectra for **EuL** in the presence of reaction components

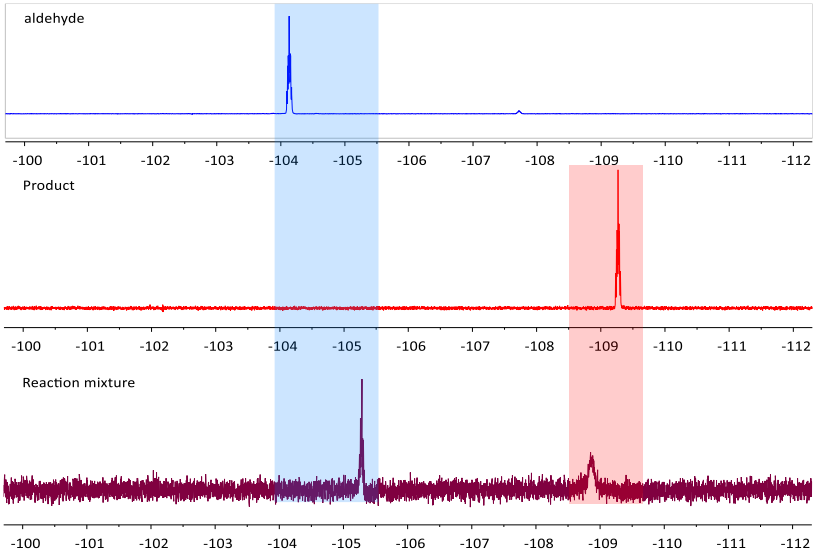


**Fig. S12** NMR spectrum for the reaction mixture in comparison with parent aldehyde and product

S1. Pavel S. Lemport, Petr I. Matveev, Alexander V. Yatsenko, Mariia V. Evsiunina, Valentine S. Petrov, Boris N. Tarasevich, Vitaly A. Roznyatovsky, Pavel V. Dorovatovskii, Victor N. Khrustalev, Sergey S. Zhokhov, Vitaly P. Solov'ev, Leonid A. Aslanov, Vladimir G. Petrov, Stepan N. Kalmykov, Valentine G. Nenajdenko and Yuri A. Ustyniuk, *RSC Adv.*, 2020, **10**, 26022; https://doi.org/10.1039/D0RA05182A.