Supplementary Information for

Spectroscopic investigation of the different complexation and extraction properties of diastereomeric diglycolamide ligands

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FI Factors

The FI factor of a complex is defined by the following equation:

$$FI_{complex} = \frac{I_{complex}}{I_{Solvens}}$$

Thereby $I_{complex}$ and $I_{Solvens}$ denote the intensity of a Cm(III) complex as well as the Cm(III) solvent complex both normalized to the energy of the excitation laser.

Due to their easier application to the experimental data, FI factors instead of fluorescence quantum yields or fluorescence quantum efficiencies are used in the presented work.
The FI factor of a species is not an absolute value. It depends on quantum yields and experimental setup. It is, therefore, not directly transferable to other systems.

Figures

Fluorescence lifetime of Cm(III) and Eu(III) in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

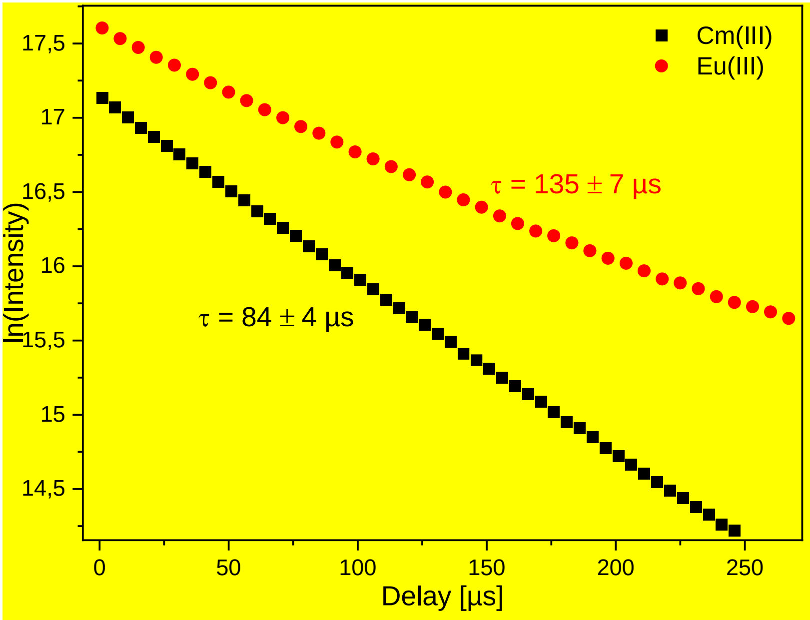

Fig. S1 *Decrease of the fluorescence intensity of Cm(III) and Eu(III) in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$ with increasing delay time (c(Cm) = 1 x 10^{-7} mol L^{-1}, c(Eu) = 1 x 10^{-5} mol L^{-1}).*

Evolution of the fluorescence intensity for the complexation of Cm(III) with cis-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

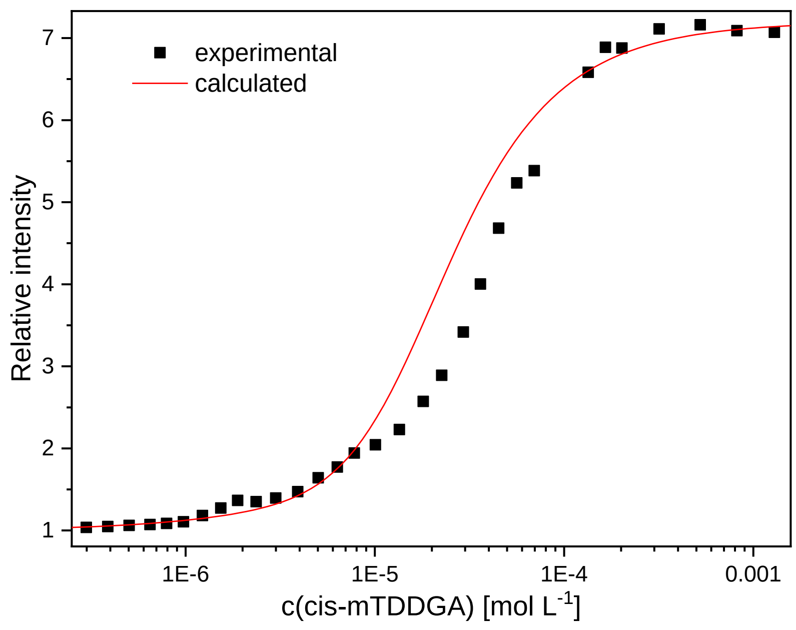

Fig. S2 *Evolution of the relative fluorescence intensity for the complexation of Cm(III) with cis-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$ as a function of the cis-mTDDGA concentration ($(c(Cm(III))_{ini} = 1 \times 10^{-7}$ mol L^{-1}).*

Slope analyses for the complexation of Cm(III) with cis-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

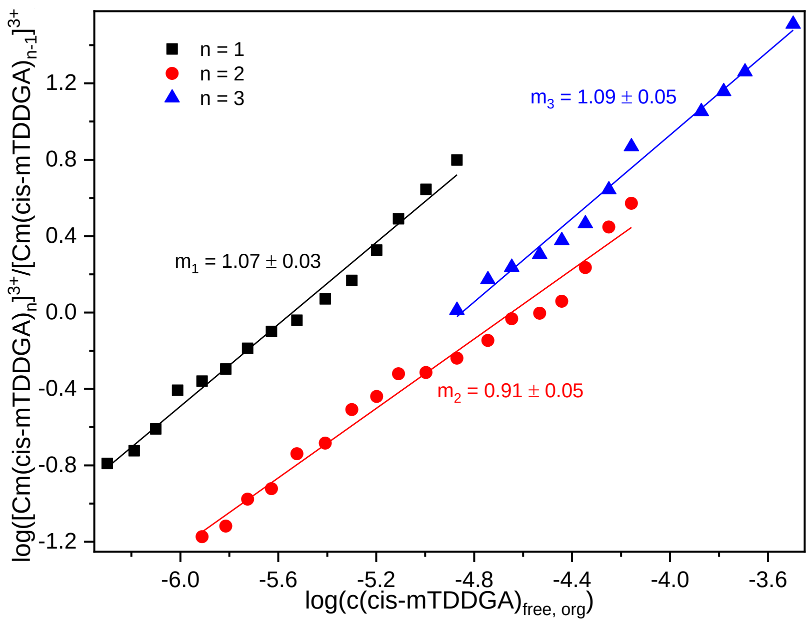

Fig. S3 *Double logarithmic plots of the concentration ratios of $[Cm(cis\text{-}mTDDGA)_n]^{3+}/[Cm(cis\text{-}mTDDGA)_{n-1}]^{3+}$ as a function of the free cis-mTDDGA concentration.*

Cm(III) emission spectra for the complexation of Cm(III) with trans-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

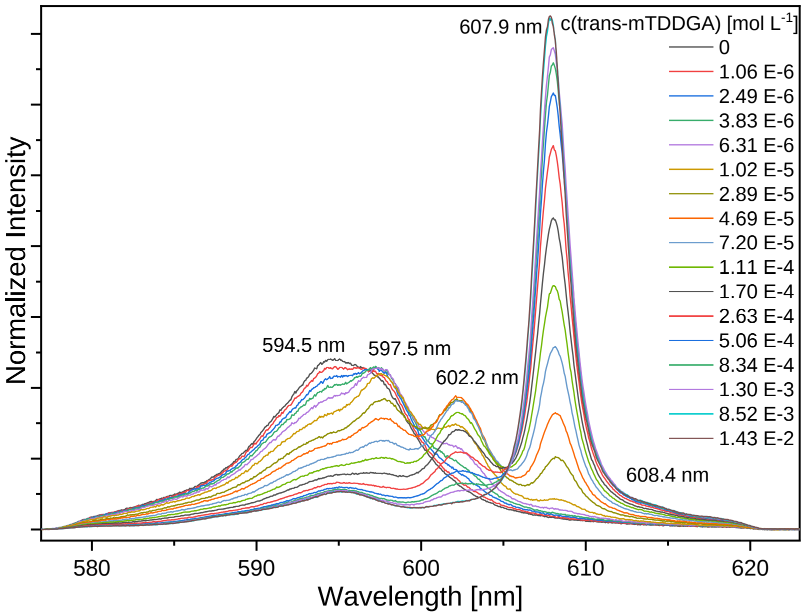

Fig. S4 *Normalized Cm(III) emission spectra for the complexation of Cm(III) with trans-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$ as a function of the trans-mTDDGA concentration ($c(Cm(III))_{ini}$ = 1 x 10^{-7} mol L^{-1}).*

Speciation diagram for the complexation of Cm(III) with trans-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

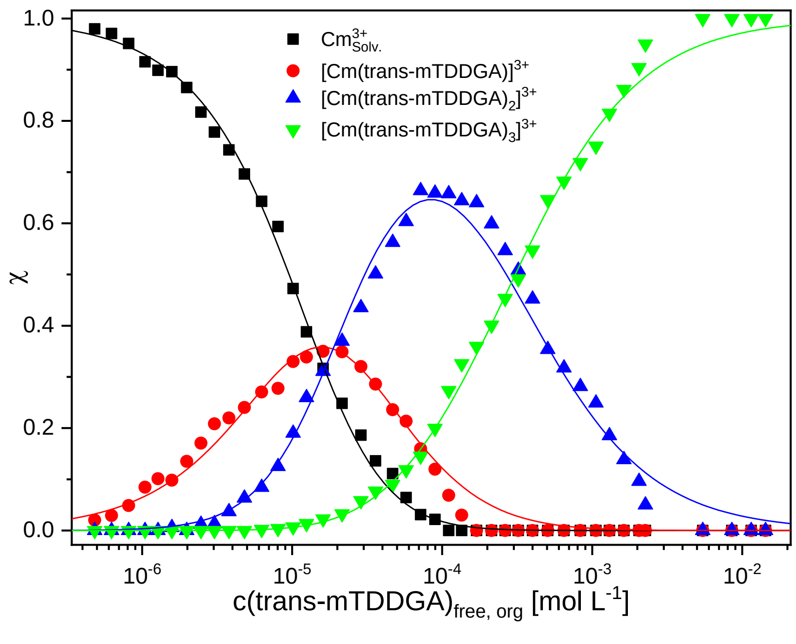

Fig. S5 *Fractions of $[Cm(Solv.)]^{3+}$ and the $[Cm(trans\text{-}mTDDGA)_n]^{3+}$ complexes (n = 1-3) as a function of the free trans-mTDDGA concentration in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$. Dots, experimental data. Lines, calculated with log β'_1 = 4.8, log β'_2 = 9.5 and log β'_3 = 13.1.*

Evolution of the fluorescence intensity for the complexation of Cm(III) with trans-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

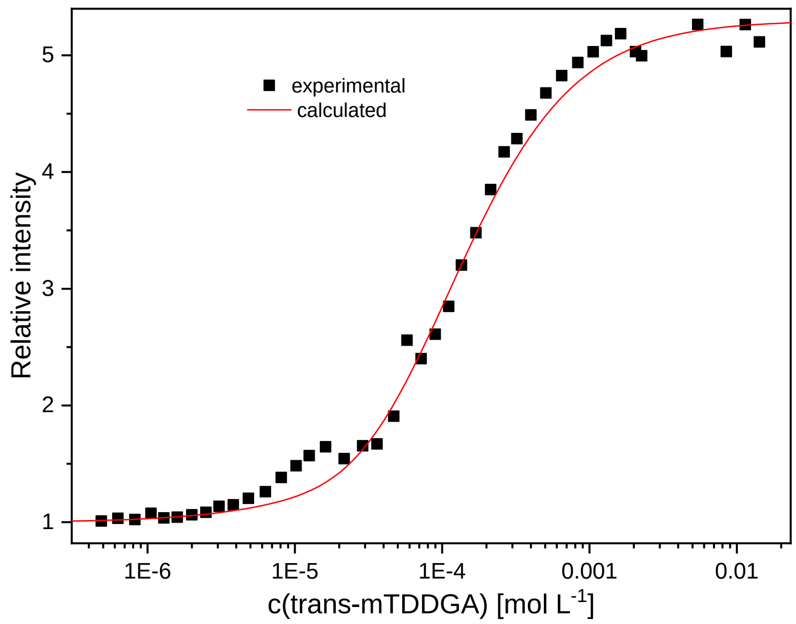

Fig. S6 *Evolution of the relative fluorescence intensity for the complexation of Cm(III) with trans-mTDDGA in 2-propanol +5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$ as a function of the trans-mTDDGA concentration ($(c(Cm(III))_{ini} = 1 \times 10^{-7}$ mol L^{-1}).*

Slope analyses for the complexation of Cm(III) with trans-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

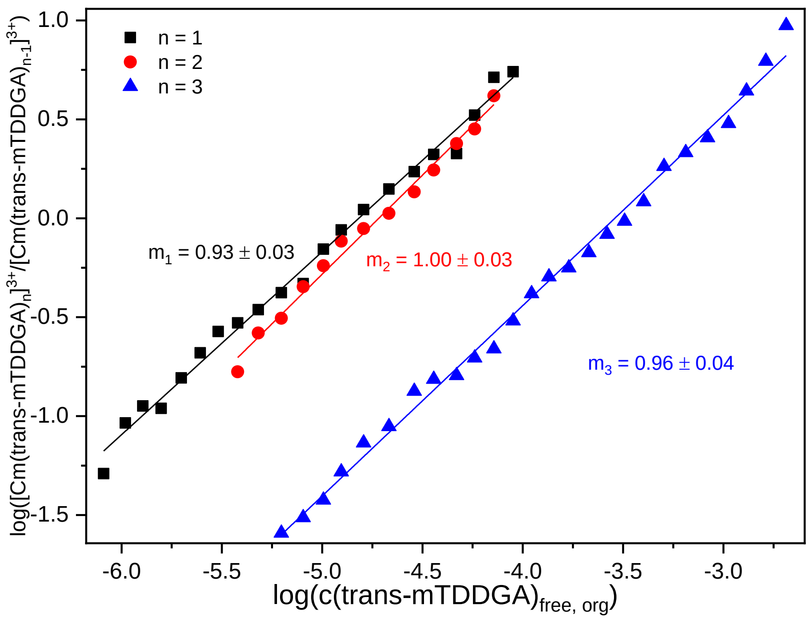

Fig. S7 *Double logarithmic plots of the concentration ratios of $[Cm(trans\text{-}mTDDGA)_n]^{3+}/[Cm(trans\text{-}mTDDGA)_{n-1}]^{3+}$ as a function of the free trans-mTDDGA concentration.*

Eu(III) emission spectra for the complexation of Eu(III) with trans-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

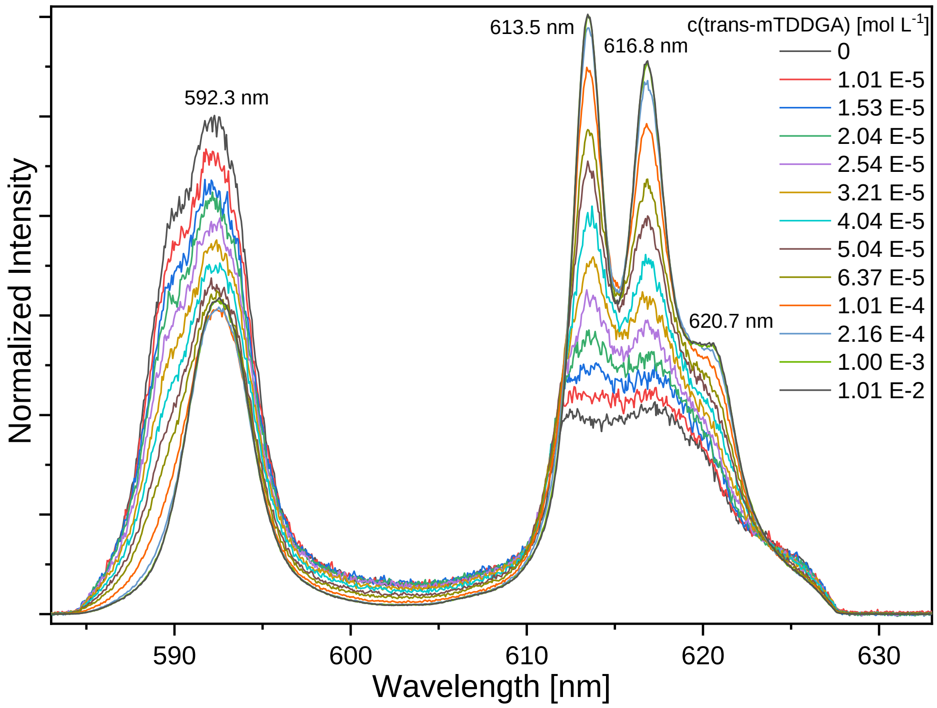

Fig. S8 *Normalized Eu(III) emission spectra for the complexation of Eu(III) with trans-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$ as a function of the trans-mTDDGA concentration ($c(Eu(III))_{ini}$ = 1 x 10^{-5} mol L^{-1}).*

Evolution of the fluorescence intensity for the complexation of Eu(III) with cis-/trans-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

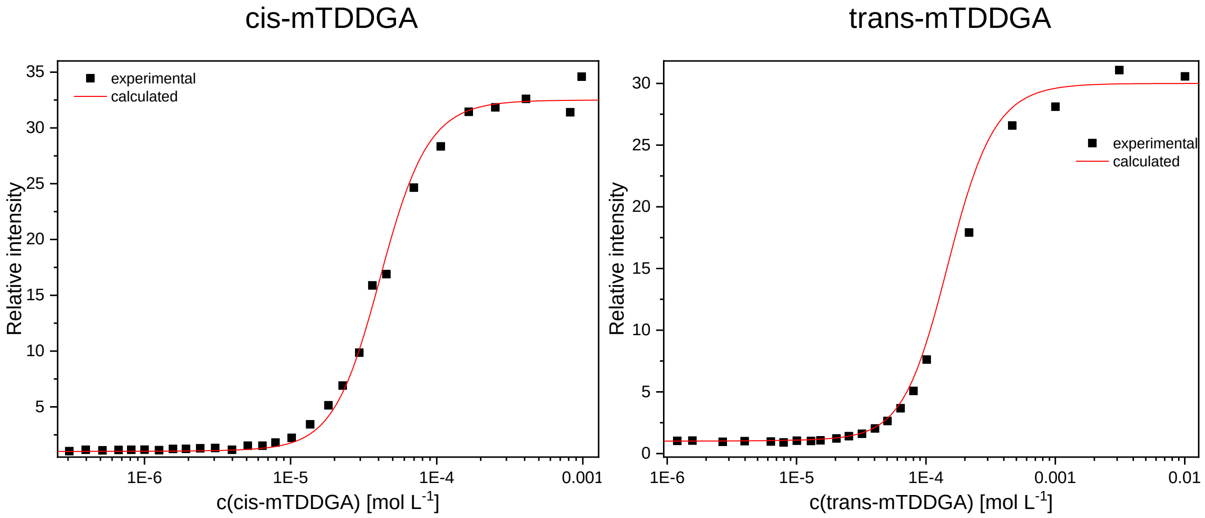

Fig. S9 *Evolution of the relative fluorescence intensity for the complexation of Cm(III) with cis- (left) and trans-mTDDGA (right) in 2-propanol and 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$ as a function of the cis-/trans-mTDDGA concentration ($c(Eu(III))_{ini}$ = 1 x 10^{-5} mol L^{-1}).*

Speciation diagram for the complexation of Eu(III) with trans-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

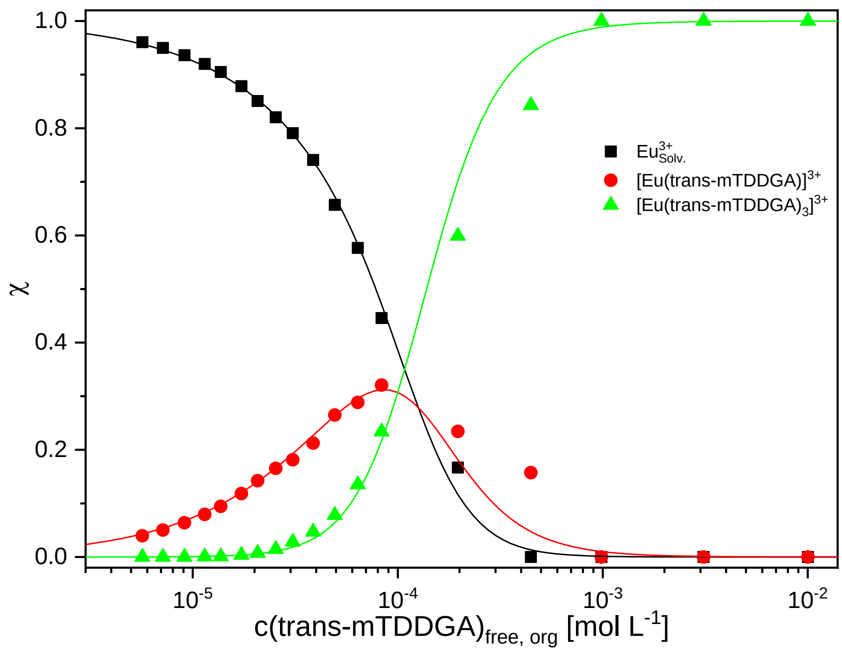

Fig. S10 *Fractions of $[Eu(Solv.)]^{3+}$ and the $[Eu(trans\text{-}mTDDGA)_n]^{3+}$ complexes (n = 1,3) as a function of the free trans-mTDDGA concentration in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$. Dots, experimental data. Lines, calculated with $\log\beta'_1$ = 3.9 and $\log\beta'_3$ = 11.9.*

Slope analyses for the complexation of Eu(III) with cis-/trans-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

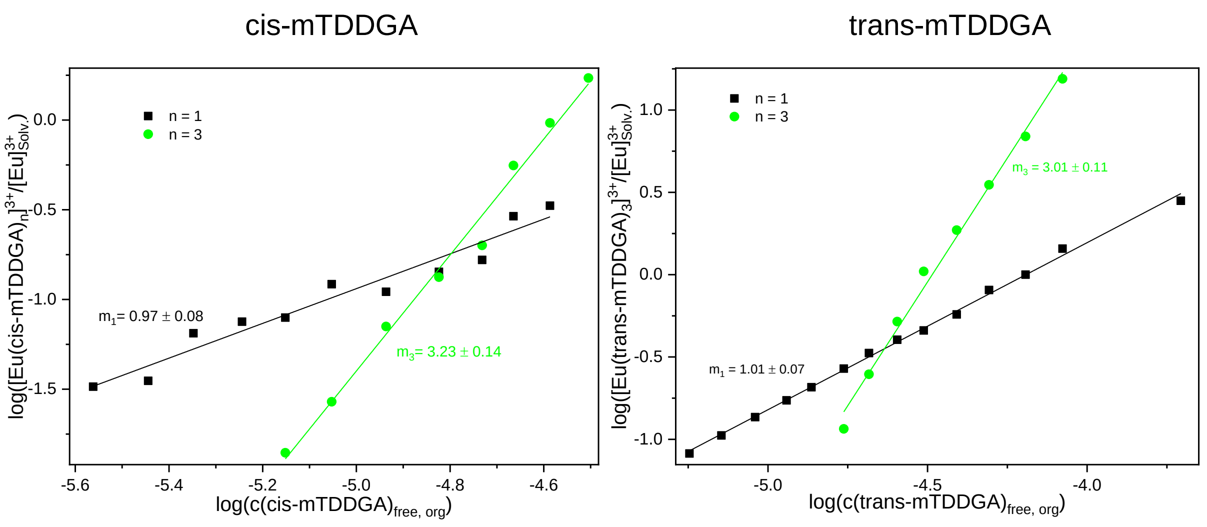

Fig. S11 *Double logarithmic plot of the concentration ratio of [Eu(L-mTDDGA)$_n$]$^{3+}$/[Eu(Solv.)]$^{3+}$ as a function of the freecis- (left) and trans-mTDDGA (right) concentration.*

Influence of the nitrate concentration on the complexation of Eu(III) with trans-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

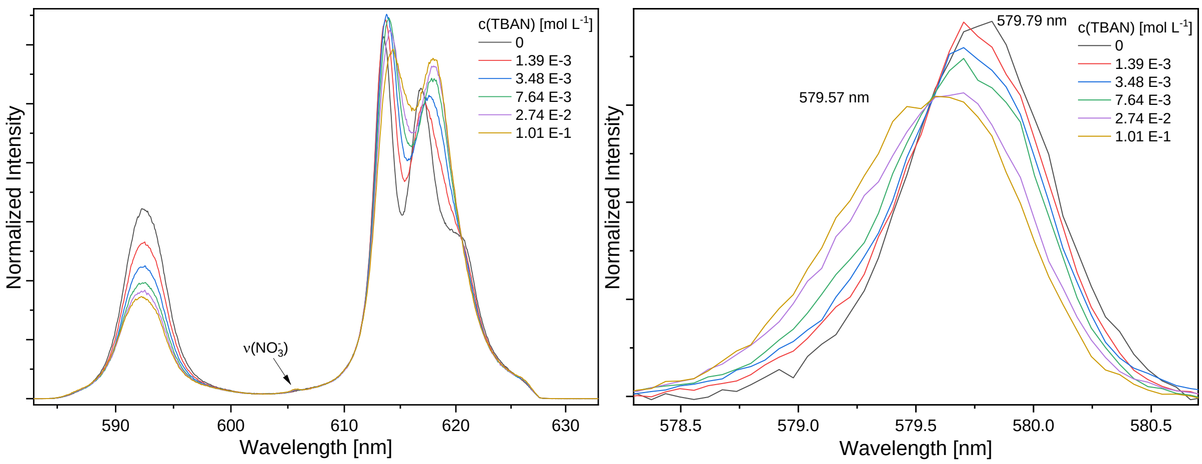

Fig. S12 *Normalized Eu(III) emission spectra of the $^5D_0 \rightarrow {}^7F_n$ (left: n = 1,2; right: n = 0) transitions with 5.7 x 10^{-3} mol L^{-1} trans-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$ as a function of the TBAN concentration.*

Influence of the nitrate concentration on the complexation of Cm(III) with cis-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

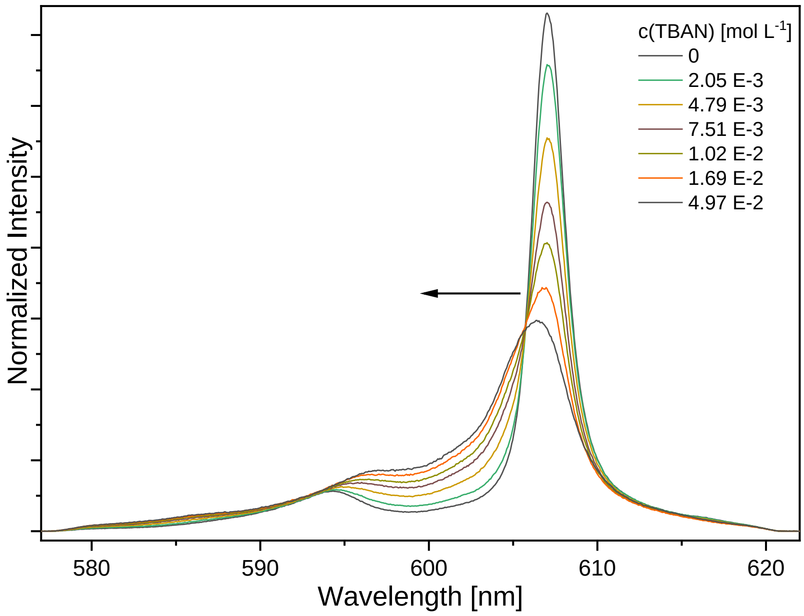

Fig. S 13 *Normalized Cm(III) emission spectra with 1.1 x 10^{-3} mol L^{-1} cis-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$ as a function of the TBAN concentration.*

Influence of the nitrate concentration on the complexation of Eu(III) with cis-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

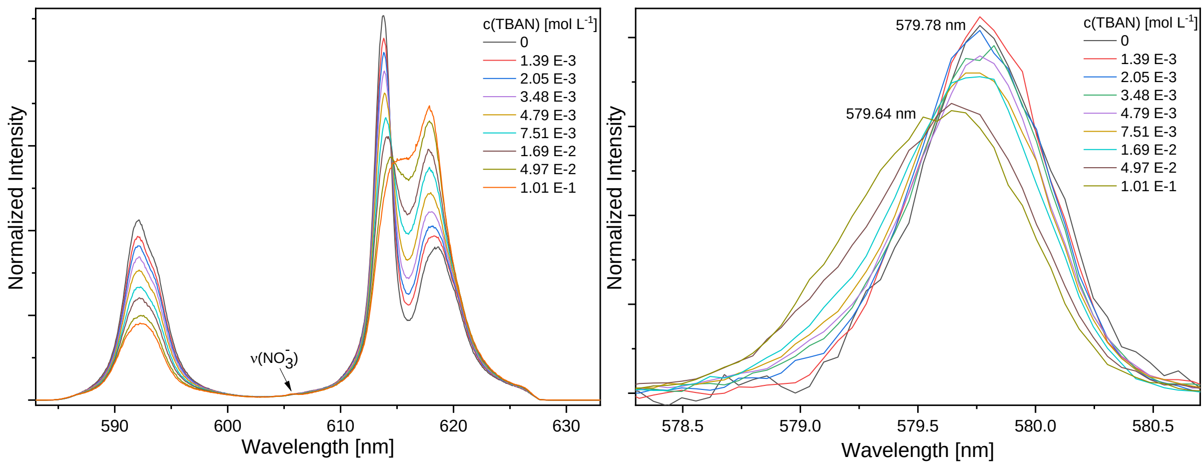

Fig. S 14 *Normalized Eu(III) emission spectra of the $^5D_0 \rightarrow {}^7F_n$ (left: n = 1,2; right: n = 0) transitions with 1.1 x 10^{-3} mol L^{-1} cis-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$ as a function of the TBAN concentration.*

Optimized structures of the $[Cm(trans\text{-}mTDDGA)_2(NO_3)_n(H_2O)_m]^{(3-n)+}$ complexes

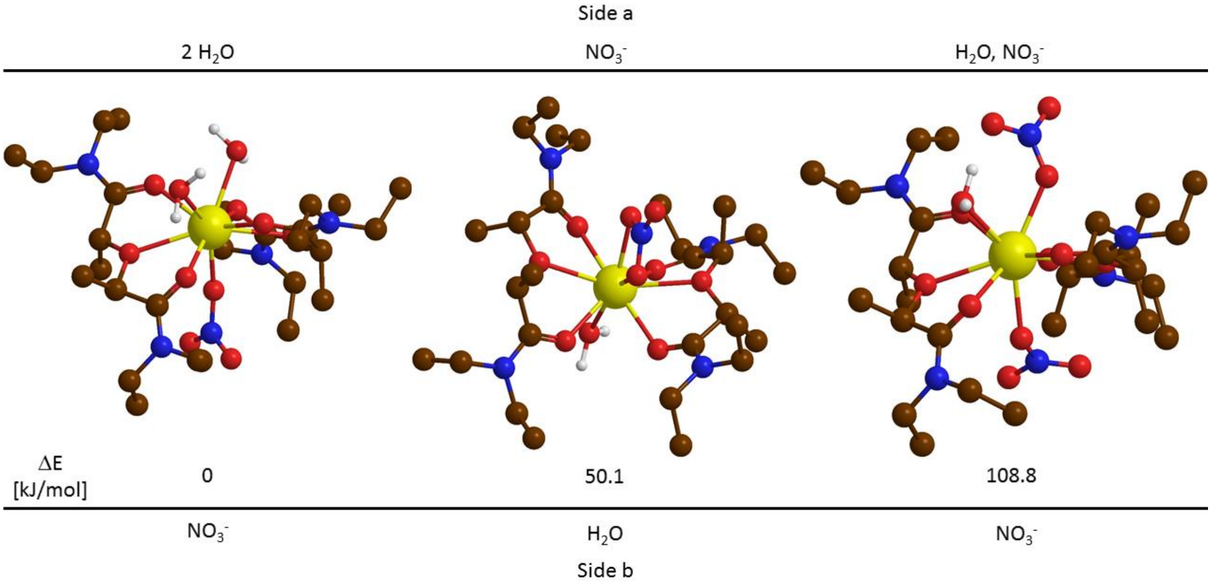

Fig. S 15 *Optimized structures of the $[Cm(trans\text{-}mTDDGA)_2(NO_3)_n(H_2O)_m]^{(3-n)+}$ complexes (with m = 1, n = 2; m = n = 1; m = 2, n = 1). Protons of the ligand framework are not shown. Carbon (brown), nitrogen (blue), oxygen (red), hydrogen (white), curium (yellow). Theoretical level: B3-LYP/def2-TZVP*

Tables

Slopes of the slope analyses for the complexation of Cm(III) and Eu(III) with cis-/trans-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$

Tab. S1 *Slopes of the slope analyses for the complexation of Cm(III) and Eu(III) with cis- and trans-mTDDGA in 2-propanol + 5 Vol.% H_2O and 1 x 10^{-2} mol L^{-1} $HClO_4$.*

	cis-mTDDGA		trans-mTDDGA	
	Cm(III)	Eu(III)	Cm(III)	Eu(III)
n = 1	1.07 ± 0.03	0.97 ± 0.08	0.93 ± 0.03	1.01 ± 0.07
n = 2	0.91 ± 0.05	-	1.00 ± 0.03	-
n = 3	1.09 ± 0.05	3.23 ± 0.14	0.96 ± 0.04	3.01 ± 0.11