

**Supplementary Information for**

**Extraction and Complexation studies with 2,6-bis(5-(tert-butyl)-1*H*-pyrazol-3-yl)pyridine in the presence of 2-bromohexanoic acid.**

Jonas Stracke,<sup>a,b</sup> Patrik Weßling,<sup>b</sup> Thomas Sittel,<sup>a</sup> Paul Meiners,<sup>b</sup> Andreas Geist,<sup>a</sup> and Petra J. Panak.<sup>a,b</sup>

<sup>a</sup>Karlsruhe Institute of Technology (KIT), Institute for Nuclear Waste Disposal (INE), P.O. Box 3640, 76021 Karlsruhe, Germany

<sup>b</sup>Heidelberg University, Institut für Physikalische Chemie, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

**KEYWORDS** Actinides, Lanthanides, Lipophilic ligands, Complexation, Selectivity, N-Donor ligand.

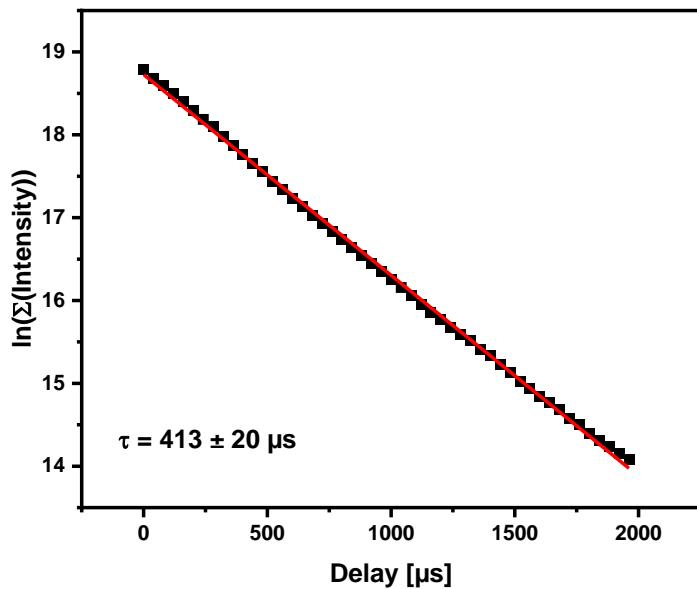
Corresponding Authors:

Jonas Stracke:            Jonas.stracke@kit.edu

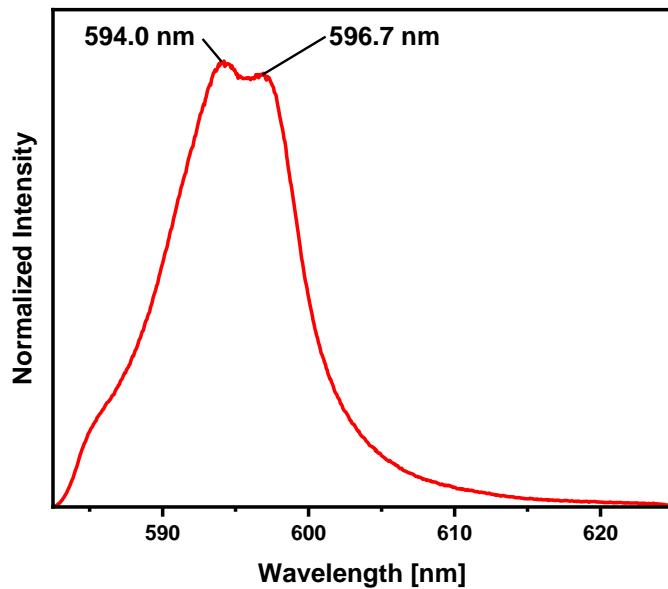
## Table of contents

TRLFS Cm(III).....	3
TRLFS Eu(III).....	5

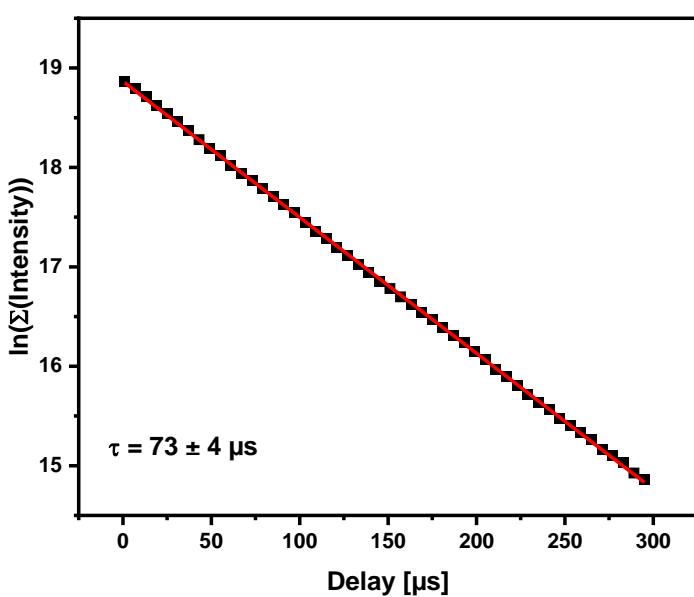
## TRLFS Cm(III)



**Figure S1:** Fluorescence lifetime of  $[\text{Cm}(\text{C4-BPP})_3]^{3+}$  in the organic phase after extraction. Organic phase  $1.0 \times 10^{-2}$  mol/L C4-BPP and  $5.0 \times 10^{-1}$  mol/L 2-bromohexanoic acid in TPH/1-octanol (10 vol.%). Aqueous phase  $3.0 \times 10^{-1}$  mol/L nitric acid. A/O = 1. T = 293 K.

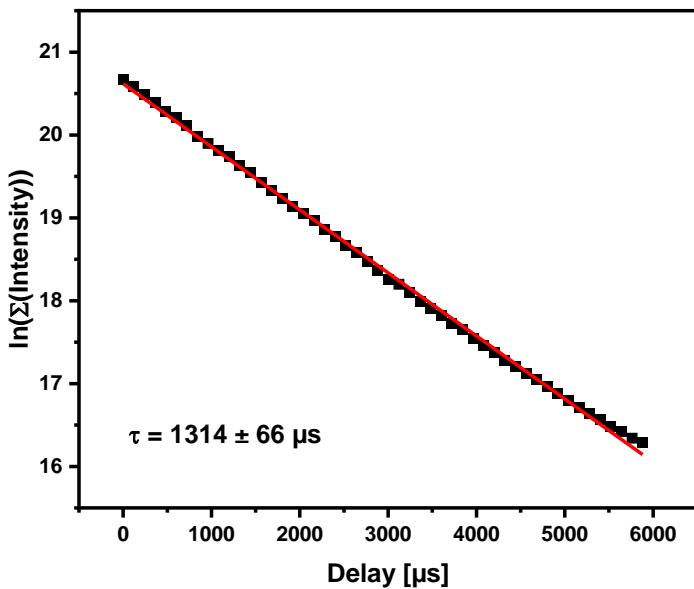


**Figure S2:** Normalized fluorescence spectra of Cm(III) in the aqueous phase after extraction. Organic phase  $1.0 \times 10^{-2}$  mol/L C4-BPP and  $5.0 \times 10^{-1}$  mol/L 2-bromohexanoic acid in TPH/1-octanol (10 vol.%). Aqueous phase  $3.0 \times 10^{-1}$  mol/L nitric acid. A/O = 1. T = 293 K.

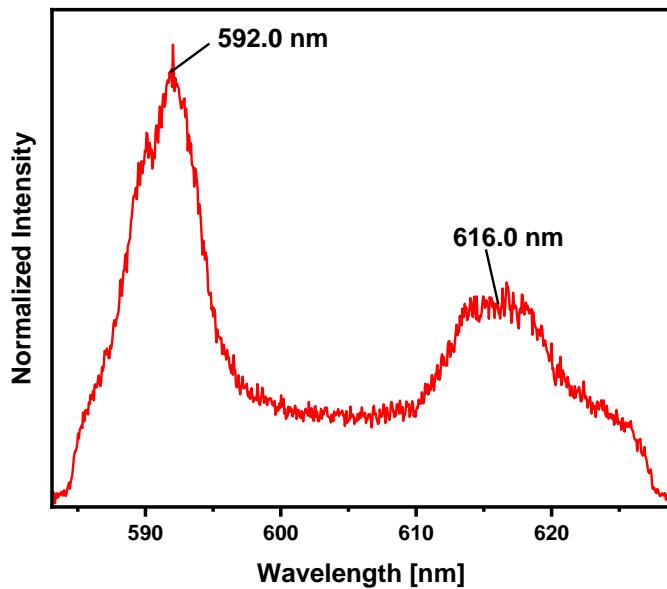


**Figure S3:** Fluorescence lifetime of  $[\text{Cm}(\text{solv.})]^{3+}$  in the aqueous phase after extraction. Organic phase  $1.0 \times 10^{-2}$  mol/L C4-BPP and  $5.0 \times 10^{-1}$  mol/L 2-bromohexanoic acid in TPH/1-octanol (10 vol.%). Aqueous phase  $3.0 \times 10^{-1}$  mol/L nitric acid. A/O = 1. T = 293 K.

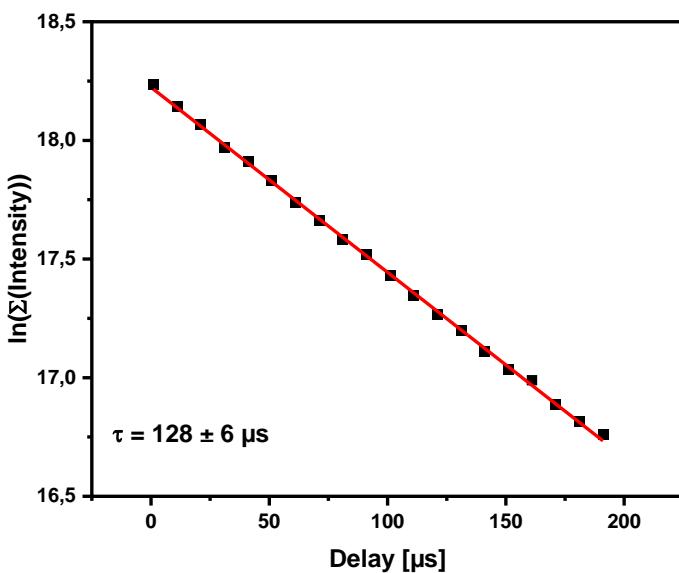
## TRLFS Eu(III)



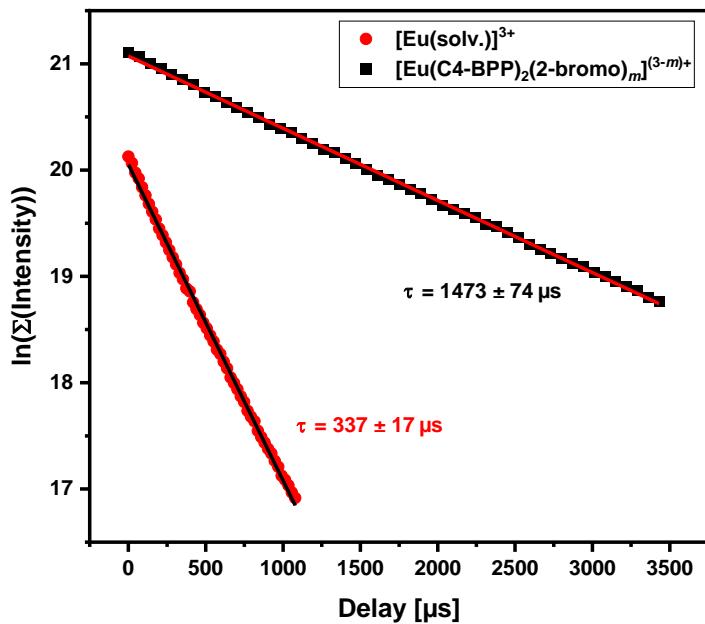
**Figure S4:** Fluorescence lifetime of  $[\text{Eu}(\text{C4-BPP})_2(\text{2-bromohexanoate})_m]^{(3-m)+}$  ( $m = 1-3$ ) in the organic phase after extraction. Organic phase  $1.0 \times 10^{-2}$  mol/L C4-BPP and  $5.0 \times 10^{-1}$  mol/L 2-bromohexanoic acid in TPH/1-octanol (10 vol.%). Aqueous phase  $3.0 \times 10^{-1}$  mol/L nitric acid. A/O = 1. T = 293 K.



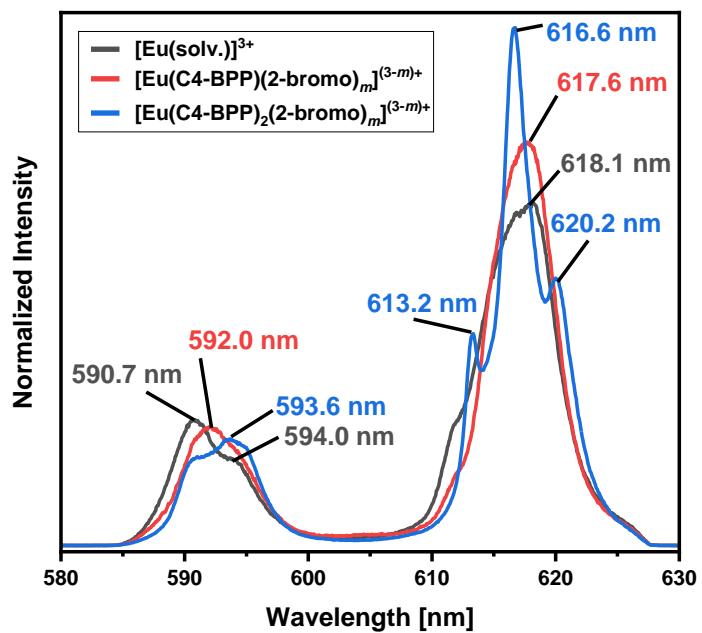
**Figure S5:** Normalized fluorescence spectra of the  $^7\text{F}_1$  and  $^7\text{F}_2$  emission bands of Eu(III) in the aqueous phase after extraction. Organic phase  $1.0 \times 10^{-2}$  mol/L C4-BPP and  $5.0 \times 10^{-1}$  mol/L 2-bromohexanoic acid in TPH/1-octanol (10 vol.%). Aqueous phase  $3.0 \times 10^{-1}$  mol/L nitric acid. A/O = 1. T = 293 K.



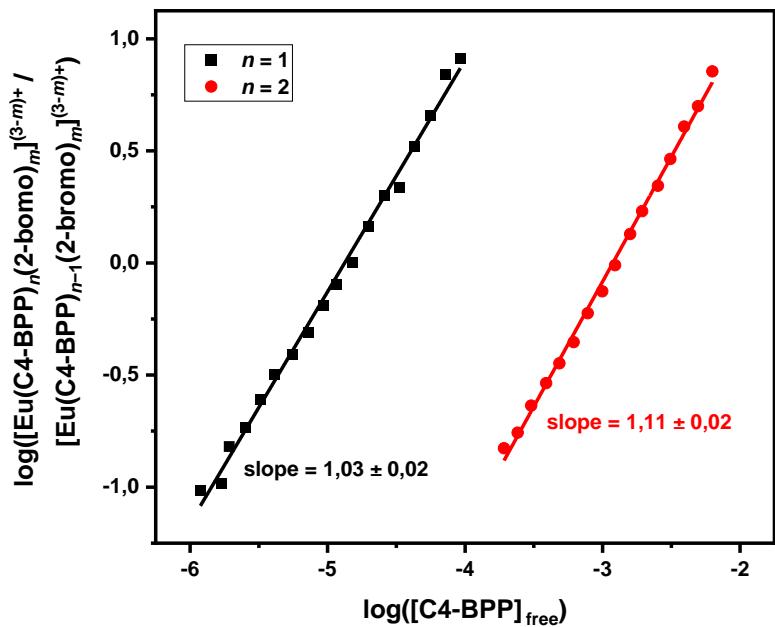
**Figure S6:** Fluorescence lifetime of  $[\text{Eu}(\text{solv.})]^{3+}$  in the aqueous phase after extraction. Organic phase  $1.0 \times 10^{-2}$  mol/L C4-BPP and  $5.0 \times 10^{-1}$  mol/L 2-bromohexanoic acid in TPH/1-octanol (10 vol.%). Aqueous phase  $3.0 \times 10^{-1}$  mol/L nitric acid. A/O = 1. T = 293 K.



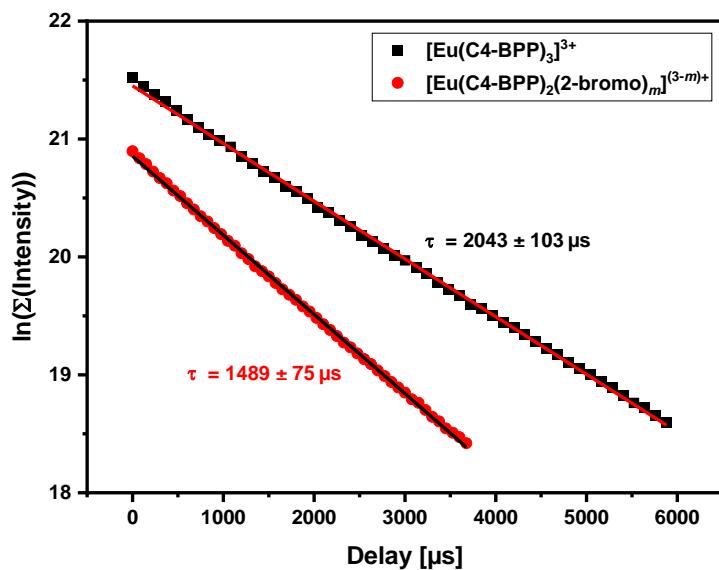
**Figure S7:** Fluorescence lifetime of  $[\text{Eu}(\text{C4-BPP})_n(\text{2-bromohexanoate})_m]^{(3-m)+}$  ( $n = 0, 2$ ;  $m = 1-3$ ) in methanol containing 1.5 vol.% water and 0.5 mol/L 2-bromohexanoic acid.  $[\text{C4-BPP}] = 0$  mol/L ( $n = 0$ ),  $1.00 \times 10^{-2}$  mol/L ( $n = 2$ ),  $[\text{Eu}]_{\text{ini}} = 1.0 \times 10^{-5}$  mol/L. (2-bromohexanoate is abbreviated as 2-bromo).



**Figure S8:** Normalized single component spectra of the  $[\text{Eu}(\text{C4-BPP})_n(2\text{-bromohexanoate})_m]^{(3-m)+}$  ( $n = 0\text{-}2$ ,  $m = 1\text{-}3$ ) complexes in methanol containing 1.5 vol.% water and  $5.0 \times 10^{-1}$  mol/L 2-bromohexanoic acid.  $[\text{Eu(III)}]_{\text{ini}} = 1.0 \times 10^{-5}$  mol/L. (2-bromohexanoate is abbreviated as 2-bromo).



**Figure S9:** Slope analyses for the complexation of Eu(III) with C4-BPP in methanol containing 1.5 vol.% water and  $5.0 \times 10^{-1}$  mol/L 2-bromohexanoic acid. Plot of  $\log\left(\frac{[\text{Eu}(\text{C4-BPP})_n(\text{2-bromohexanoate})_m]^{(3-m)+}}{[\text{Eu}(\text{C4-BPP})_{n-1}(\text{2-bromohexanoate})_m]^{(3-m)+}}\right)$  ( $m = 1-3$ ) vs. the logarithm of the free C4-BPP concentration (2-bromohexanoate is abbreviated as 2-bromo).



**Figure S10:** Fluorescence lifetime of  $[\text{Eu}(\text{C4-BPP})_n(\text{2-bromohexanoate})_m]^{(3-m)+}$  ( $n = 2, 3$ ;  $m = 0-3$ ) in methanol containing 1.5 vol.% water and  $3.98 \times 10^{-2}$  mol/L C4-BPP. [2-bromohexanoic acid] = 0 mol/L ( $n = 0$ ),  $5.01 \times 10^{-1}$  mol/L ( $n = 2$ ),  $[\text{Eu}]_{\text{ini}} = 1.0 \times 10^{-5}$  mol/L. (2-bromohexanoate is abbreviated as 2-bromo).