4,4′-Bis(trifluoromethyl)-2,2′-Bipyridine – A Multipurpose Ligand Scaffold for Lanthanoid-Based Luminescence/^{19}F NMR Probes

Tuba Güden-Silber, Kathrin Klein and Michael Seitz*

Inorganic Chemistry I, Department of Chemistry and Biochemistry,
Ruhr-University Bochum, 44780 Bochum, Germany

Email: michael.seitz@rub.de. Fax: ++49 (0)234 32-14378.

Supporting Information

Table of Contents Page

1 Average Tb-F Distances in Tb-7

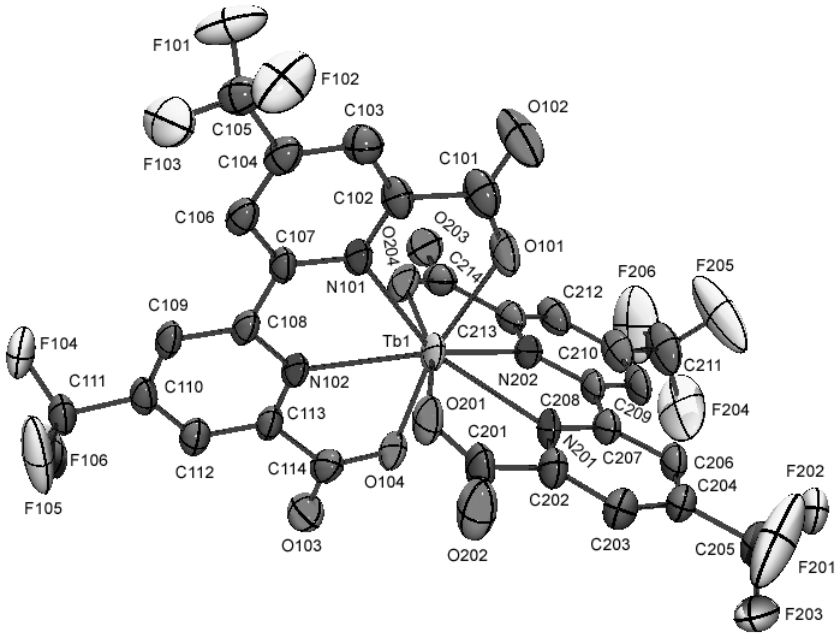

Figure S1. Thermal ellipsoid plot for **Tb-7**. The hydrogen atoms and the Et_3NH^+ cation are omitted for clarity.

Weigthed average: $r_{mean} = \sum_{i=1}^{n} w_i \cdot r_i$ (with $w_i = \frac{(r_i)^{-6}}{\sum_{j=1}^{m} (r_j)^{-6}}$)

Distances Tb-F in Å:

Tb1–F101: 7.414

Tb1–F102: 7.247

Tb1–F103: 7.356

Tb1–F104: 7.419

Tb1–F105: 7.286

Tb1–F106: 7.367

Tb1–F201: 7.293

Tb1–F202: 7.344

Tb1–F203: 7.428

Tb1–F204: 7.358

Tb1–F205: 7.338

Tb1–F206: 7.359

r_{mean} = 7.35 Å

2 ^{19}F NMR Relaxation Measurements

Fluorine NMR measurements were performed using a Bruker DPX-250 (5.87 T, ^{19}F: 235 MHz) spectrometer. Longitudinal relaxation times T_1 were determined at 298K with solutions of **RE-7** (1-2 mM) in HEPES buffer (10 mM, pH 7.4) using standard inversion-recovery techniques. T_1 values were obtained by fitting the data with an exponential function (Levenberg-Marquardt algorithm on χ^2).

Representative inversion-recovery plots for **RE-7** (HEPES buffer, pH 7.4, 298 K) are shown in Figures S2-S4:

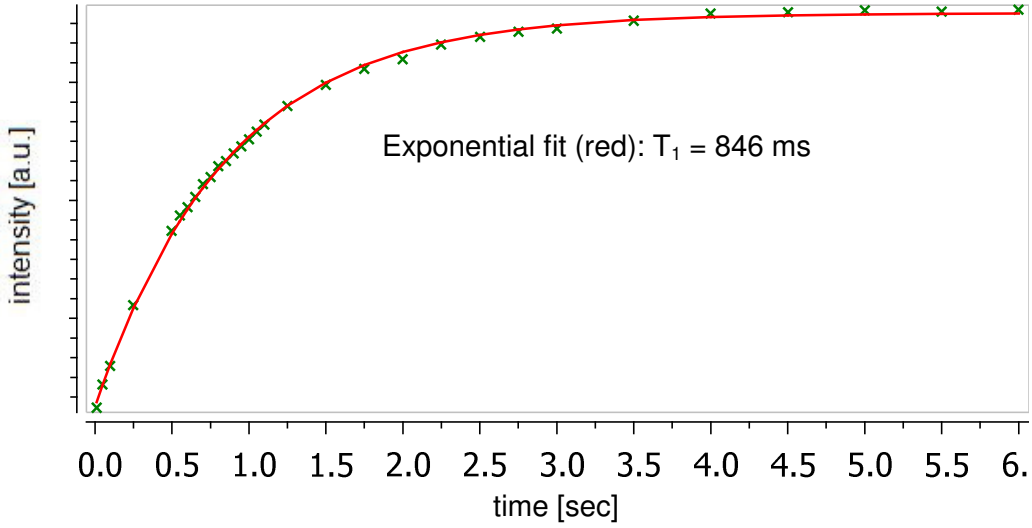

Figure S2. Inversion-recovery profile of **Y-7** with exponential fit (red).

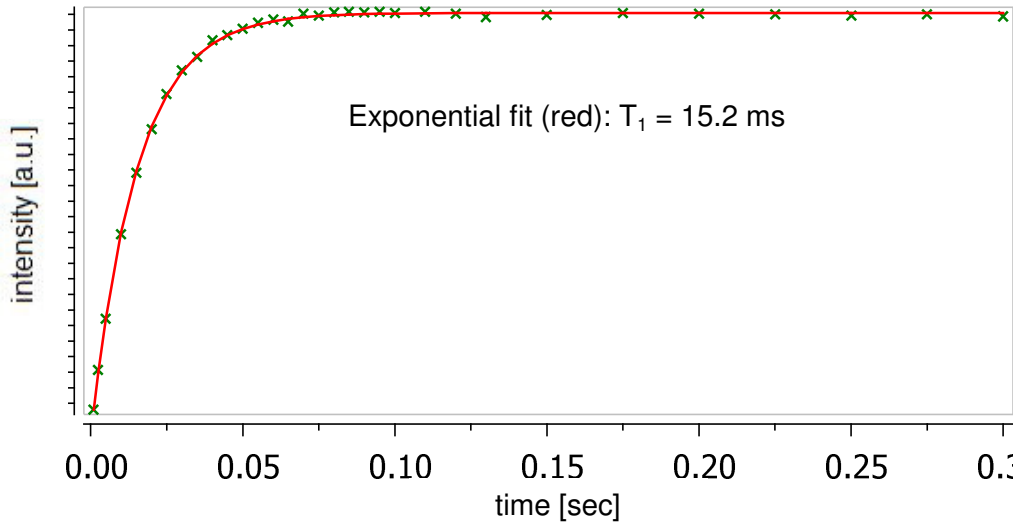

Figure S3. Inversion-recovery profile of **Tb-7** with exponential fit (red).

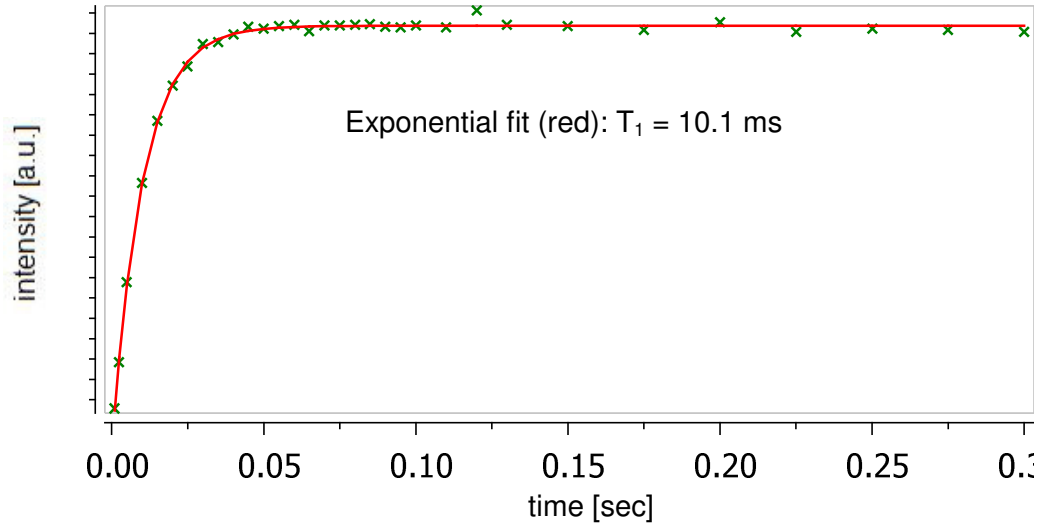

Figure S4. Inversion-recovery profile of **Dy-7** with exponential fit (red).