Crystal structure of $[Eu(CyMe_4\text{-}BTBP)_2\kappa^2O,O'\text{-}(NO_3)](NO_3)_2\cdot n\text{-}C_8H_{17}OH$ and its structure in 1-octanol solution.

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SUPPORTING INFORMATION

Table S1. Previously reported structures containing a $[Eu(NO_3)_n]^{(3-n)}$ complex, where n = 5 or 6, as listed in the Cambridge Structural Database (CSD), ref. 10, including their CSD reference code, coordination number (CN), and mean Eu-O bond distance. For all Eu-O structures, see ref. 10.

CSD code	CN	$d_{(Eu\text{-}O)}$/Å	note
REPBUK	10	2.437	
FONDAN	10	2.456	
WEZTOL	10	2.467	
OPAGUI	10	2.476	
LAHHIN	10	2.480	
OPAHAP	10	2.480	
PHASEU	10	2.481	
AXAPIY	10	2.481	
VIHJIF	10	2.482	
not available	10	2.482	ref. 7
ROZZIQ	10	2.484	
WELBUK	11	2.522	coordinates one H_2O
WELBUK01	11	2.537	coordinates one H_2O
FOCDIK	11	2.545	coordinates one H_2O
SERWER	12	2.576	
GEZHOI	12	2.582	
SUXXIS	12	2.594	

Table S2. Selected basic crystallographic information (top) and selected distances and angles for **1** (bottom).

Formula	$[Eu(C_{32}H_{38}N_8)_2(NO_3)](NO_3)_2\cdot C_8H_{17}OH$
M_W	1537.62
Crystal system	Orthorhombic
Space group	*Pcc*n (No. 56)
a (Å)	23.946(6)
b (Å)	16.623(6)
c (Å)	20.508(6)
α, β, γ (°)	90
V (Å^3)	8163(3)
Z	4
T (K)	296(2)
μ (mm^{-1})	0.832
F(000)	3208
Refl. meas./obs./$I>2\sigma$	49992/5788/4008
No. param./restraints	549/132
R1 all/$I>2\sigma$	0.0652/0.0428
*w*R2 all/$I>2\sigma$	0.1437/0.1245
θ_{max} (coverage)	23.2° (99.2%)
Goodness-of-fit	1.088

Atoms	Bond dist./Å	Atoms	Bond angle/°
Eu1-O11	2.562(5)	O11-Eu1-N10	93.5(2)
Eu1-N10	2.548(4)	O11-Eu1-N18	139.4(2)
Eu1-N18	2.571(4)	O11-Eu1-N30	63.0(2)
Eu1-N30	2.578(5)	O11-Eu1-N38	77.7(2)
Eu1-N38	2.604(4)	N10-Eu1-N18	62.9(1)
N1-O11	1.233(6)	N10-Eu1-N30	62.9(1)
N1-O12	1.202(11)	N10-Eu1-N38	122.4(1)
		N18-Eu1-N30	121.6(1)
		N18-Eu1-N38	142.6(1)
		N30-Eu1-N38	62.6(1)

Table S3. Previously reported 1-octanol crystal structures as listed in the Cambridge Structural Database (CSD), including their CSD reference code, role of the 1-octanol molecule (classified as non-coordinating solvate (solv.), coordinating ligand (coord.) or pure solvent (pure), final R value, measurement temperature, and reference. The findings of the present structure, **1**, is listed for comparison.

CSD code	Type	R value	*T*/K	Reference
AKEFOM	solv.	5.78 %	173	N. Stieger et al. *Struct. Chem.* **2010**, *21*, 771-777
COMPUQ	solv.	3.13%	200	T. Shiga et al. *Inorg. Chim. Acta.* **2008**, *361*, 4113-4117
COMQAX	solv.	5.05%	200	
COMQEB	solv.	4.37%	200	
FEJQOA	solv.	11.95%	223	I. L. Karle et al. *Proc. Nat. Acad. Sci. USA* **1998**, *95*, 5501-5504
PEKVAD	solv.	11.78%	153	H. Furukawa et al. *J. Am. Chem. Soc.* **2006**, *128*, 8398-8399
PUKPIU	solv.	6.95%	295	K. A. Udachin and J. A. Ripmeester *J. Am. Chem. Soc.* **1998**, *120*, 1080-1081
QAYWAP	solv.	*not rep.*	198	N. Yoswathananont et al. *Eur. J. Org. Chem.* **2005**, 5330-5338
QUSGIU	solv.	6.90%	173	K. A. Udachin et al. *J. Supramol. Chem.* **2001**, *1*, 97-100
RECHEN	coord.	6.17%	153	A. K. Sah et al. *Inorg. Chem.* **2006**, *45*, 2083-2092
ZZZVYK	pure	*not rep.*	248*	J. M. Dunoyer *C. R. Acad. Sci.* **1951**, *233*, 41-42
ZZZVYK01	pure	12.54%	190	H. A. Shallard-Brown et al. *Acta Crystallogr. Sect. E* **2005**, *61*, o213-o214
this work, **1**	solv.	4.28%	296	

* CSD lists this temperature as 295 K due to a misinterpretation of the original article.

Figure S1. Fit of the EXAFS data for solid **1** and the corresponding complex in 1-octanol solution (offset: 6).

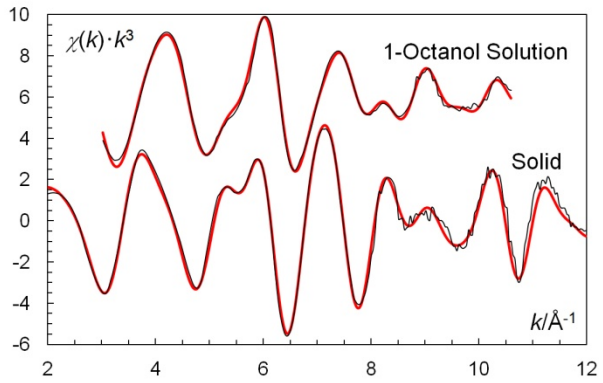

Figure S2. Fourier transform of the EXAFS data in Fig. S1 (offset: 1). A dotted line has been added to aid comparison.