Electronic Supplementary Information (ESI) – Table of Contents

Luminescent Tb(III) and Sm(III) complexes with a 1,4,7-triazacyclononane-based tris-aryloxide ligand for high-performance oxygen sensors

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Tables

Figures

Legends of Supporting Videos

Tables

Table S1 Crystallographic data for $\mathbf{1}^{Sm}$

	$\mathbf{1}^{Sm}$
Formula	$C_{37}H_{50}N_3O_4Sm$
Fw	751.22
Crystal system	triclinic
Space group	*P*-1 (No. 2)
a (Å)	7.930(3)
b (Å)	14.405(5)
c (Å)	16.407(4)
α (deg)	68.230(11)
β (deg)	76.869(14)
γ (deg)	84.941(14)
V (Å^3)	1694.9(10)
Z	2
μ (cm^{-1})	17.79
F(000)	774.00
D_{calcd}(g/cm^3)	1.472
Temperature (K)	93
Reflections collected	20543
Independent reflection	7698
	(R_{int} = 0.032)
Data/parameters	7698/412
R_1 [$I > 2\sigma(I)$]	0.0305
wR_2 (all data)	0.0699
Goodness-of-fit	1.099

Table S2 Continuous shape measures (CSM) values calculated for the Sm^{3+} in $\mathbf{1}^{Sm}$

	HP–7	HPY–7	PBPY–7	COC–7	CTPR–7	JPBPY–7	JETPY–7
$\mathbf{1}^{Sm}$	33.718	20.512	8.700	1.039	2.437	11.363	13.857

HP-7 (D_{7h})	Heptagon
HPY-7 (C_{6v})	Hexagonal pyramid
PBPY-7 (D_{5h})	Pentagonal bipyramid
COC-7 (C_{3v})	Monocapped octahedron (Capped octahedron)
CTPR-7 (C_{2v})	Monocapped trigonal prism (Capped trigonal prism)
JPBPY-7 (D_{5h})	Johnson pentagonal bipyramid (J13)
JETPY-7 (C_{3v})	Johnson elongated triangular pyramid (J7)

M, Llunell, D. Casanova, J. Cirera, P. Alemany and S. Alvarez, *SHAPE*, *version 2.1*, Barcelona, 2013.

D. Casanova, P. Alemany, J. M. Bofill and S. Alvarez, *Chem. – Eur. J.*, 2003, **9**, 1281.

Figures

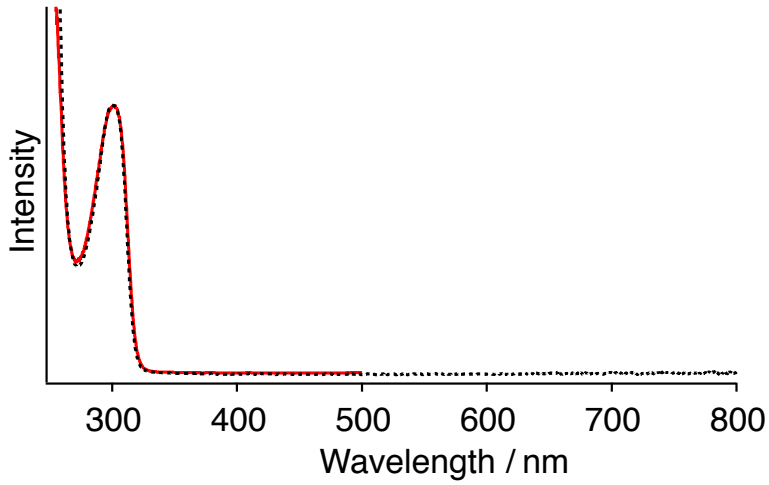

Fig. S1 Absorption (black dot) and excitation (red) spectra of $\mathbf{1}^{Sm}$ in THF at room temperature. The excitation spectrum was detected at 648 nm.

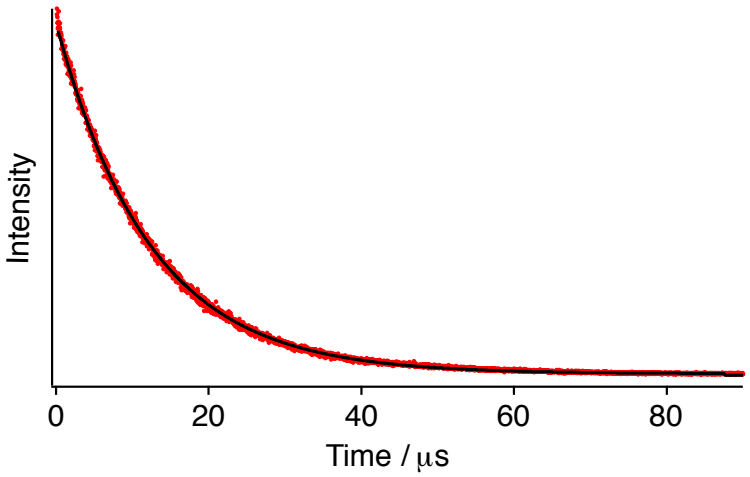

Fig. S2 Luminescence decay curve of $\mathbf{1}^{Sm}$ under air (red, 12.2 μs) in THF at room temperature. The decay was monitored by a TBX-850 detector (250–850 nm) with a Y47 color filter (λ_{ex} = 300 nm). Fitted by single exponential curve (black).

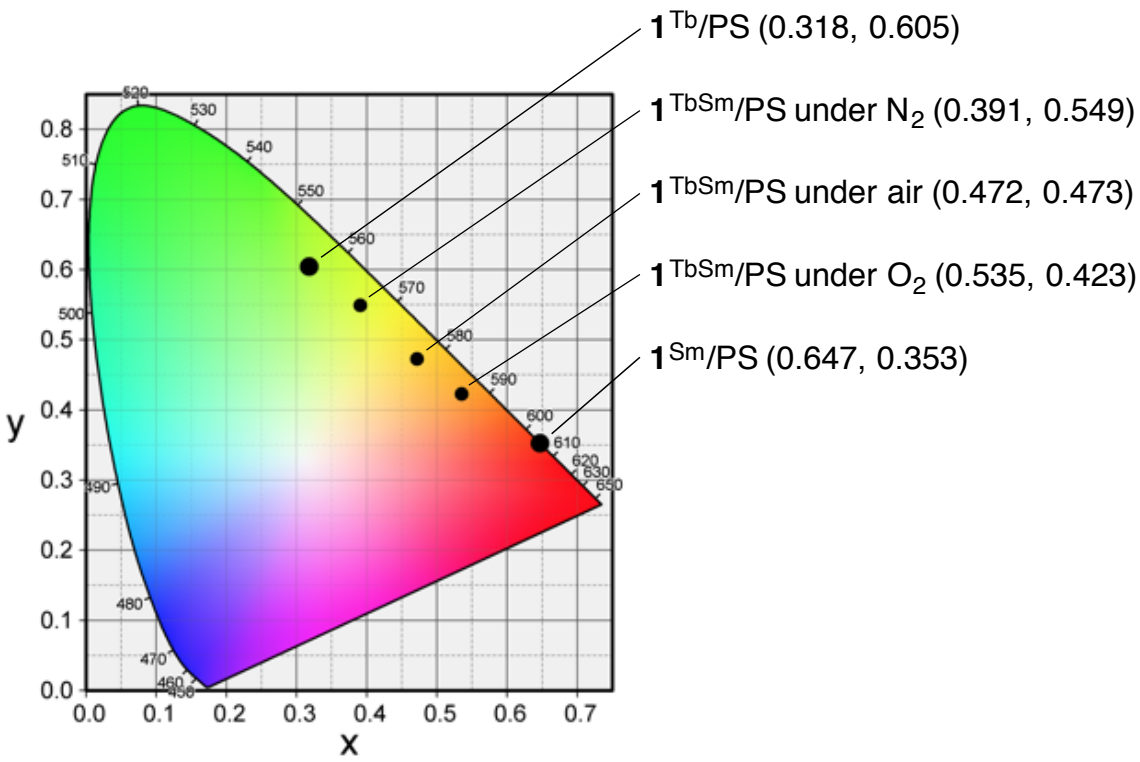

Fig. S3 CIE 1931 chromaticity diagram of $\mathbf{1}^{Tb}$/PS, $\mathbf{1}^{Sm}$/PS and $\mathbf{1}^{TbSm}$/PS (λ_{ex} = 300 nm).

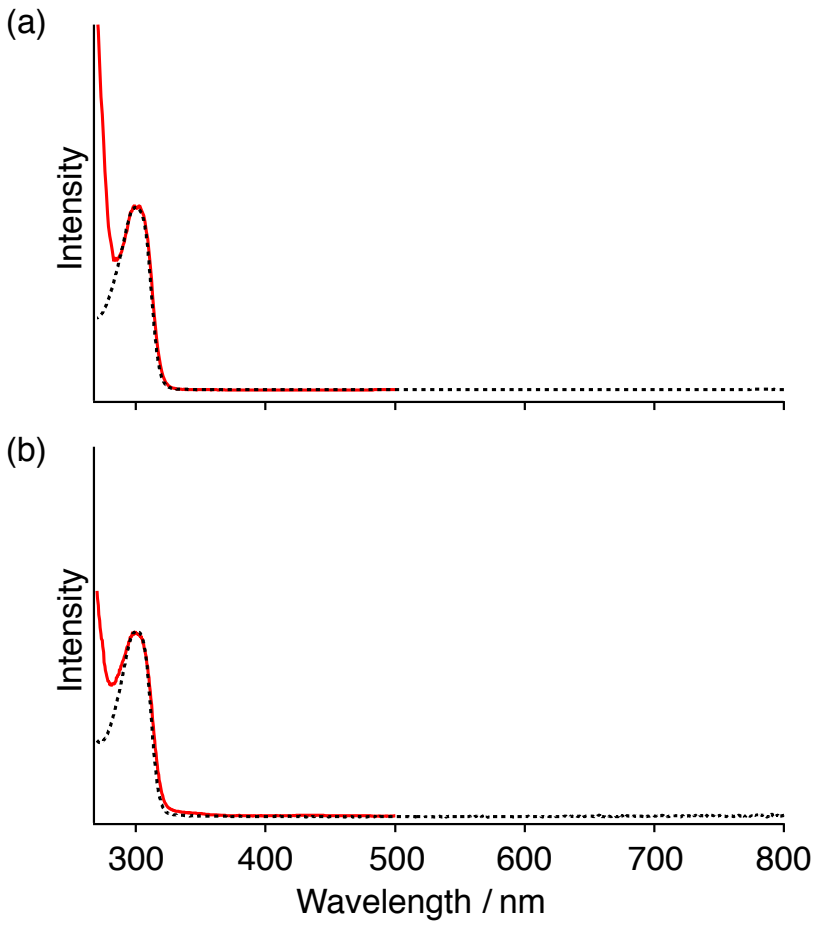

Fig. S4 Excitation spectra (red) of (a) $\mathbf{1}^{Tb}$/PS and (b) $\mathbf{1}^{Sm}$/PS at room temperature (Excitation spectra of $\mathbf{1}^{Tb}$/PS and $\mathbf{1}^{Sm}$/PS were detected at 547 and 647 nm, respectively) and absorption spectra (black dot) of (a) $\mathbf{1}^{Tb}$ and (b) $\mathbf{1}^{Sm}$ in THF at room temperature.

Legends of Supporting Videos

Video S1. Reversible changes of luminescent intensity of $\mathbf{1}^{Tb}$/PS by alternating changes in the oxygen concentration (λ_{ex} = 300 nm).

Video S2. Reversible changes of luminescent color of $\mathbf{1}^{TbSm}$/PS by alternating changes in the oxygen concentration (λ_{ex} = 300 nm).