Electronic Supplementary Information (ESI) – Table of Contents

An oxygen-sensitive luminescent Dy(III) complex

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Tables

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

	$\mathbf{1}^{Dy}$
Formula	$C_{37}H_{50}N_3O_4Dy$
Fw	763.32
Crystal system	triclinic
Space group	P-1 (No. 2)
a (Å)	7.9076(14)
b (Å)	14.308(3)
c (Å)	16.300(3)
α (deg)	68.911(6)
β (deg)	76.832(9)
γ (deg)	85.214(9)
V (Å^3)	1675.4(6)
Z	2
μ (cm^{-1})	22.77
F(000)	782.00
D_{calcd}(g/cm^3)	1.513
Temperature (K)	112
Reflections collected	20482
Independent reflection	7646
	($R_{int} = 0.032$)
Data/parameters	7646/412
R_1 [$I > 2\sigma(I)$]	0.0421
wR_2 (all data)	0.1283
Goodness-of-fit	1.166

Table S2 Continuous shape measures (CSM) values calculated for the Dy^{3+} in **1**^{Dy}

	HP–7	HPY–7	PBPY–7	COC–7	CTPR–7	JPBPY–7	JETPY–7
1^{Dy}	33.596	20.405	8.428	0.919	2.315	11.180	14.067

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)

Figures
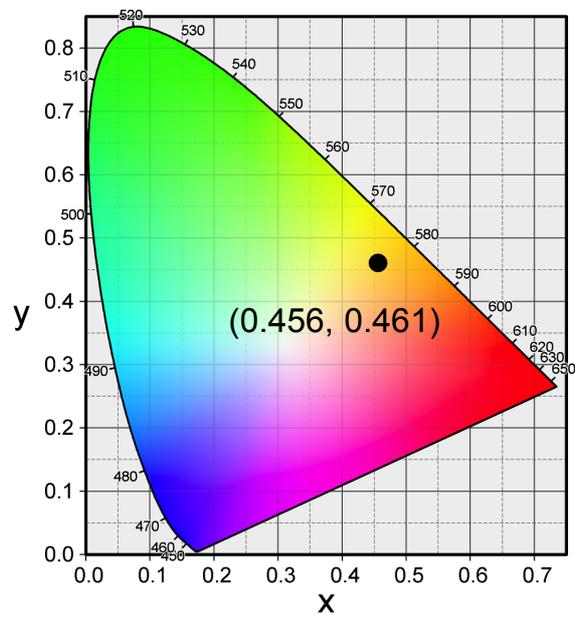
Fig. S1 CIE 1931 chromaticity diagram of $\mathbf{1}^{\text{Dy}}$ in THF at room temperature (λ_{ex} = 300 nm).

Fig. S2 Absorption (black dot) and excitation (red) spectra of **1**^{Dy} under air in THF at room temperature. The excitation spectrum was detected at 575 nm.
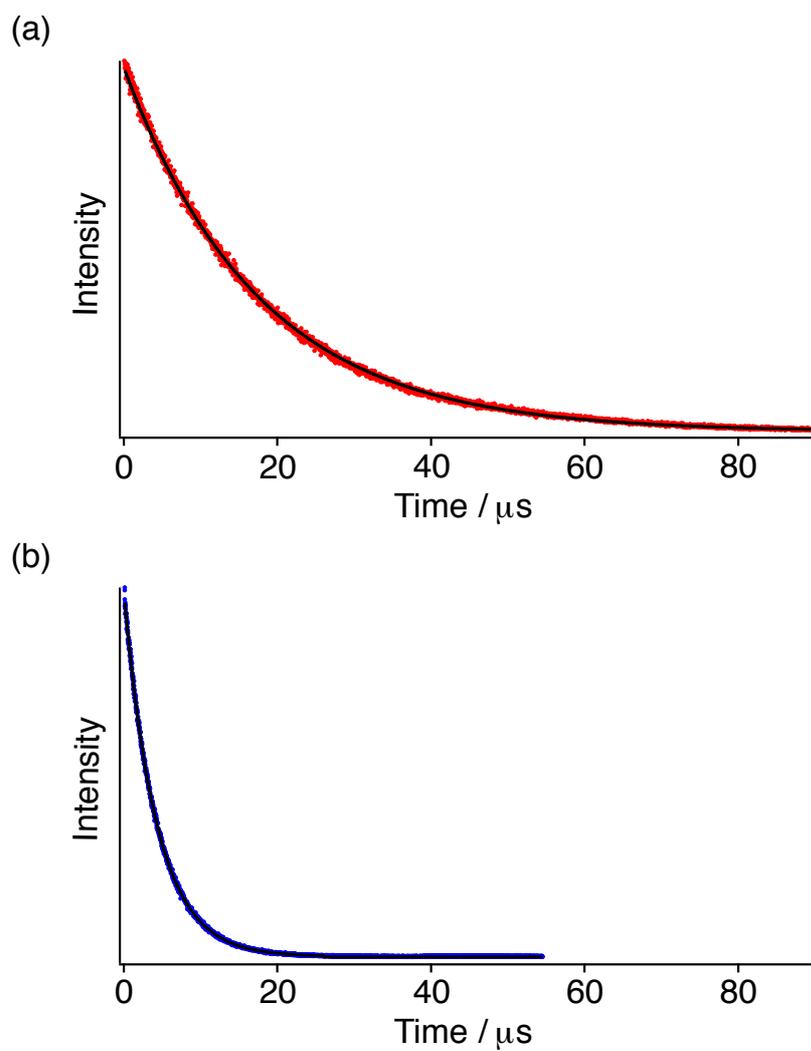
Fig. S3 Luminescence decay curves of 1^{Dy} under (a) N_2 (red, 17.7 μs) and (b) O_2 (blue, 4.1 μs) in THF at room temperature. The decay was monitored by a TBX-850 detector (250–850 nm) with an L42 color filter (λ_{ex} = 300 nm). Fitted by single exponential curve (black).
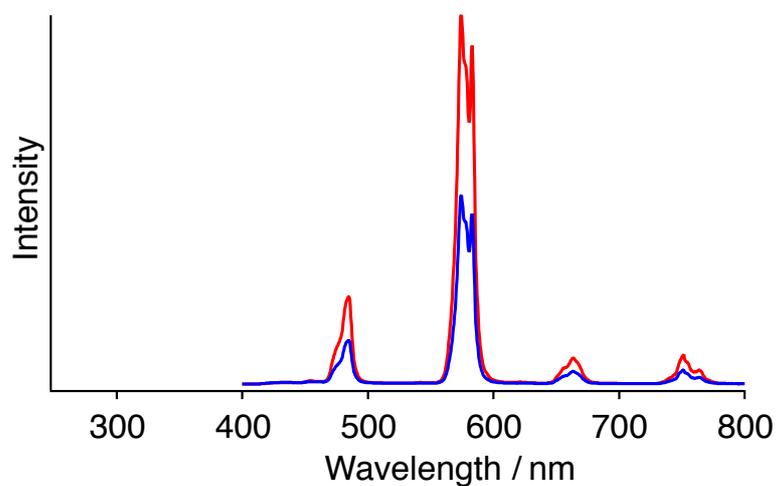
Fig. S4 Corrected luminescence spectra of 1^{Dy}/PS under N_2 (red) and O_2 (blue) at room temperature ($\lambda_{ex} = 300$ nm).
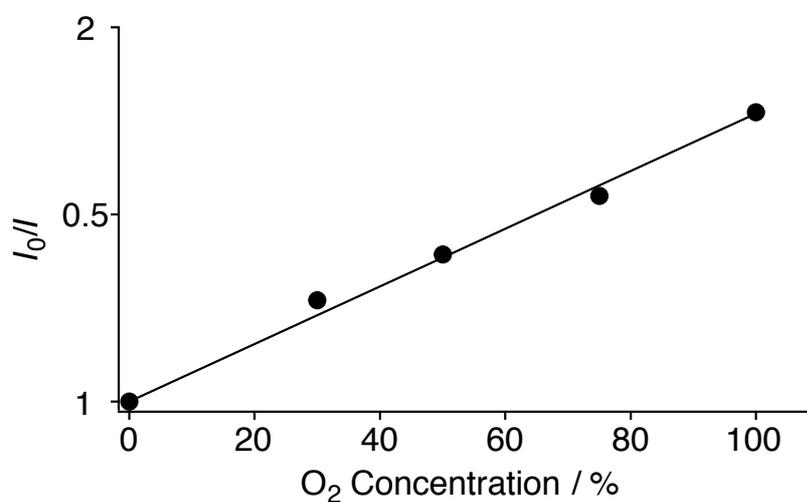
Fig. S5 Stern–Volmer plot of the luminescence intensity against the oxygen concentration for 1^{Dy}/PS (I_0/I vs. [O_2]). The I_0 and I are the luminescence intensities at 0% of O_2 and at the indicated O_2 concentrations, respectively. The luminescence intensities were monitored at 575 nm.
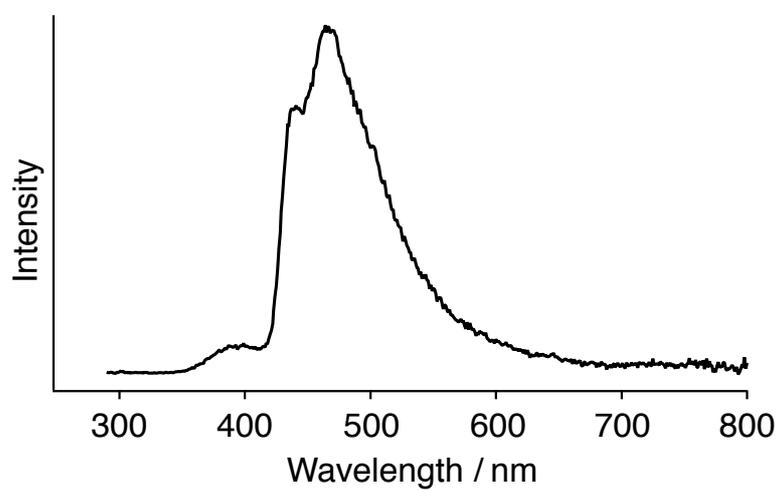
Fig. S6 Corrected luminescence spectrum of **1**^{Gd} under Ar in the crystalline-state at room temperature. (λ_{ex} = 250 nm). The spectrum was acquired with a delay time of 50 µs in order to show the phosphorescence from the lowest triplet state (T1) of the ligand clearly.
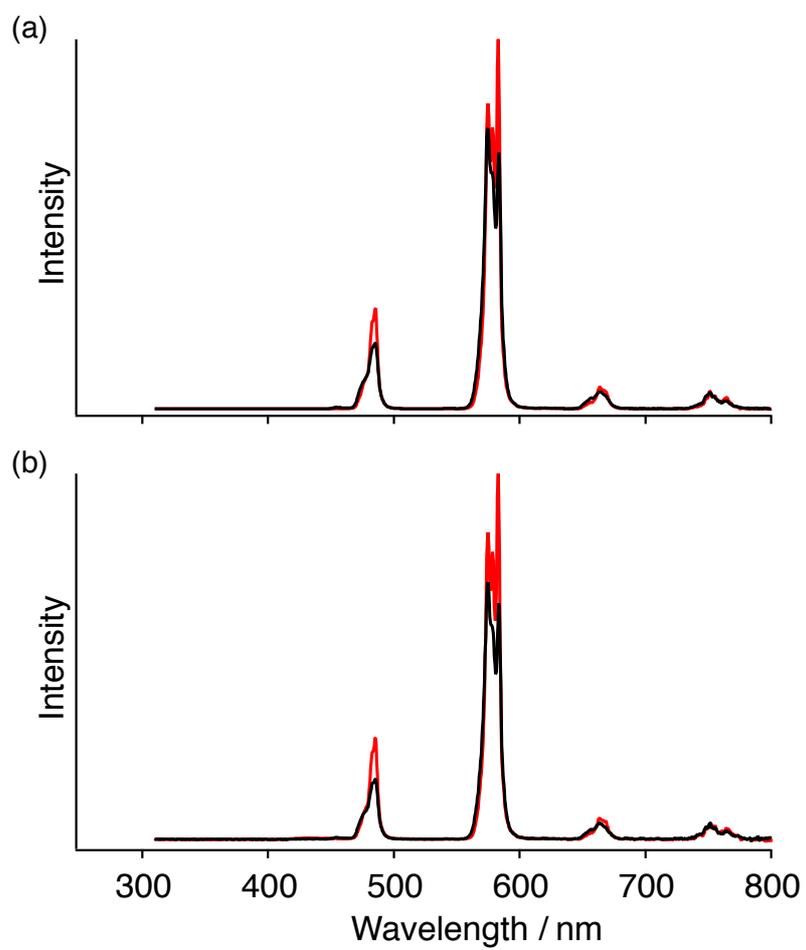
Fig. S7 Corrected luminescence spectra of $\mathbf{1}^{Dy}$ under (a) N_2 and (b) O_2 at room temperature (black) and $-100\ ^\circ$C (red) in THF (λ_{ex} = 300 nm).
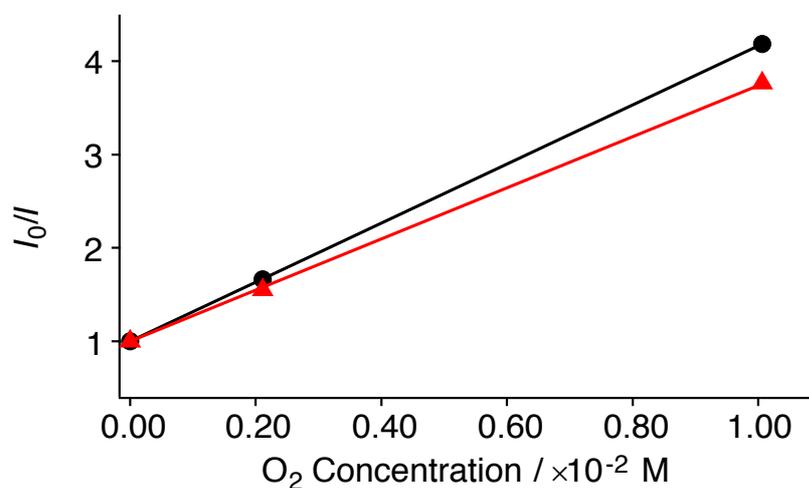
Fig. S8 Stern–Volmer plots of the luminescence intensity (I_0/I) against the oxygen concentration ([O_2]) for $\mathbf{1^{Dy}}$ at −100 ºC (▲) (1.5 × 10^{-5} M, K_{SV} = 274 M^{-1}, R^2 = 0.9998) and room temperature (●) (1.5 × 10^{-5} M, K_{SV} = 317 M^{-1}, R^2 = 0.9999). The I_0 and I are the luminescence intensities at 0% of O_2 and at the indicated O_2 concentrations, respectively. The luminescence intensities were monitored at 485 nm.
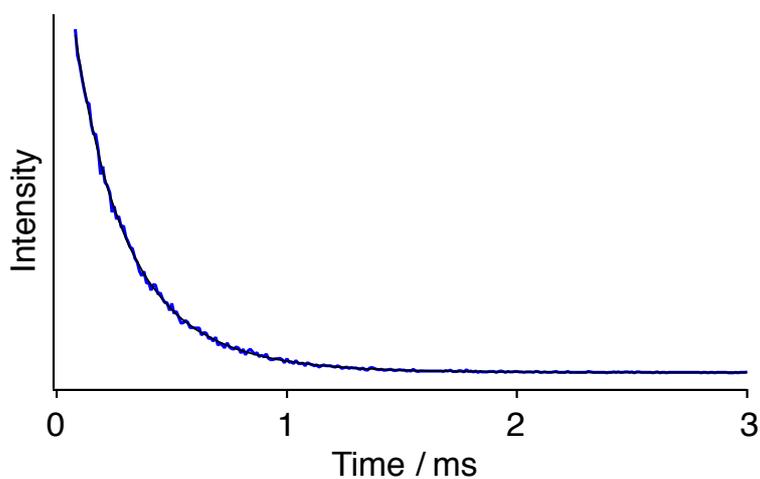
Fig. S9 Luminescence decay curve of $\mathbf{1}^{Gd}$ under Ar (blue) in the crystalline-state at room temperature. The decay was monitored at 436 nm (λ_{ex} = 250 nm). The decay curve was fitted by bi-exponential curve (black: τ_1 = 315 μs, amplitude A_1 = 0.704; τ_2 = 155 μs, amplitude A_1 = 0.296) since the emission at 436 nm contains two emissions (λ_{em}^{max} = 397 and 466 nm: see Fig. S6).
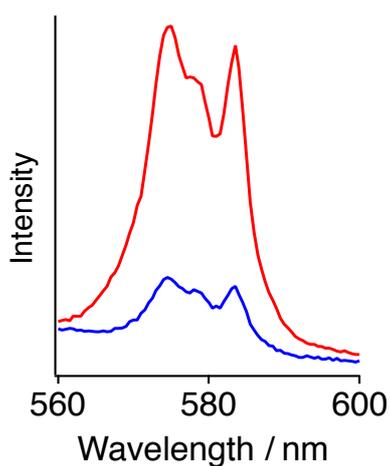
Fig. S10 Corrected luminescence spectra of $\mathbf{1}^{Dy}$ ($^4F_{9/2} \rightarrow {}^6H_{13/2}$) under N_2 (red) and O_2 (blue) in THF at room temperature (λ_{ex} = 470 nm).