

ELECTRONIC SUPPLEMENTARY INFORMATION

Crystalline-to-Semicrystalline Transition in Lanthanide Trifluoroacetates: Implications for Optical Pressure and Temperature Sensing

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1. Powder X-ray Diffraction

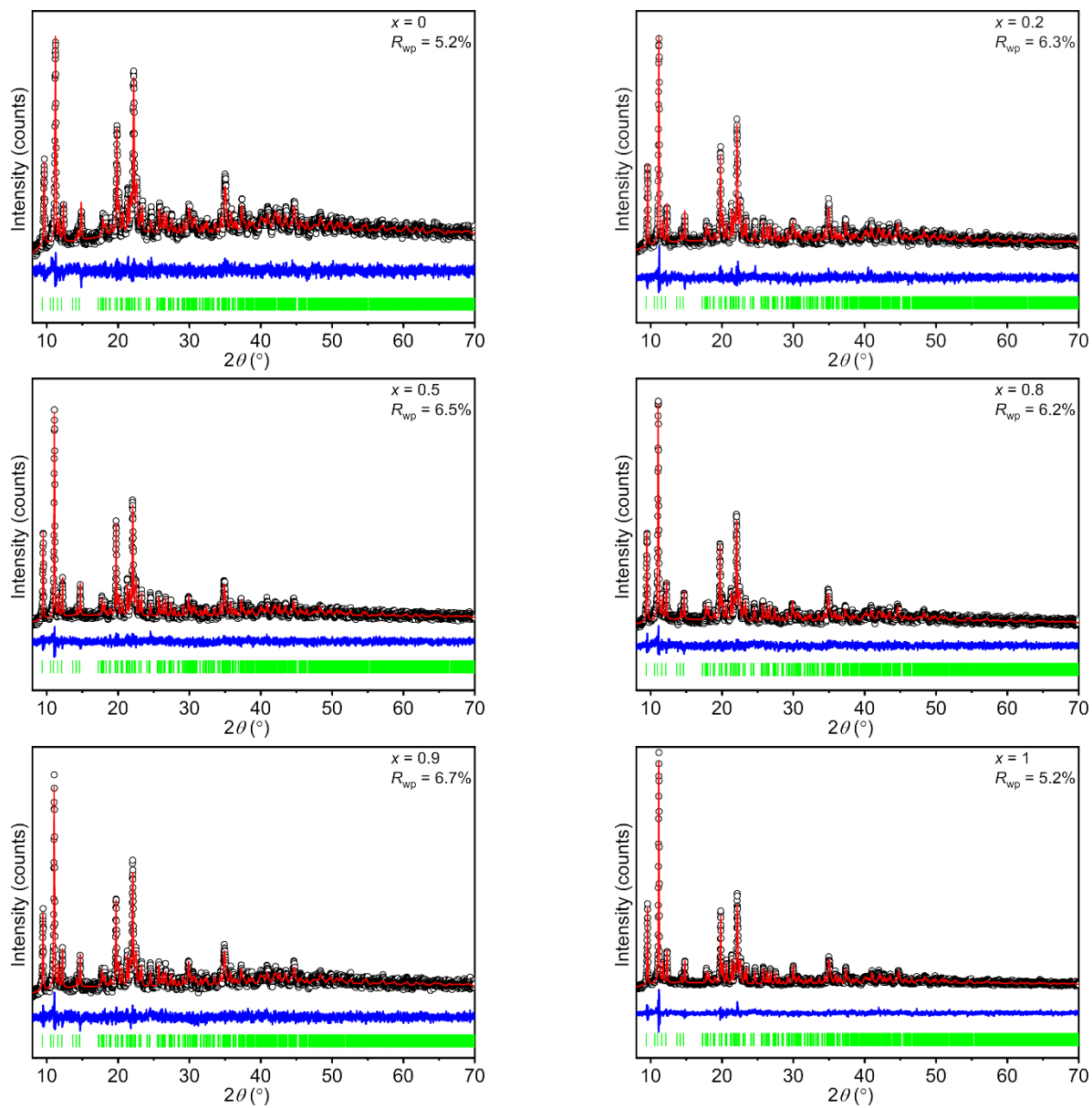


Figure S1. Rietveld analysis of the PXRD patterns of $\text{Eu}_{1-x}\text{Tb}_x(\text{tfa})_3(\text{H}_2\text{O})_3$. Experimental data (\circ), calculated patterns ($—$), difference curves ($—$, offset for clarity), and tick marks ($|$) corresponding to the calculated positions of the diffraction maxima are shown.

Table S1. Unit Cell Constants and Volume of $\text{Eu}_{1-x}\text{Tb}_x(\text{tfa})_3(\text{H}_2\text{O})_3$

x	a (Å)	b (Å)	c (Å)	β (°)	V (Å ³)
0	9.2096 (7)	18.8873 (10)	9.7935 (7)	113.967 (5)	1556.65 (19)
0.1	9.2036 (5)	18.8814 (10)	9.7909 (6)	113.960 (3)	1554.82 (17)
0.2	9.2014 (6)	18.8833 (13)	9.7850 (7)	113.971 (4)	1553.5 (2)
0.5	9.1883 (5)	18.8661 (11)	9.7786 (6)	113.961 (3)	1549.02 (18)
0.8	9.1732 (6)	18.8468 (13)	9.7669 (8)	113.952 (4)	1543.1 (2)
0.9	9.1675 (8)	18.8384 (18)	9.7647 (11)	113.951 (5)	1541.2 (3)
1	9.1648 (4)	18.8409 (10)	9.7575 (6)	113.956 (3)	1539.72 (15)

Table S2. Fractional Atomic Coordinates and Isotropic Displacement Parameters (\AA^2)
of $\text{Eu}(\text{tfa})_3(\text{H}_2\text{O})_3$

	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}
Eu	0.2941 (5)	1.0697 (2)	0.4750 (5)	0.0021 (9)
O1A	0.535 (3)	1.0902 (12)	0.423 (3)	0.011 (3)
O1B	0.762 (3)	1.0536 (8)	0.413 (3)	0.011 (3)
C1A	0.6540 (18)	1.0983 (6)	0.3960 (16)	0.011 (3)
C1B	0.6707 (15)	1.1707 (5)	0.3353 (14)	0.011 (3)
F1A	0.555 (3)	1.1797 (10)	0.1993 (16)	0.011 (3)
F1B	0.640 (3)	1.2213 (6)	0.402 (2)	0.011 (3)
F1C	0.798 (2)	1.1796 (12)	0.313 (3)	0.011 (3)
O2A	0.264 (3)	0.9855 (15)	0.268 (2)	0.011 (3)
O2B	0.4916 (19)	0.9371 (17)	0.2800 (19)	0.011 (3)
C2A	0.3496 (18)	0.9553 (9)	0.2160 (11)	0.011 (3)
C2B	0.2751 (14)	0.9386 (7)	0.0488 (11)	0.011 (3)
F2A	0.348 (3)	0.9595 (14)	-0.0238 (17)	0.011 (3)
F2B	0.265 (3)	0.8698 (8)	0.028 (2)	0.011 (3)
F2C	0.1247 (16)	0.9536 (15)	-0.015 (2)	0.011 (3)
O3A	0.147 (3)	1.1146 (15)	0.626 (3)	0.011 (3)
O3B	0.216 (3)	1.2280 (13)	0.689 (3)	0.011 (3)
C3A	0.1503 (18)	1.1713 (10)	0.6918 (16)	0.011 (3)
C3B	0.0539 (14)	1.1712 (7)	0.7889 (14)	0.011 (3)
F3A	-0.0458 (18)	1.1275 (10)	0.761 (3)	0.011 (3)
F3B	0.037 (2)	1.2249 (11)	0.843 (3)	0.011 (3)
F3C	0.142 (3)	1.1394 (14)	0.9122 (16)	0.011 (3)
O1W	0.1645	1.1392	0.2513	0.011 (3)
H1WA	0.119	1.13	0.162	0.011 (3)
H1WB	0.159	1.182	0.259	0.011 (3)
O2W	0.3799	1.19157	0.52769	0.011 (3)
H2WA	0.43	1.21501	0.60299	0.011 (3)
H2WB	0.33001	1.22001	0.454	0.011 (3)
O3W	0.016	1.0349	0.35209	0.011 (3)
H3WA	-0.057	1.056	0.368	0.011 (3)
H3WB	-0.025	0.998	0.30301	0.011 (3)

Table S3. Fractional Atomic Coordinates and Isotropic Displacement Parameters (\AA^2)
of $\text{Eu}_{0.9}\text{Tb}_{0.1}(\text{tfa})_3(\text{H}_2\text{O})_3$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
Eu	0.2946 (5)	1.0694 (3)	0.4726 (5)	0.031 (3)
Tb	0.2946 (5)	1.0694 (3)	0.4726 (5)	0.031 (3)
O1A	0.533 (3)	1.0877 (14)	0.429 (3)	0.039 (4)
O1B	0.749 (3)	1.0441 (8)	0.409 (3)	0.039 (4)
C1A	0.650 (2)	1.0921 (8)	0.3985 (17)	0.039 (4)
C1B	0.6764 (13)	1.1640 (7)	0.3418 (16)	0.039 (4)
F1A	0.559 (2)	1.1770 (10)	0.2083 (17)	0.039 (4)
F1B	0.657 (3)	1.2152 (8)	0.414 (2)	0.039 (4)
F1C	0.803 (2)	1.1689 (12)	0.316 (3)	0.039 (4)
O2A	0.276 (3)	0.9935 (16)	0.280 (3)	0.039 (4)
O2B	0.494 (2)	0.9355 (17)	0.292 (2)	0.039 (4)
C2A	0.355 (2)	0.9579 (11)	0.2283 (17)	0.039 (4)
C2B	0.2751 (15)	0.9395 (7)	0.0621 (16)	0.039 (4)
F2A	0.349 (3)	0.9549 (14)	-0.013 (2)	0.039 (4)
F2B	0.253 (3)	0.8709 (8)	0.045 (2)	0.039 (4)
F2C	0.1275 (17)	0.9593 (13)	-0.001 (2)	0.039 (4)
O3A	0.160 (4)	1.1178 (13)	0.614 (3)	0.039 (4)
O3B	0.227 (3)	1.2293 (13)	0.695 (3)	0.039 (4)
C3A	0.1615 (18)	1.1715 (9)	0.6883 (19)	0.039 (4)
C3B	0.0627 (12)	1.1658 (6)	0.7827 (15)	0.039 (4)
F3A	-0.037 (2)	1.1218 (11)	0.746 (3)	0.039 (4)
F3B	0.045 (3)	1.2167 (9)	0.844 (2)	0.039 (4)
F3C	0.149 (2)	1.1303 (12)	0.9013 (19)	0.039 (4)
O1W	0.1645	1.1392	0.2513	0.039 (4)
H1WA	0.119	1.13	0.162	0.039 (4)
H1WB	0.159	1.182	0.259	0.039 (4)
O2W	0.3799	1.19157	0.52769	0.039 (4)
H2WA	0.43	1.21501	0.60299	0.039 (4)
H2WB	0.33001	1.22001	0.454	0.039 (4)
O3W	0.016	1.0349	0.35209	0.039 (4)
H3WA	-0.057	1.056	0.368	0.039 (4)
H3WB	-0.025	0.998	0.30301	0.039 (4)

Table S4. Fractional Atomic Coordinates and Isotropic Displacement Parameters (\AA^2)
of $\text{Eu}_{0.8}\text{Tb}_{0.2}(\text{tfa})_3(\text{H}_2\text{O})_3$

	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}
Eu	0.2926 (7)	1.0701 (3)	0.4742 (6)	0.033 (3)
Tb	0.2926 (7)	1.0701 (3)	0.4742 (6)	0.033 (3)
O1A	0.529 (3)	1.0859 (16)	0.422 (4)	0.028 (5)
O1B	0.757 (4)	1.0474 (10)	0.419 (3)	0.028 (5)
C1A	0.652 (3)	1.0934 (9)	0.402 (2)	0.028 (5)
C1B	0.6783 (16)	1.1667 (8)	0.3518 (18)	0.028 (5)
F1A	0.568 (3)	1.1796 (11)	0.215 (2)	0.028 (5)
F1B	0.648 (3)	1.2162 (10)	0.421 (3)	0.028 (5)
F1C	0.810 (2)	1.1748 (14)	0.337 (4)	0.028 (5)
O2A	0.280 (4)	0.9865 (18)	0.287 (3)	0.028 (5)
O2B	0.499 (2)	0.9347 (19)	0.283 (3)	0.028 (5)
C2A	0.358 (2)	0.9549 (12)	0.2277 (19)	0.028 (5)
C2B	0.2713 (19)	0.9392 (8)	0.0607 (19)	0.028 (5)
F2A	0.338 (3)	0.9590 (16)	-0.018 (2)	0.028 (5)
F2B	0.255 (3)	0.8706 (9)	0.038 (3)	0.028 (5)
F2C	0.122 (2)	0.9564 (15)	0.006 (3)	0.028 (5)
O3A	0.147 (4)	1.1148 (14)	0.612 (3)	0.028 (5)
O3B	0.224 (4)	1.2260 (15)	0.688 (4)	0.028 (5)
C3A	0.155 (2)	1.1696 (11)	0.685 (2)	0.028 (5)
C3B	0.0588 (15)	1.1674 (8)	0.7821 (17)	0.028 (5)
F3A	-0.044 (2)	1.1251 (14)	0.749 (3)	0.028 (5)
F3B	0.046 (3)	1.2197 (11)	0.843 (3)	0.028 (5)
F3C	0.144 (3)	1.1320 (14)	0.901 (2)	0.028 (5)
O1W	0.1645	1.1392	0.2513	0.028 (5)
H1WA	0.119	1.13	0.162	0.028 (5)
H1WB	0.159	1.182	0.259	0.028 (5)
O2W	0.3799	1.19157	0.52769	0.028 (5)
H2WA	0.43	1.21501	0.60299	0.028 (5)
H2WB	0.33001	1.22001	0.454	0.028 (5)
O3W	0.016	1.0349	0.35209	0.028 (5)
H3WA	-0.057	1.056	0.368	0.028 (5)
H3WB	-0.025	0.998	0.30301	0.028 (5)

Table S5. Fractional Atomic Coordinates and Isotropic Displacement Parameters (\AA^2)
of $\text{Eu}_{0.5}\text{Tb}_{0.5}(\text{tfa})_3(\text{H}_2\text{O})_3$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
Eu	0.2925 (6)	1.0693 (3)	0.4712 (6)	0.022 (3)
Tb	0.2925 (6)	1.0693 (3)	0.4712 (6)	0.022 (3)
O1A	0.536 (4)	1.0883 (16)	0.428 (4)	0.036 (5)
O1B	0.753 (4)	1.0465 (10)	0.407 (3)	0.036 (5)
C1A	0.652 (3)	1.0935 (9)	0.396 (2)	0.036 (5)
C1B	0.6736 (16)	1.1653 (8)	0.3355 (18)	0.036 (5)
F1A	0.555 (3)	1.1767 (12)	0.202 (2)	0.036 (5)
F1B	0.653 (3)	1.2167 (9)	0.406 (3)	0.036 (5)
F1C	0.799 (3)	1.1711 (15)	0.308 (4)	0.036 (5)
O2A	0.269 (4)	0.9921 (19)	0.274 (3)	0.036 (5)
O2B	0.491 (3)	0.937 (2)	0.287 (3)	0.036 (5)
C2A	0.351 (3)	0.9579 (13)	0.223 (2)	0.036 (5)
C2B	0.2731 (19)	0.9394 (9)	0.0566 (19)	0.036 (5)
F2A	0.347 (3)	0.9561 (16)	-0.018 (3)	0.036 (5)
F2B	0.255 (4)	0.8706 (9)	0.039 (3)	0.036 (5)
F2C	0.125 (2)	0.9576 (16)	-0.007 (3)	0.036 (5)
O3A	0.164 (4)	1.1131 (16)	0.628 (3)	0.036 (5)
O3B	0.215 (4)	1.2283 (15)	0.684 (4)	0.036 (5)
C3A	0.157 (2)	1.1699 (12)	0.689 (2)	0.036 (5)
C3B	0.0566 (15)	1.1673 (8)	0.7823 (17)	0.036 (5)
F3A	-0.037 (3)	1.1210 (13)	0.754 (3)	0.036 (5)
F3B	0.031 (3)	1.2205 (11)	0.832 (3)	0.036 (5)
F3C	0.146 (3)	1.1381 (15)	0.909 (2)	0.036 (5)
O1W	0.1645	1.1392	0.2513	0.036 (5)
H1WA	0.119	1.13	0.162	0.036 (5)
H1WB	0.159	1.182	0.259	0.036 (5)
O2W	0.3799	1.19157	0.52769	0.036 (5)
H2WA	0.43	1.21501	0.60299	0.036 (5)
H2WB	0.33001	1.22001	0.454	0.036 (5)
O3W	0.016	1.0349	0.35209	0.036 (5)
H3WA	-0.057	1.056	0.368	0.036 (5)
H3WB	-0.025	0.998	0.30301	0.036 (5)

Table S6. Fractional Atomic Coordinates and Isotropic Displacement Parameters (\AA^2)
of $\text{Eu}_{0.2}\text{Tb}_{0.8}(\text{tfa})_3(\text{H}_2\text{O})_3$

	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}
Eu	0.2925 (6)	1.0691 (3)	0.4718 (6)	0.039 (3)
Tb	0.2925 (6)	1.0691 (3)	0.4718 (6)	0.039 (3)
O1A	0.527 (3)	1.0819 (17)	0.422 (4)	0.040 (5)
O1B	0.756 (4)	1.0426 (10)	0.421 (3)	0.040 (5)
C1A	0.652 (3)	1.0890 (9)	0.404 (2)	0.040 (5)
C1B	0.6802 (16)	1.1623 (8)	0.3546 (18)	0.040 (5)
F1A	0.572 (3)	1.1755 (11)	0.217 (2)	0.040 (5)
F1B	0.649 (3)	1.2118 (10)	0.424 (3)	0.040 (5)
F1C	0.813 (2)	1.1699 (14)	0.341 (4)	0.040 (5)
O2A	0.288 (4)	0.9910 (18)	0.291 (3)	0.040 (5)
O2B	0.502 (3)	0.933 (2)	0.294 (3)	0.040 (5)
C2A	0.363 (2)	0.9554 (13)	0.2351 (19)	0.040 (5)
C2B	0.2777 (18)	0.9372 (8)	0.0692 (18)	0.040 (5)
F2A	0.348 (3)	0.9525 (16)	-0.010 (2)	0.040 (5)
F2B	0.255 (4)	0.8686 (9)	0.052 (3)	0.040 (5)
F2C	0.130 (2)	0.9572 (16)	0.011 (3)	0.040 (5)
O3A	0.153 (4)	1.1144 (15)	0.608 (3)	0.040 (5)
O3B	0.228 (4)	1.2255 (15)	0.688 (4)	0.040 (5)
C3A	0.159 (2)	1.1687 (11)	0.682 (2)	0.040 (5)
C3B	0.0617 (15)	1.1654 (7)	0.7781 (17)	0.040 (5)
F3A	-0.041 (2)	1.1226 (14)	0.743 (3)	0.040 (5)
F3B	0.048 (4)	1.2171 (11)	0.840 (3)	0.040 (5)
F3C	0.147 (3)	1.1296 (14)	0.897 (2)	0.040 (5)
O1W	0.1645	1.1392	0.2513	0.040 (5)
H1WA	0.119	1.13	0.162	0.040 (5)
H1WB	0.159	1.182	0.259	0.040 (5)
O2W	0.3799	1.19157	0.52769	0.040 (5)
H2WA	0.43	1.21501	0.60299	0.040 (5)
H2WB	0.33001	1.22001	0.454	0.040 (5)
O3W	0.016	1.0349	0.35209	0.040 (5)
H3WA	-0.057	1.056	0.368	0.040 (5)
H3WB	-0.025	0.998	0.30301	0.040 (5)

Table S7. Fractional Atomic Coordinates and Isotropic Displacement Parameters (\AA^2)
of $\text{Eu}_{0.1}\text{Tb}_{0.9}(\text{tfa})_3(\text{H}_2\text{O})_3$

	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}
Eu	0.2910 (11)	1.0703 (5)	0.4710 (11)	0.0103 (8)
Tb	0.2910 (11)	1.0703 (5)	0.4710 (11)	0.0103 (8)
O1A	0.518 (9)	1.088 (6)	0.408 (9)	0.0154 (12)
O1B	0.749 (9)	1.047 (4)	0.415 (9)	0.0154 (12)
C1A	0.646 (14)	1.094 (8)	0.395 (17)	0.0154 (12)
C1B	0.679 (16)	1.167 (8)	0.350 (16)	0.0154 (12)
F1A	0.576 (8)	1.182 (4)	0.210 (7)	0.0154 (12)
F1B	0.647 (9)	1.217 (4)	0.418 (8)	0.0154 (12)
F1C	0.816 (8)	1.174 (4)	0.342 (8)	0.0154 (12)
O2A	0.270 (10)	0.982 (5)	0.281 (10)	0.0154 (12)
O2B	0.494 (8)	0.934 (5)	0.280 (8)	0.0154 (12)
C2A	0.352 (13)	0.953 (8)	0.223 (13)	0.0154 (12)
C2B	0.271 (15)	0.939 (9)	0.055 (14)	0.0154 (12)
F2A	0.339 (6)	0.961 (4)	-0.021 (8)	0.0154 (12)
F2B	0.259 (8)	0.870 (3)	0.029 (8)	0.0154 (12)
F2C	0.120 (6)	0.954 (4)	-0.003 (7)	0.0154 (12)
O3A	0.153 (10)	1.118 (4)	0.620 (11)	0.0154 (12)
O3B	0.212 (9)	1.232 (4)	0.684 (9)	0.0154 (12)
C3A	0.152 (18)	1.173 (6)	0.687 (16)	0.0154 (12)
C3B	0.057 (18)	1.170 (8)	0.785 (17)	0.0154 (12)
F3A	-0.039 (8)	1.125 (4)	0.757 (8)	0.0154 (12)
F3B	0.037 (9)	1.223 (4)	0.840 (8)	0.0154 (12)
F3C	0.148 (9)	1.139 (4)	0.907 (9)	0.0154 (12)
O1W	0.1645	1.1392	0.2513	0.0154 (12)
H1WA	0.119	1.13	0.162	0.0154 (12)
H1WB	0.159	1.182	0.259	0.0154 (12)
O2W	0.3799	1.19157	0.52769	0.0154 (12)
H2WA	0.43	1.21501	0.60299	0.0154 (12)
H2WB	0.33001	1.22001	0.454	0.0154 (12)
O3W	0.016	1.0349	0.35209	0.0154 (12)
H3WA	-0.057	1.056	0.368	0.0154 (12)
H3WB	-0.025	0.998	0.30301	0.0154 (12)

Table S8. Fractional Atomic Coordinates and Isotropic Displacement Parameters (\AA^2)
of $\text{Tb}(\text{tfa})_3(\text{H}_2\text{O})_3$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
Tb	0.2927 (5)	1.0697 (3)	0.4703 (4)	0.038 (2)
O1A	0.535 (3)	1.0822 (13)	0.427 (3)	0.033 (4)
O1B	0.759 (3)	1.0417 (8)	0.418 (3)	0.033 (4)
C1A	0.656 (2)	1.0885 (7)	0.4040 (15)	0.033 (4)
C1B	0.6833 (13)	1.1613 (6)	0.3518 (14)	0.033 (4)
F1A	0.571 (2)	1.1744 (9)	0.2156 (16)	0.033 (4)
F1B	0.657 (3)	1.2114 (8)	0.422 (2)	0.033 (4)
F1C	0.8137 (19)	1.1682 (12)	0.333 (3)	0.033 (4)
O2A	0.279 (3)	0.9913 (15)	0.289 (2)	0.033 (4)
O2B	0.496 (2)	0.9338 (16)	0.2965 (19)	0.033 (4)
C2A	0.358 (2)	0.9568 (10)	0.2348 (15)	0.033 (4)
C2B	0.2772 (15)	0.9407 (7)	0.0676 (14)	0.033 (4)
F2A	0.351 (2)	0.9574 (13)	-0.0069 (19)	0.033 (4)
F2B	0.254 (3)	0.8723 (7)	0.046 (2)	0.033 (4)
F2C	0.1298 (17)	0.9610 (13)	0.006 (2)	0.033 (4)
O3A	0.155 (3)	1.1152 (12)	0.617 (2)	0.033 (4)
O3B	0.228 (3)	1.2264 (12)	0.697 (3)	0.033 (4)
C3A	0.1605 (16)	1.1693 (9)	0.6917 (16)	0.033 (4)
C3B	0.0650 (12)	1.1651 (6)	0.7893 (12)	0.033 (4)
F3A	-0.0364 (19)	1.1219 (11)	0.755 (2)	0.033 (4)
F3B	0.051 (3)	1.2165 (9)	0.852 (2)	0.033 (4)
F3C	0.152 (2)	1.1294 (11)	0.9073 (17)	0.033 (4)
O1W	0.1645	1.1392	0.2513	0.033 (4)
H1WA	0.119	1.13	0.162	0.033 (4)
H1WB	0.159	1.182	0.259	0.033 (4)
O2W	0.3799	1.19157	0.52769	0.033 (4)
H2WA	0.43	1.21501	0.60299	0.033 (4)
H2WB	0.33001	1.22001	0.454	0.033 (4)
O3W	0.016	1.0349	0.35209	0.033 (4)
H3WA	-0.057	1.056	0.368	0.033 (4)
H3WB	-0.025	0.998	0.30301	0.033 (4)

2. Luminescence: Concentration Dependence

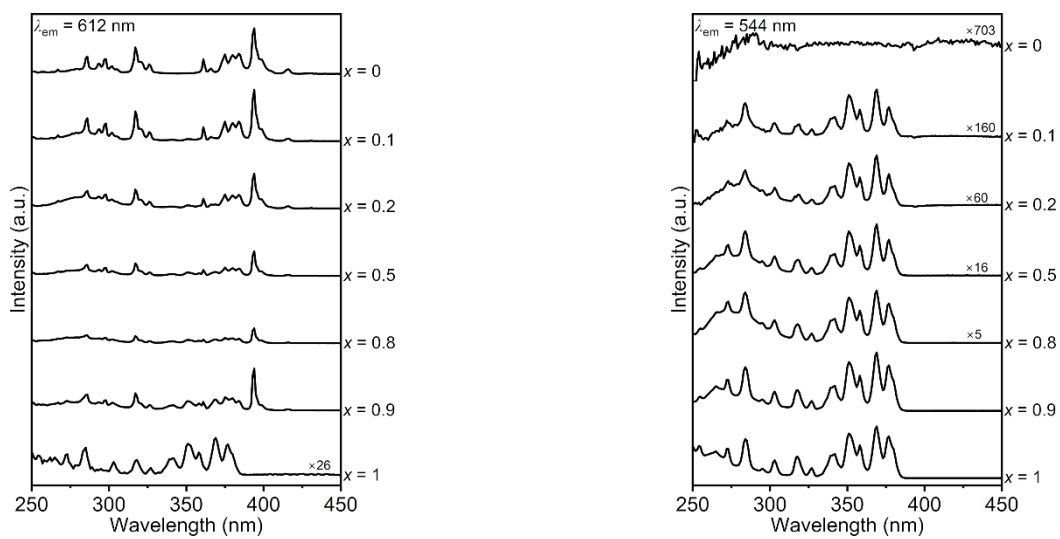


Figure S2. Room-temperature excitation spectra of $\text{Eu}_{1-x}\text{Tb}_x(\text{tfa})_3(\text{H}_2\text{O})_3$.

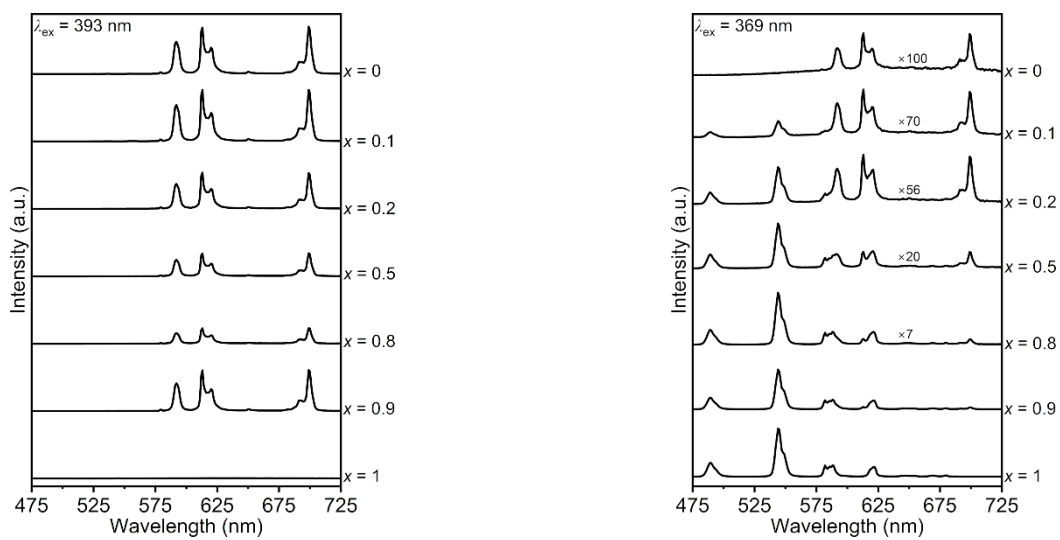


Figure S3. Room-temperature emission spectra of $\text{Eu}_{1-x}\text{Tb}_x(\text{tfa})_3(\text{H}_2\text{O})_3$.

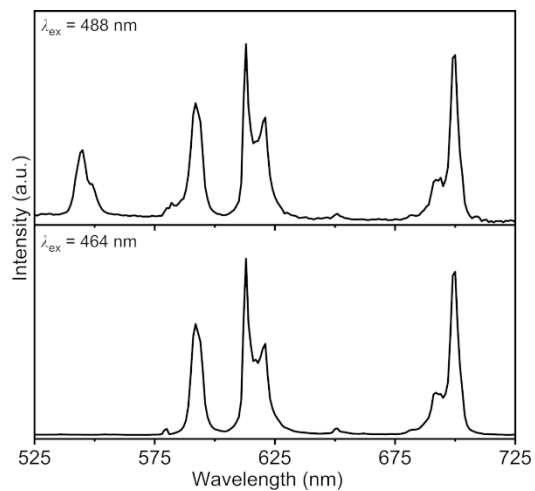


Figure S4. Room-temperature emission spectra of $\text{Eu}_{0.9}\text{Tb}_{0.1}(\text{tfa})_3(\text{H}_2\text{O})_3$ excited at 488 nm ($\text{Tb}^{3+} \text{}^7\text{F}_6 \rightarrow \text{}^5\text{D}_4$) and 464 nm ($\text{Eu}^{3+} \text{}^7\text{F}_0 \rightarrow \text{}^5\text{D}_2$).

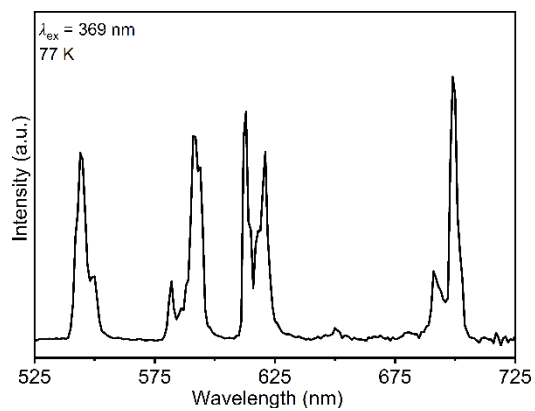


Figure S5. Low-temperature emission spectra of $\text{Eu}_{0.9}\text{Tb}_{0.1}(\text{tfa})_3(\text{H}_2\text{O})_3$.

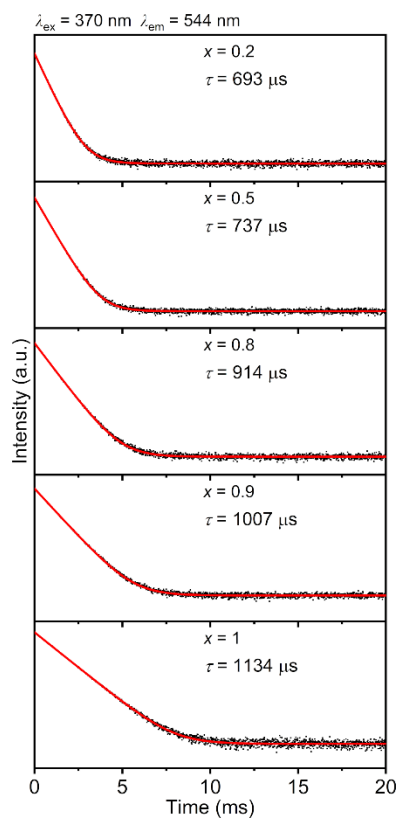


Figure S6. Room-temperature luminescence decays of $\text{Eu}_{1-x}\text{Tb}_x(\text{tfa})_3(\text{H}_2\text{O})_3$ excited at 370 nm and monitored at 544 nm ($\text{Tb}^{3+} \ ^5\text{D}_4 \rightarrow \ ^7\text{F}_5$). Decays are shown in logarithmic scale and the corresponding monoexponential fits are depicted as solid red lines. Lifetimes (τ) are given.

3. Luminescence: Pressure and Temperature Dependence

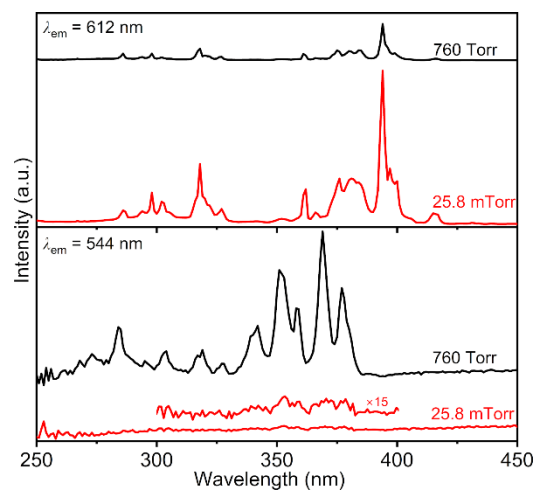


Figure S7. Room-temperature excitation spectra of $\text{Eu}_{0.9}\text{Tb}_{0.1}(\text{tfa})_3(\text{H}_2\text{O})_3$ at atmospheric pressure and under dynamic vacuum.

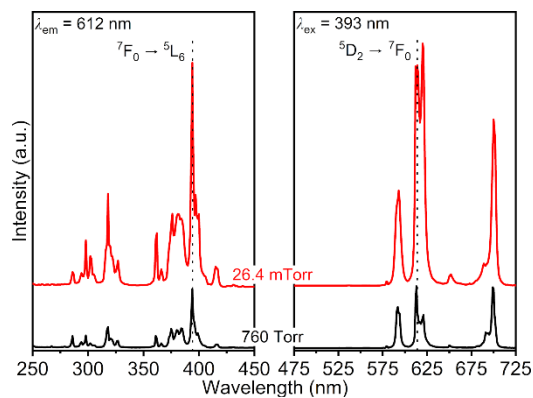


Figure S8. Room-temperature excitation and emission spectra of $\text{Eu}(\text{tfa})_3(\text{H}_2\text{O})_3$ under atmospheric pressure and under dynamic vacuum. Selected $f-f$ transitions are labeled.

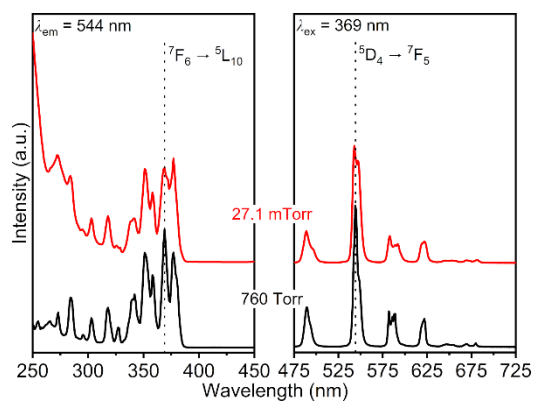


Figure S9. Room-temperature excitation and emission spectra of $\text{Tb}(\text{tfa})_3(\text{H}_2\text{O})_3$ under atmospheric pressure and under dynamic vacuum. Selected $f-f$ transitions are labeled.

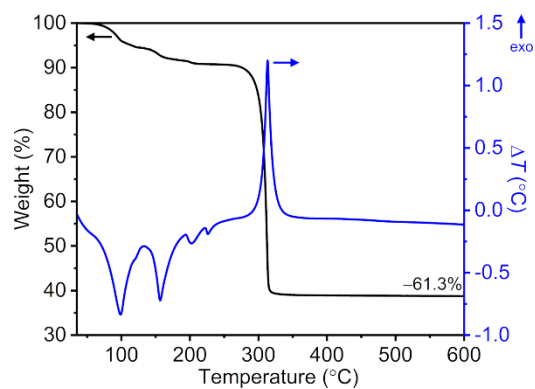


Figure S10. Thermogravimetric (TGA) and differential thermal analyses (DTA) of $\text{Eu}_{0.9}\text{Tb}_{0.1}(\text{tfa})_3(\text{H}_2\text{O})_3$. Total weight loss is given. Analysis was conducted under flowing nitrogen (100 mL min^{-1}) using an SDT2960 TGA–DTA analyzer (TA Instruments). $\approx 5\text{--}10 \text{ mg}$ of trifluoroacetate powder were placed in an alumina crucible, held at $35 \text{ }^\circ\text{C}$ for 30 min, and then heated to $600 \text{ }^\circ\text{C}$ using a heating rate of $10 \text{ }^\circ\text{C min}^{-1}$.

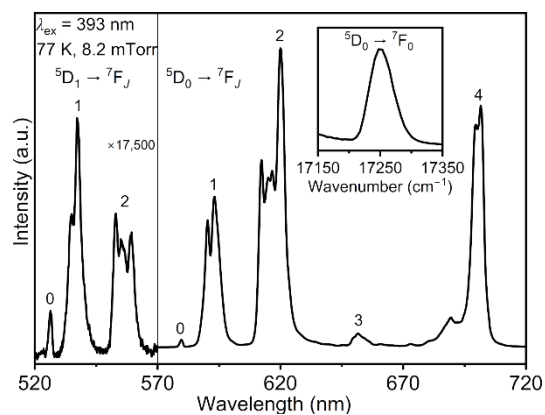


Figure S11. High-resolution low-temperature emission spectrum of $\text{Eu}(\text{tfa})_3(\text{H}_2\text{O})_3$ under dynamic vacuum. Selected $f-f$ transitions are labeled. A detailed view of the asymmetry of the emission band arising from the ${}^5\text{D}_0 \rightarrow {}^7\text{F}_0$ transition ($fwhm = 45 \text{ cm}^{-1}$) is shown in the inset. The wavelength-to-wavenumber Jacobian transformation was applied to obtain this spectrum.

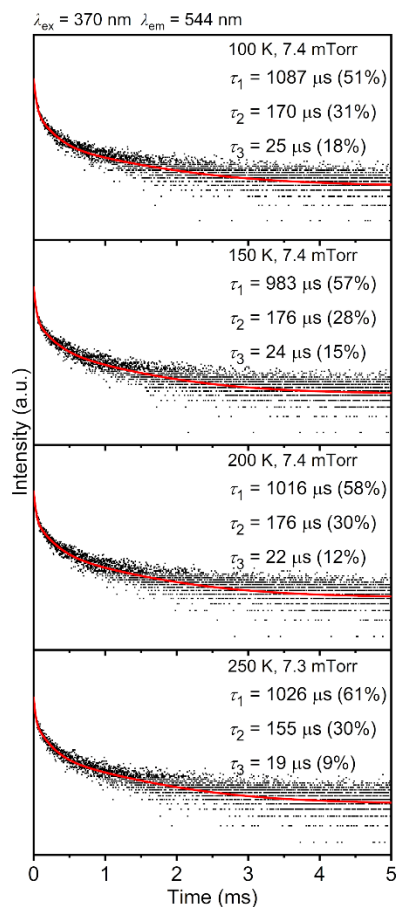


Figure S12. Variable-temperature luminescence decays of $\text{Eu}_{0.9}\text{Tb}_{0.1}(\text{tfa})_3(\text{H}_2\text{O})_3$ under dynamic vacuum. Luminescence was excited at 370 nm and monitored at 544 nm ($\text{Tb}^{3+} \ ^5\text{D}_4 \rightarrow \ ^7\text{F}_5$). Decays are shown in logarithmic scale and the corresponding triexponential fits are depicted as solid red lines. Lifetimes and percent contributions are given. Amplitude-weighted average lifetimes equal 106, 118, 132, and 140 μs at 100, 150, 200, and 250 K, respectively.

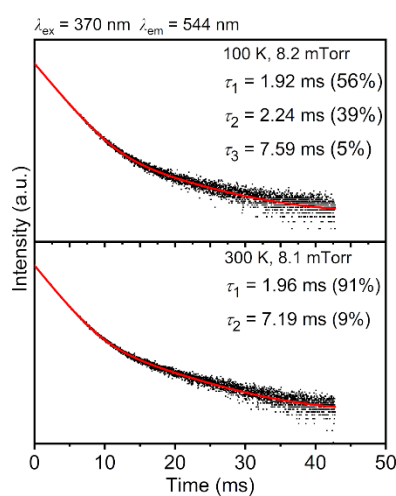


Figure S13. Luminescence decays of $\text{Tb}(\text{tfa})_3(\text{H}_2\text{O})_3$ under dynamic vacuum at 100 and 300 K. Luminescence was excited at 370 nm and monitored at 544 nm ($\text{Tb}^{3+} \ ^5\text{D}_4 \rightarrow \ ^7\text{F}_5$). The sample was degassed under vacuum at 325 K for 12 h prior to data collection. Decays are shown in logarithmic scale and the corresponding tri- and biexponential fits are depicted as solid red lines. Lifetimes and percent contributions are given. Amplitude-weighted average lifetimes equal 2.1 ms at 100 and 300 K.

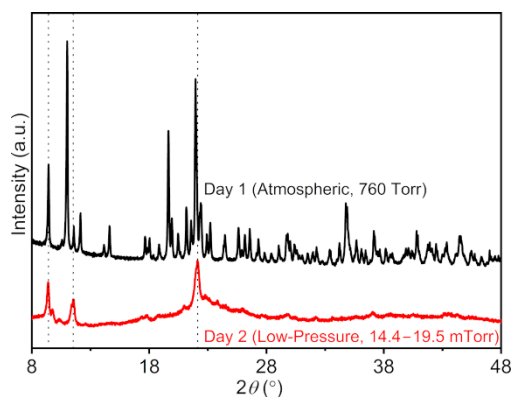


Figure S14. PXRD patterns of $\text{Eu}_{0.9}\text{Tb}_{0.1}(\text{tfa})_3(\text{H}_2\text{O})_3$ in cycle 1 (days 1 and 2). Dotted lines are guides-to-the-eye to facilitate comparison between the positions of the three major diffraction maxima of the low-pressure phase with those of the atmospheric phase.

4. Pressure and Temperature Sensing Using $\text{Eu}_{0.9}\text{Tb}_{0.1}(\text{tfa})_3(\text{H}_2\text{O})_3$

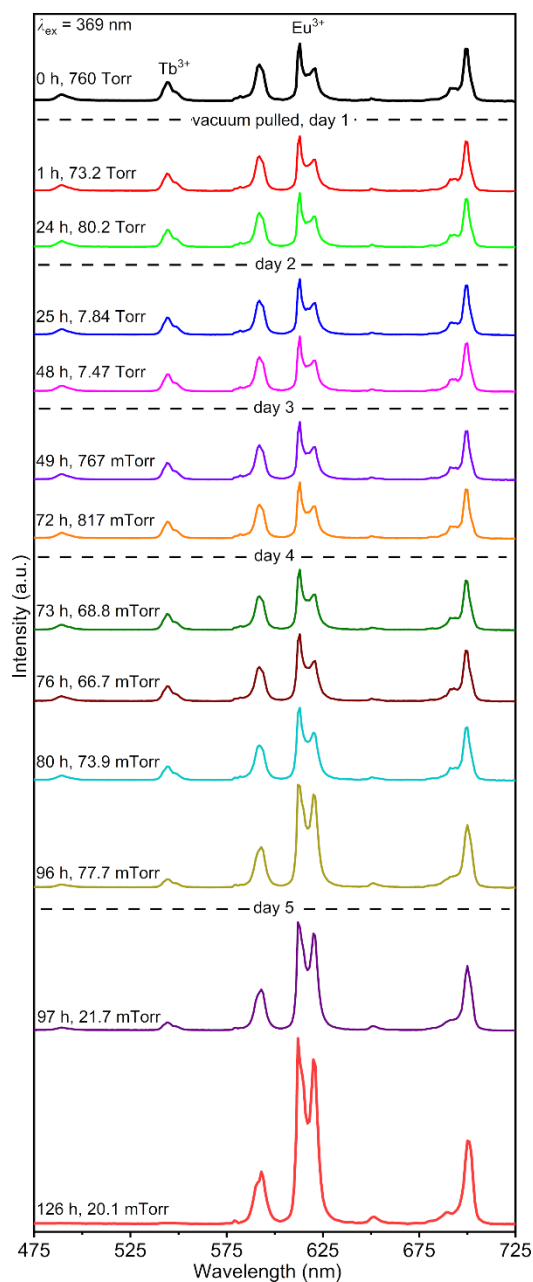


Figure S15. Room-temperature emission spectra of $\text{Eu}_{0.9}\text{Tb}_{0.1}(\text{tfa})_3(\text{H}_2\text{O})_3$ at atmospheric pressure and under controlled dynamic vacuum. Spectra are labeled with the time and pressure at which they were collected. Thicker lines are used to highlight the spectra of the atmospheric and low-pressure phases at 0 and 126 h, respectively.

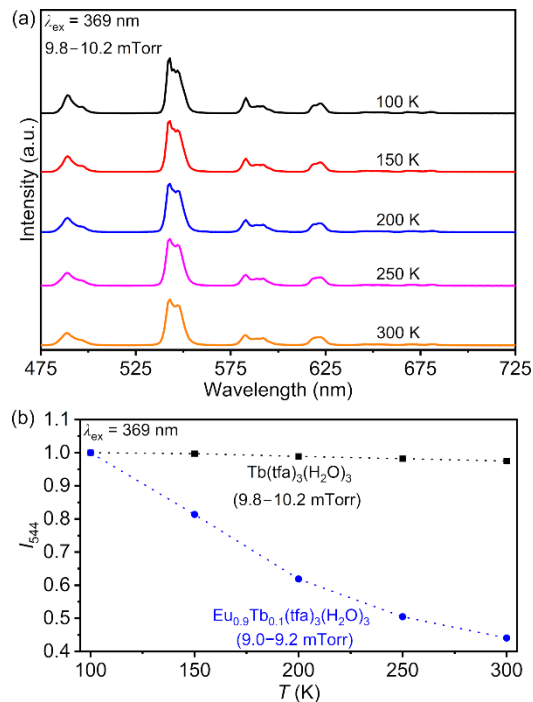


Figure S16. (a) Variable-temperature emission spectra of $\text{Tb}(\text{tfa})_3(\text{H}_2\text{O})_3$ under dynamic vacuum. The sample was degassed under vacuum at 325 K for 12 h prior to data collection. (b) Temperature dependence of the integrated intensity of the 544 nm emission band (I_{544}) in the low-pressure phase of $\text{Tb}(\text{tfa})_3(\text{H}_2\text{O})_3$ and $\text{Eu}_{0.9}\text{Tb}_{0.1}(\text{tfa})_3(\text{H}_2\text{O})_3$. Intensities are normalized to their values at 100 K. Dotted lines are guides-to-the-eye.

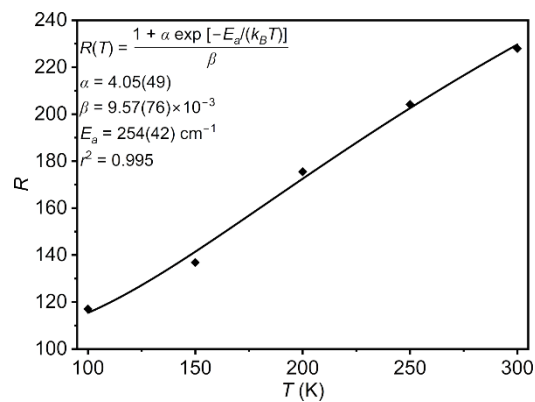


Figure S17. Fit of a Mott–Seitz model with one nonradiative deactivation channel to experimental luminescence intensity ratio values (R). α and β are constants and E_a is the activation energy for thermal quenching of green emission. Fit is depicted as a solid black line. Fit parameters and residual (r^2) are given.

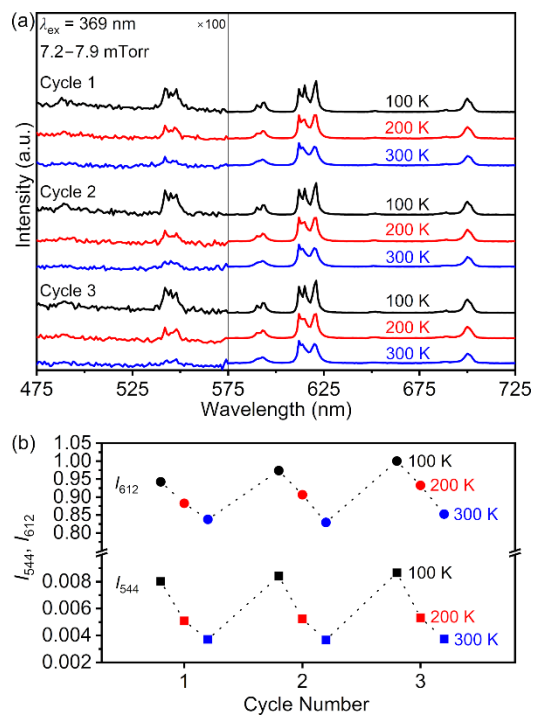


Figure S18. Cyclability of $\text{Eu}_{0.9}\text{Tb}_{0.1}(\text{tfa})_3(\text{H}_2\text{O})_3$ under dynamic vacuum. (a) Variable-temperature emission spectra at 100, 200, and 300 K. (b) Integrated intensities of the 544 and 612 nm emission bands (I_{544} , I_{612}) as a function of heating–cooling cycle. Dotted lines are guides-to-the-eye.

Table S9. Repeatability, Temperature Accuracy, and Resolution of $\text{Eu}_{0.9}\text{Tb}_{0.1}(\text{tfa})_3(\text{H}_2\text{O})_3$

Cycle #	P (mTorr)	100 K		200 K		300 K	
		R	$T_{\text{calculated}}$ (K)	R	$T_{\text{calculated}}$ (K)	R	$T_{\text{calculated}}$ (K)
1	7.2–7.4	117.65556	105.63246	173.42849	202.12542	225.72171	292.59812
2	7.5–7.7	115.79119	102.40690	173.50396	202.25599	226.07977	293.21759
3	7.8–7.9	115.45158	101.81934	175.30496	205.37190	228.22933	296.93656
$\langle R \rangle$		116.29944		174.07914		226.67694	
Repeatability (%) ^a		99		99		99	
$\langle T_{\text{calculated}} \rangle$ (K) ^b			103.3		203.3		294.3
ΔT (K) ^c			2.1		1.8		2.3

^a Repeatability = $100 \times \left[1 - \frac{\max |R_i - \langle R \rangle|}{\langle R \rangle} \right]$ where R_i is the value of R in the i th cycle.

^b $T_{\text{calculated}} = \frac{R - 56.6}{0.578}$.

^c Standard deviation of $T_{\text{calculated}}$.