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Supplementary materials

Photoluminescent lanthanide(III) coordination polymers with 2-{[(4-methylphenyl)amino]methylene}-5,5-dimethylcyclohexane-1,3-dione

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Table S1. Crystallographic data of the ligand and complexes.

Identification code	**L**	**1^{Eu}**	**2^{Sm}**	**3^{Tb}**	**4^{Dy}**	**5^{Gd}**
Empirical formula	$C_{16}H_{19}NO_2$	$C_{32}H_{38}N_5O_{13}Eu$	$C_{32}H_{38}N_5O_{13}Sm$	$C_{32}H_{38}N_5O_{13}Tb$	$C_{32}H_{38}N_5O_{13}Dy$	$C_{32}H_{38}N_5O_{13}Gd$
Formula weight	257.32	852.63	852.63	859.59	859.59	859.59
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $C2/c$	Monoclinic, $C2/c$	Monoclinic, $C2/c$	Monoclinic, $C2/c$	Monoclinic, $C2/c$
a/Å	11.8139(10)	14.5613(5)	14.6306(4)	14.5270(3)	14.4892(6)	14.5319(5)
b/Å	5.8067(4)	11.6777(6)	11.6855(3)	11.6368(2)	11.6159(4)	11.6177(5)
c/Å	20.3464(13)	20.3665(8)	20.3367(5)	20.4175(3)	20.4562(8)	20.4408(7)
β/°	100.245(4)	93.018(2)	93.0550(10)	93.1040(10)	93.116(2)	93.279(3)
Volume/Å^3	1373.51(17)	3458.4(3)	3471.94(16)	3446.47(11)	3437.8(2)	3445.3(2)
Z	4	4	4	4	4	4
ρ_{calc} g/cm^3	1.244	1.638	1.628	1.657	1.668	1.654
μ/mm^{-1}	0.082	1.887	1.764	2.125	2.247	1.998
Crystal size/mm	0.13 × 0.05 × 0.04	0.16 × 0.14 × 0.05	0.2 × 0.1 × 0.08	0.09 × 0.04 × 0.02	0.14 × 0.09 × 0.02	0.15 × 0.11 × 0.08
2θ range for data collection/°	4.07 – 63.05	4.01 – 54.24	4.46 – 66.30	4.00 – 66.31	4.50 – 63.02	4.49 – 57.70
Index ranges	-17 ≤ h ≤ 17, -8 ≤ k ≤ 8, -29 ≤ l ≤ 29	-18 ≤ h ≤ 18, -14 ≤ k ≤ 14, -25 ≤ l ≤ 26	-22 ≤ h ≤ 22, -17 ≤ k ≤ 17, -31 ≤ l ≤ 30	-18 ≤ h ≤ 22, -13≤ k ≤ 17, -31 ≤ l ≤ 29	-21 ≤ h ≤ 21, -17 ≤ k ≤ 16, -27 ≤ l ≤ 30	-18 ≤ h ≤ 18, -15 ≤ k ≤ 9, -17 ≤ l ≤ 26
Reflections collected	36346 / 4583	26306 / 3801	23929 / 6619	22222 / 6564	23349 / 5731	7383 / 3995
Independent reflections	R_{int} = 0.0778, R_{sigma} = 0.0432	R_{int} = 0.0666, R_{sigma} = 0.0417	R_{int} = 0.0291, R_{sigma} = 0.0284	R_{int} = 0.0402, R_{sigma} = 0.0435	R_{int} = 0.0467, R_{sigma} = 0.0448	R_{int} = 0.0178, R_{sigma} = 0.0296
Restraints/ parameters	0 / 175	0 / 235	0 / 235	0 / 235	0 / 235	0 / 235
Goodness-of-fit on F^2	1.058	1.041	1.041	1.044	1.044	1.089
Final R indexes [I>=2σ (I)]	R_1 = 0.0580, wR_2 = 0.1356	R_1 = 0.0275, wR_2 = 0.0522	R_1 = 0.0204, wR_2 = 0.0466	R_1 = 0.0273, wR_2 = 0.0567	R_1 = 0.0276, wR_2 = 0.0525	R_1 = 0.0251, wR_2 = 0.0545
Final R indexes [all data]	R_1 = 0.0950, wR_2 = 0.1604	R_1 = 0.0321, wR_2 = 0.0547	R_1 = 0.0228, wR_2 = 0.0474	R_1 = 0.0318, wR_2 = 0.0588	R_1 = 0.0330, wR_2 = 0.0540	R_1 = 0.0271, wR_2 = 0.0552
Largest diff. peak/hole / e/Å^{-3}	0.24 / -0.26	0.51 / -0.47	0.62 / -0.82	0.64 / -0.54	0.64 / -0.54	0.64 / -0.54
CCDC	2370261	2370259	2370257	2370256	2370260	2370258

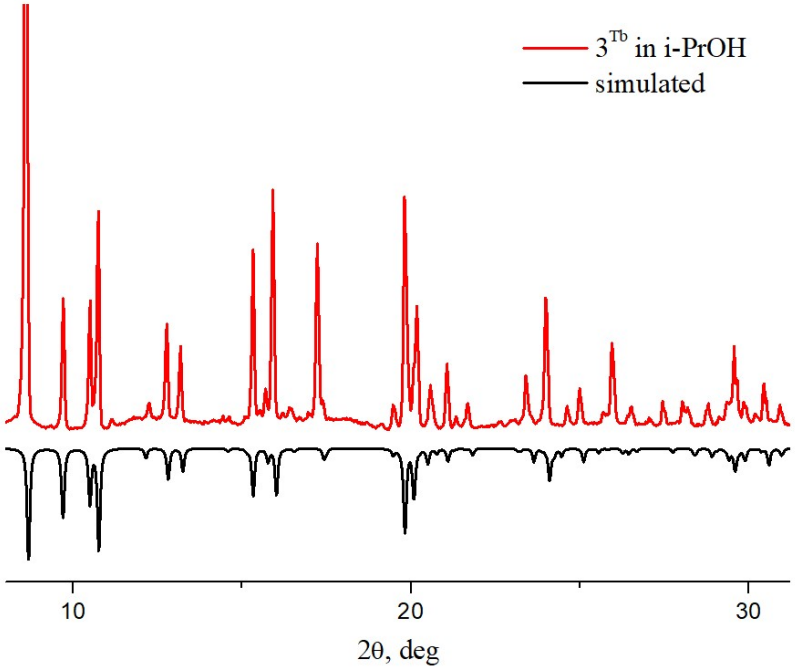

Figure S1. The experimental pattern for terbium complex **3**$^{\mathbf{Tb}}$ synthesized in isopropanol and the simulated one according to the single-crystal XRD analysis.

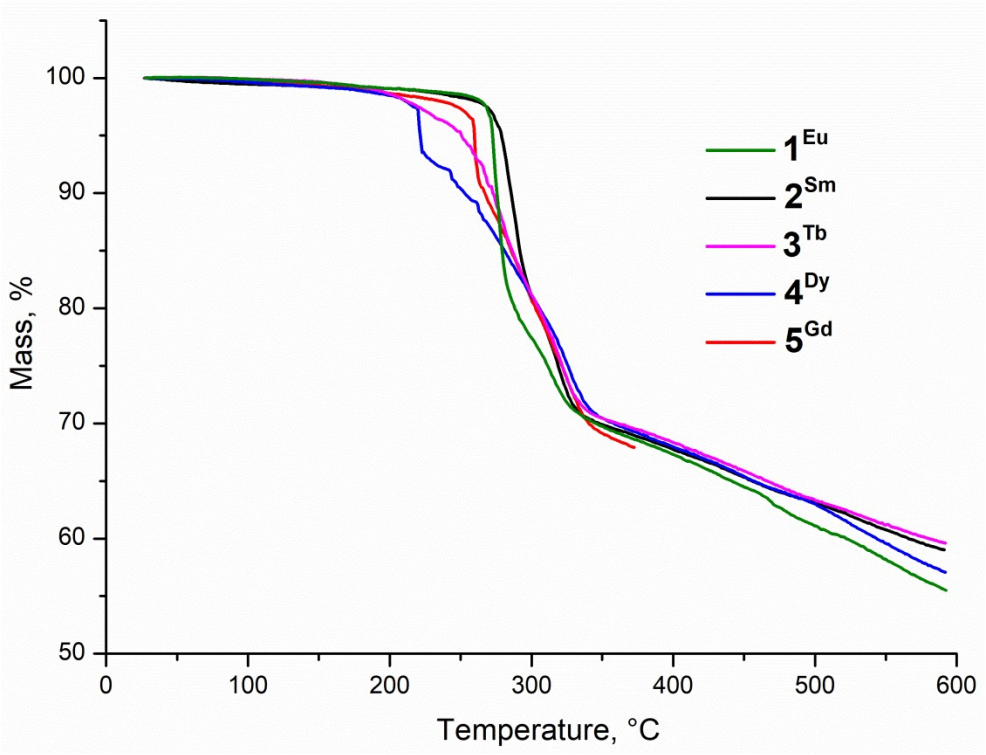

Figure S2. The thermogravimetric curves of obtained complexes.

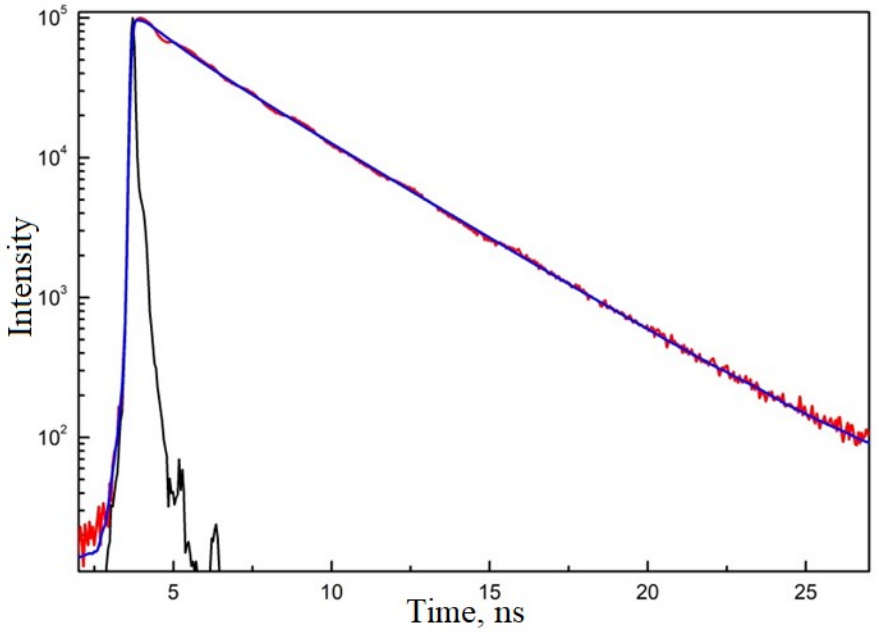

Figure S3. Photoluminescence kinetics curve of the ligand (red curve) and biexponential fit (blue curve) with lifetimes of 3.2 ns (80%) and 1.1 ns (20%). The black curve is the instrument response function (λ_{ex}=375 nm and λ_{em}=470 nm).

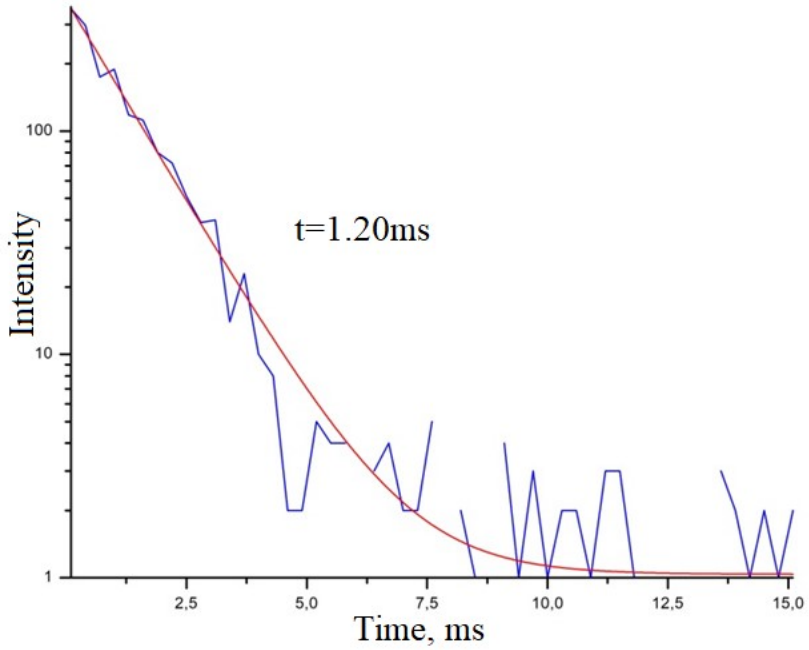

Figure S4. Photoluminescence kinetics curve of the europium(III) complex $\mathbf{1}^{\mathbf{Eu}}$ (λ_{ex}=350 nm and λ_{em}=613 nm). The red line is an exponential approximation.

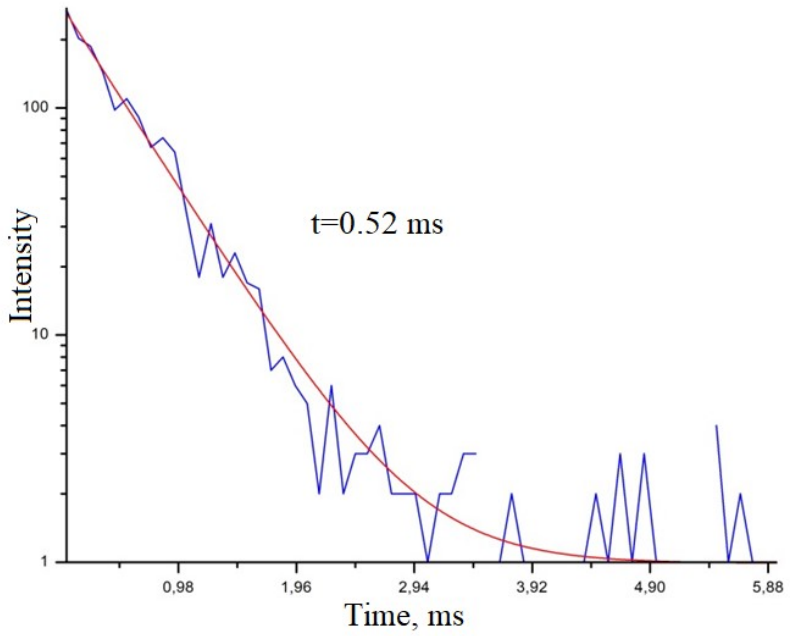

Figure S5. Photoluminescence kinetics curve of the terbium(III) complex $\mathbf{3}^{\mathbf{Tb}}$ (λ_{ex}=280 nm and λ_{em}=545 nm). The red line is an exponential approximation.

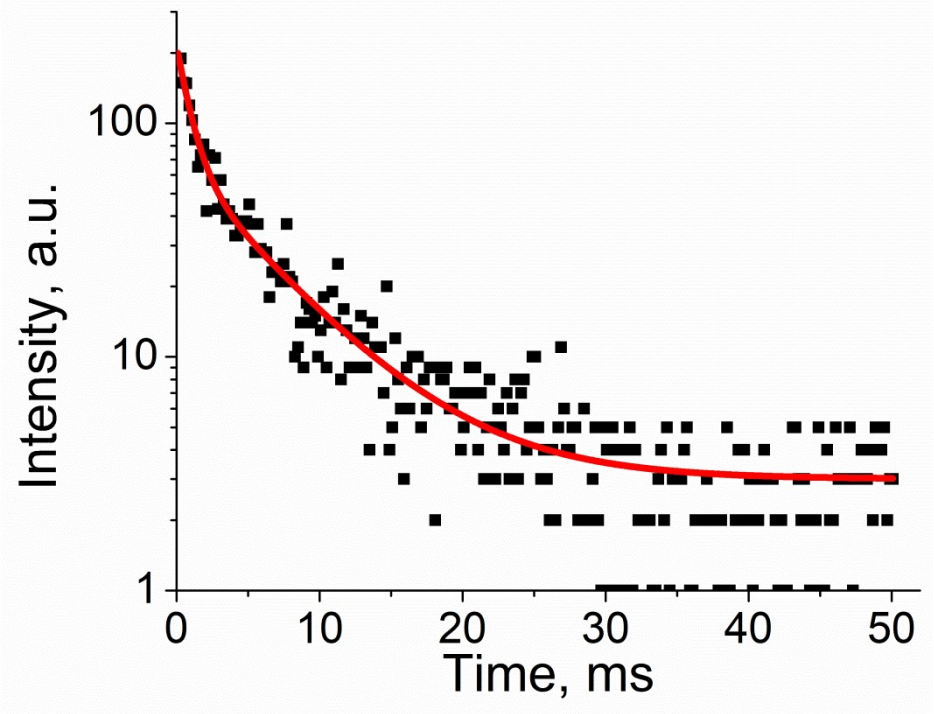

Figure S6. Photoluminescence kinetics curve of the gadolinium(III) complex $\mathbf{5}^{\mathbf{Gd}}$ (λ_{ex}=390 nm). The red line is an exponential approximation.

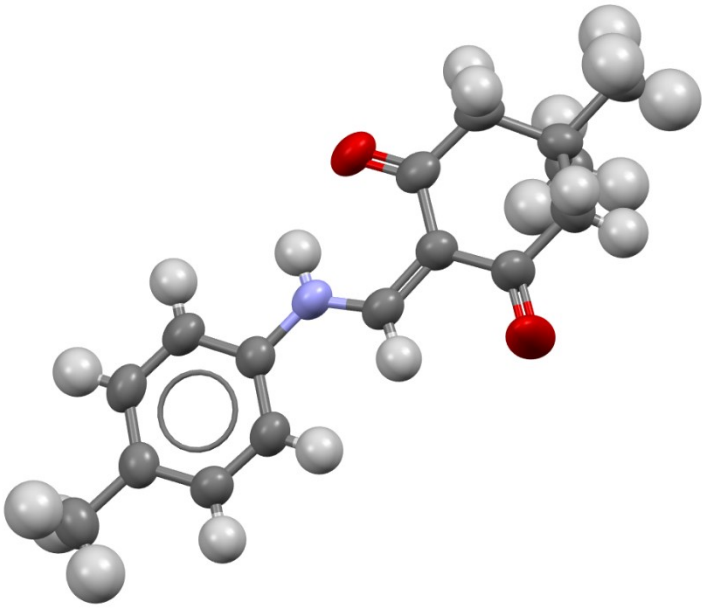

Figure S7. Structure of ligand with anisotropic displacement parameters depicted at 80% probability level.

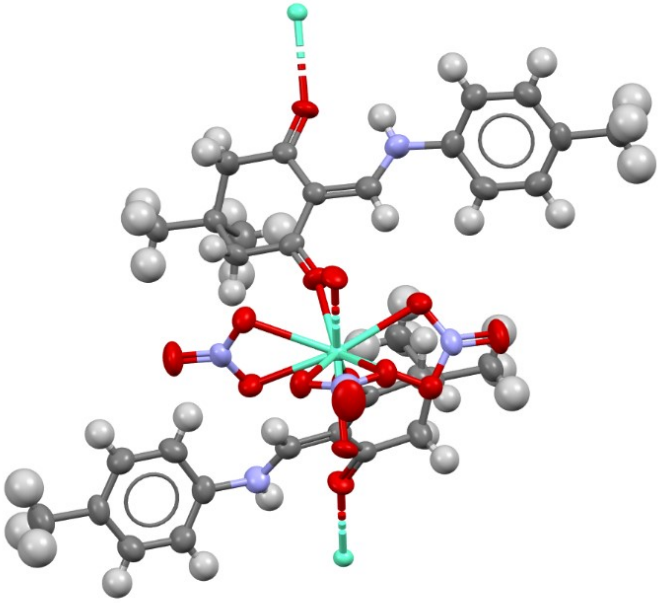

Figure S8. Structure of $\mathbf{1}^{Eu}$ with anisotropic displacement parameters depicted at 80% probability level.

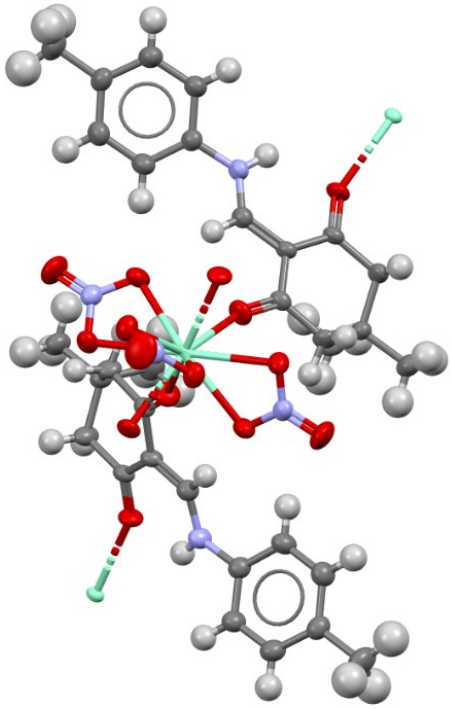

Figure S9. Structure of **2**^{Sm} with anisotropic displacement parameters depicted at 80% probability level.

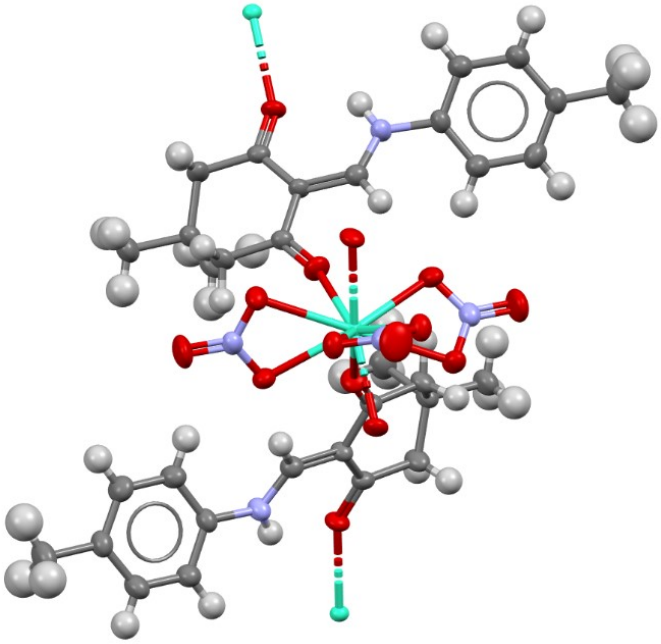

Figure S10. Structure of **3**^{Tb} with anisotropic displacement parameters depicted at 80% probability level.

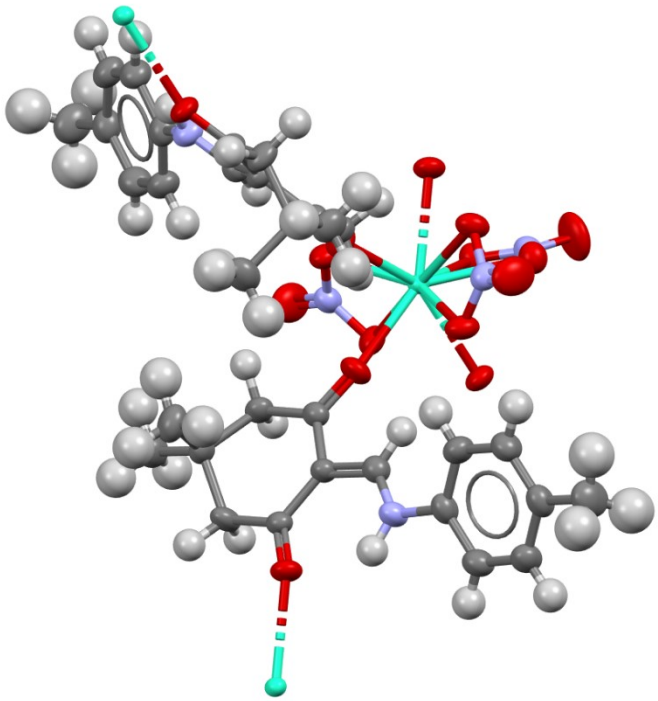

Figure S11. Structure of $\mathbf{4}^{\mathbf{Dy}}$ with anisotropic displacement parameters depicted at 80% probability level.

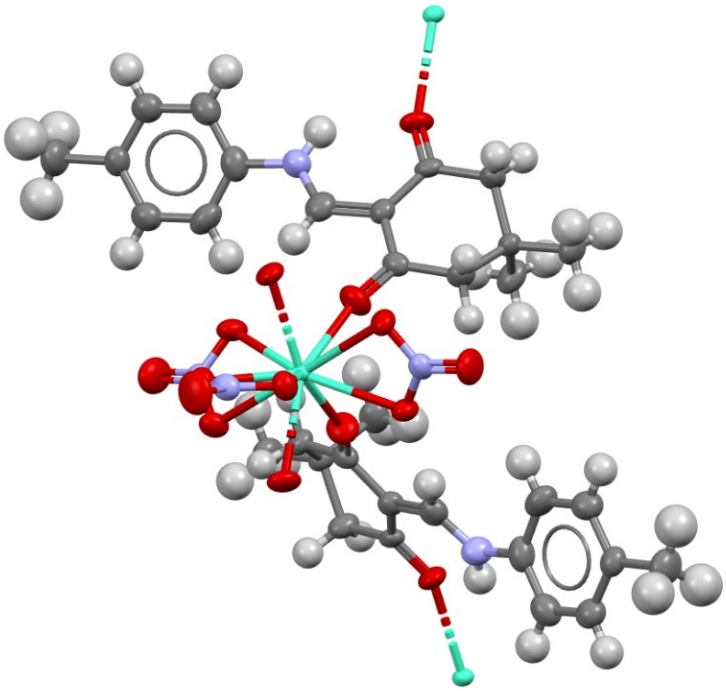

Figure S12. Structure of $\mathbf{5}^{\mathbf{Gd}}$ with anisotropic displacement parameters depicted at 80% probability level.