Supplemental Information

Tunable Ligand Emission of Napthylsalophen Triple-Decker Dinuclear Lanthanide (III) Sandwich Complexes

Emily E. Hardy, Kevin M. Wyss, Rebecca J. Keller, John D. Gorden, Anne E. V. Gorden*

Department of Chemistry and Biochemistry, Auburn University, 179 Chemistry Building, Auburn, Alabama 36849, USA.

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Additional Crystallographic Data

Table SI1: Crystallographic Data for Tb_2L_3, Dy_2L_3, and Lu_2L_3.

Identification code	Tb2L3-MeOH	Dy2L3-MeOH	Lu2L3-MeOH
Empirical formula	$C_{85}H_{58}N_6O_7Tb_2$	$C_{85}H_{58}N_6O_7Dy_2$	$C_{85}H_{58}N_6O_7Lu_2$
Formula weight	1593.29	1600.44	1625.38
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a/Å	17.4947(6)	17.4758(9)	17.3981(17)
b/Å	20.5096(7)	20.4943(11)	20.4310(19)
c/Å	20.6071(8)	20.6011(11)	20.6803(19)
α/°	90	90	90
β/°	96.4934(9)	96.445(1)	96.1767(13)
γ/°	90	90	90
Volume/Å³	7347.3(4)	7331.7(7)	7308.4(12)
Z	4	4	4
ρcalc (g cm⁻³)	1.4404	1.4498	1.4771
m/mm-1	1.969	2.082	2.745
Temperature/K	180.45	180.45	180.45
Radiation	0.71073	0.71073	0.71073
collected reflns	107251	97079	80420
Independent reflns	16189	12348	16055
GoF (on F2)	1.078	1.085	1.987
R1 [I=2σ (I)]	0.0495	0.0622	0.1491
wR2 [I=2σ (I)]	0.0954	0.1037	0.4186
(Δρ)max/(Δρ)min (e Å⁻³)	3.04/-1.35	2.26/-3.45	8.78/-2.86

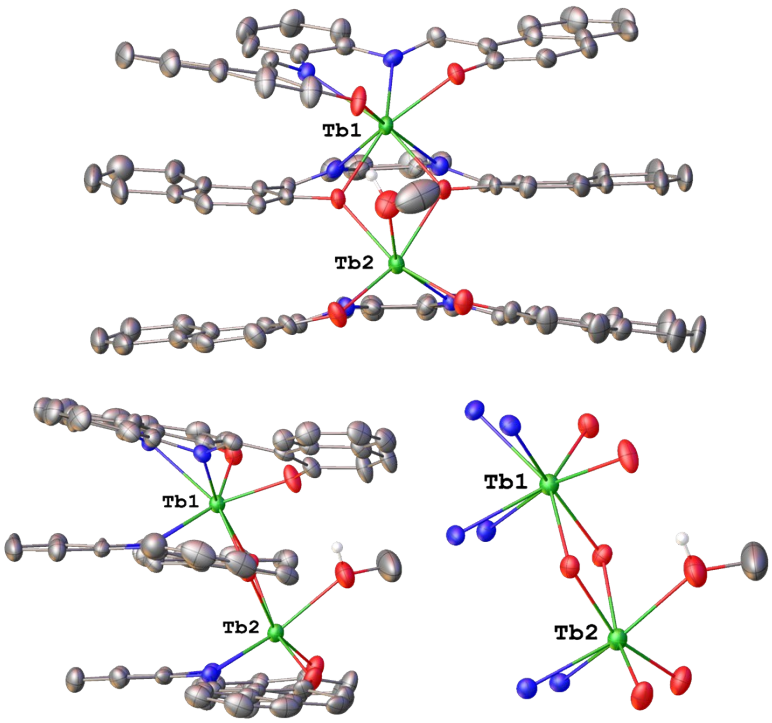

Figure SI1: Projections of Tb_2L_3. Carbon atoms shown in grey, hydrogen in white, oxygen in red, nitrogen in blue, and terbium in green.

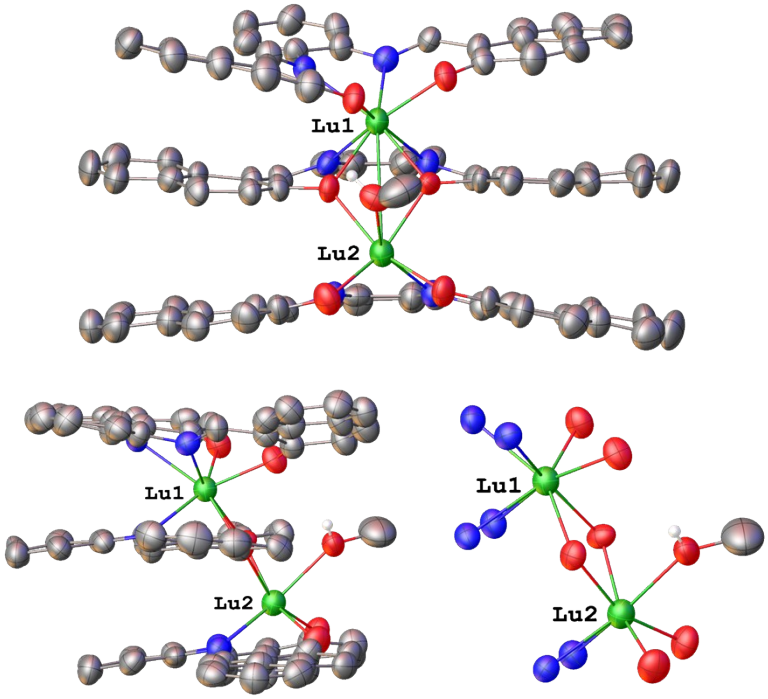

Figure SI2. Projections of Lu_2L_3. Carbon atoms shown in grey, hydrogen in white, oxygen in red, nitrogen in blue, and lutetium in green.

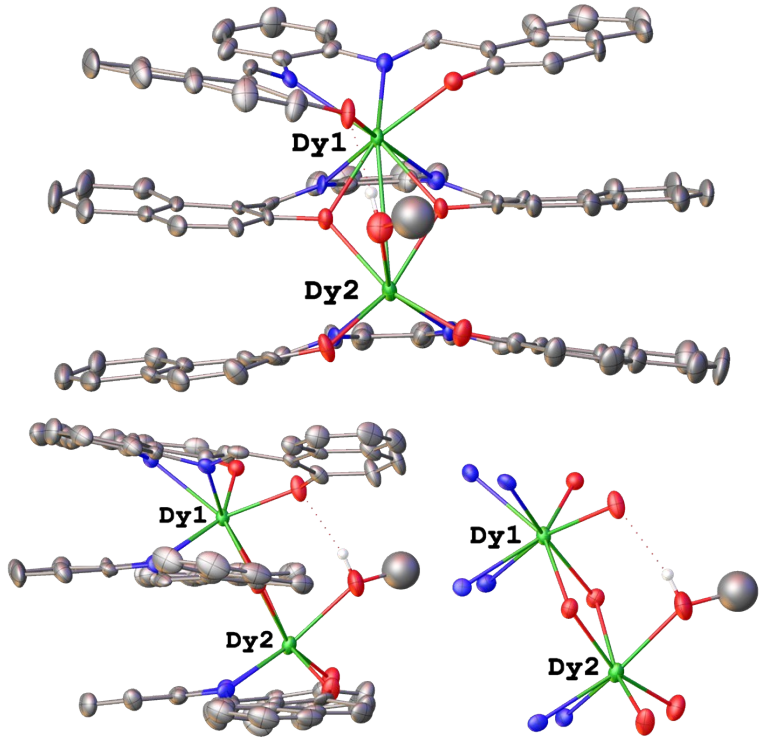

Figure SI3. Projections of Dy_2L_3. Carbon atoms shown in grey, hydrogen in white, oxygen in red, nitrogen in blue, and dysprosium in green.

Electronic Spectroscopy

Solid-State Excitation and Emission Spectra

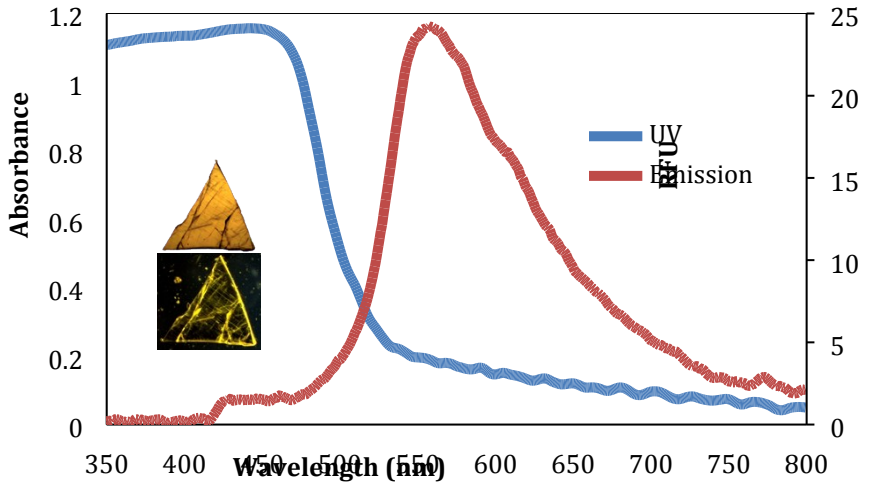

Figure SI4: Solid-state absorbance and emission after 365 nm excitation of Pr_2L_3. Images of single crystals of Pr_2L_3 taken on a CRAIC Microspectrophotometer under ambient light and 365 nm light.

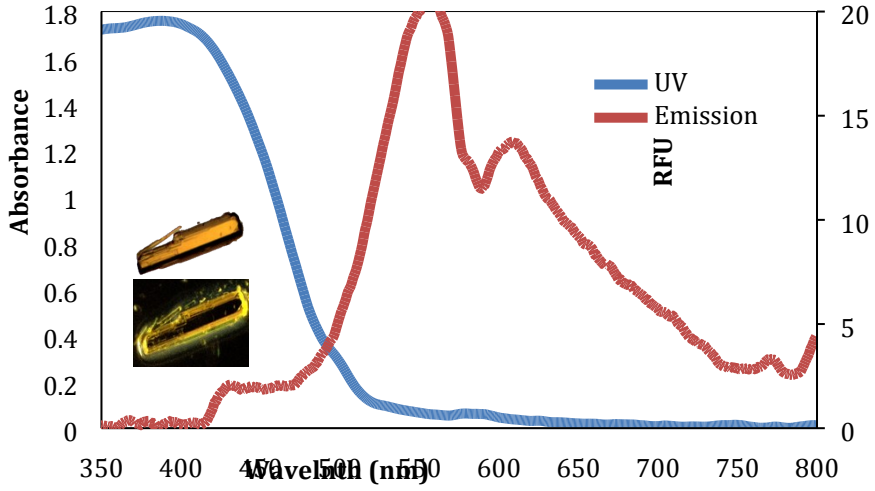

Figure SI5: Solid-state absorbance and emission after 365 nm excitation of Nd_2L_3. Images of single crystals of Nd_2L_3 taken on a CRAIC Microspectrophotometer under ambient light and 365 nm light.

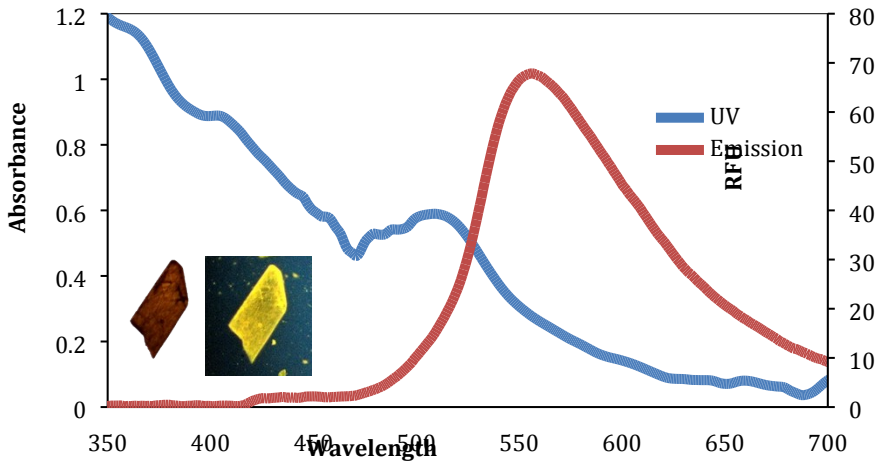

Figure SI6: Solid-state absorbance and emission after 365 nm excitation of Sm_2L_3. Images of single crystals of Sm_2L_3 taken on a CRAIC Microspectrophotometer under ambient light and 365 nm light.

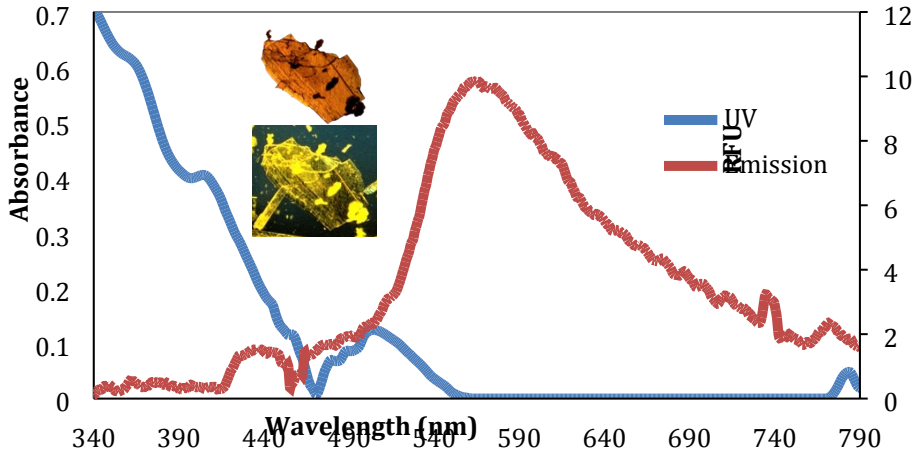

Figure SI7: Solid-state absorbance and emission after 365 nm excitation of Eu_2L_3. Images of single crystals of Eu_2L_3 taken on a CRAIC Microspectrophotometer under ambient light and 365 nm light.

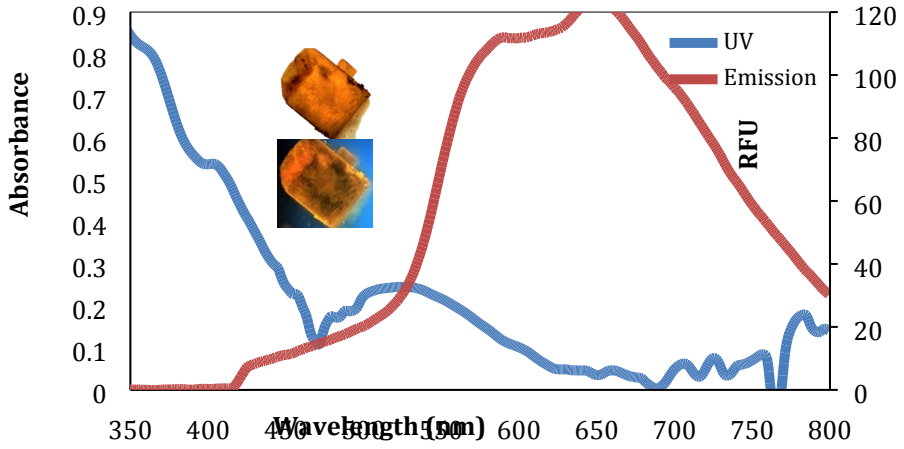

Figure SI8: Solid state absorbance and emission after 365 nm excitation of Gd_2L_3. Images of single crystals of Gd_2L_3 taken on a CRAIC Microspectrophotometer under ambient light and 365 nm light.

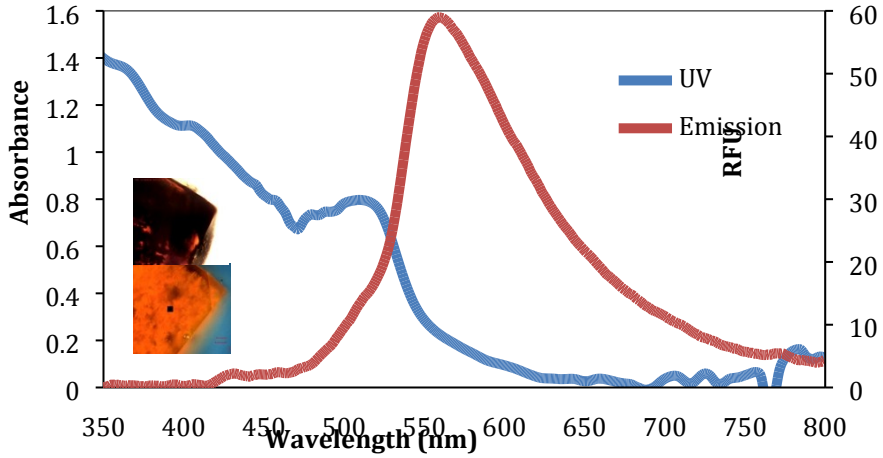

Figure SI9: Solid-state absorbance and emission after 365 nm excitation of Tb_2L_3. Images of single crystals of Tb_2L_3 taken on a CRAIC Microspectrophotometer under ambient light and 365 nm light.

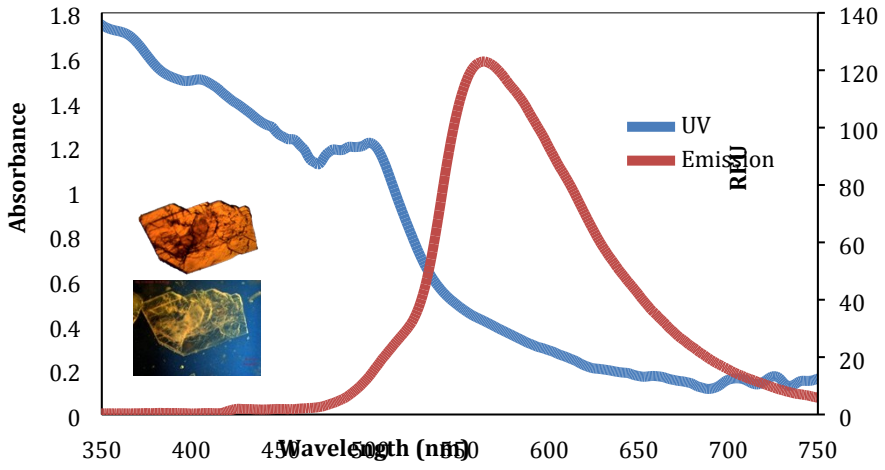

Figure SI10: Solid-state absorbance and emission after 365 nm excitation of Dy_2L_3. Images of single crystals of Dy_2L_3 taken on a CRAIC Microspectrophotometer under ambient light and 365 nm light.

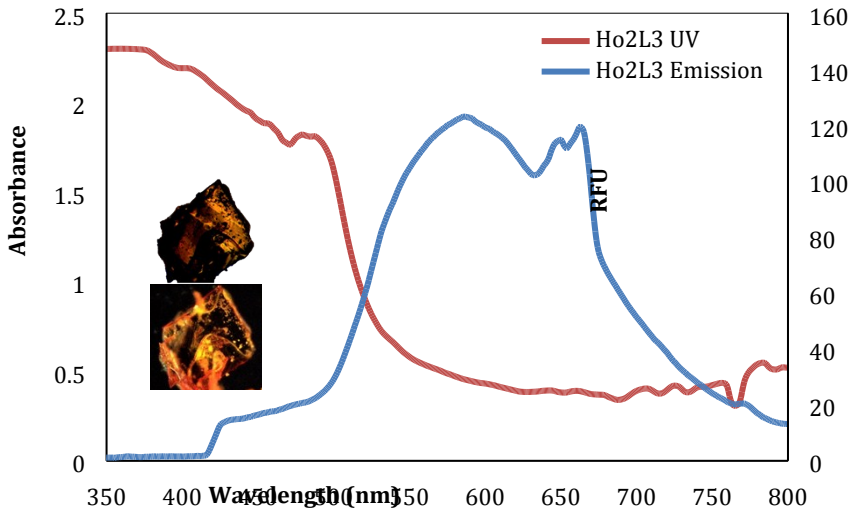

Figure SI11: Solid state absorbance and emission after 365 nm excitation of Ho_2L_3. Images of single crystals of Ho_2L_3 taken on a CRAIC Microspectrophotometer under ambient light and 365 nm light.

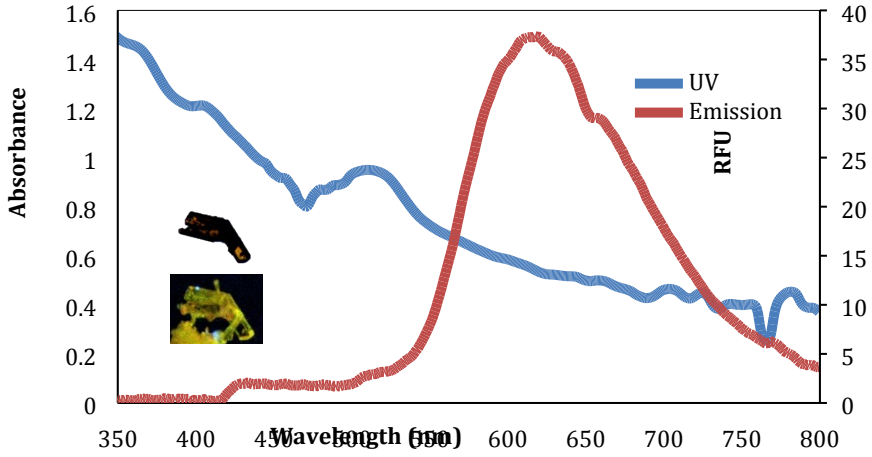

Figure SI12: Solid state absorbance and emission after 365 nm excitation of Er_2L_3 Images of single crystals of Er_2L_3 taken on a CRAIC Microspectrophotometer under ambient light and 365 nm light.

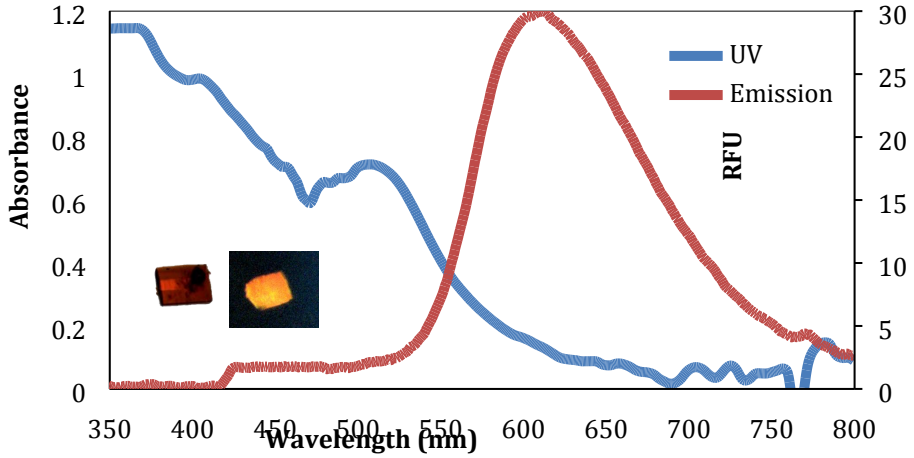

Figure SI13: Solid-state absorbance and emission after 365 nm excitation of Yb_2L_3. Images of single crystals of Yb_2L_3 taken on a CRAIC Microspectrophotometer under ambient light and 365 nm light.

Additional Solution Phase Absorption and Emission Spectra

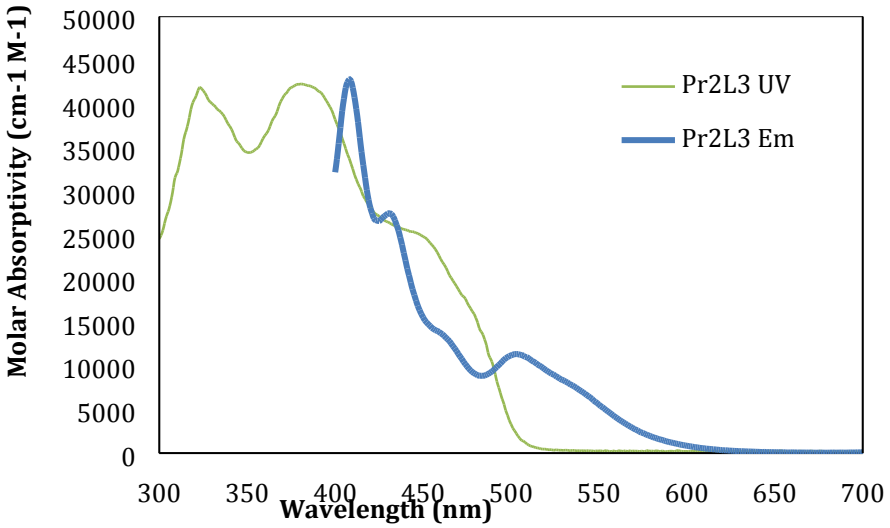

Figure SI14: Solution phase absorbance and emission after 365 nm excitation of Pr_2L_3 (15 µM in $CHCl_3$).

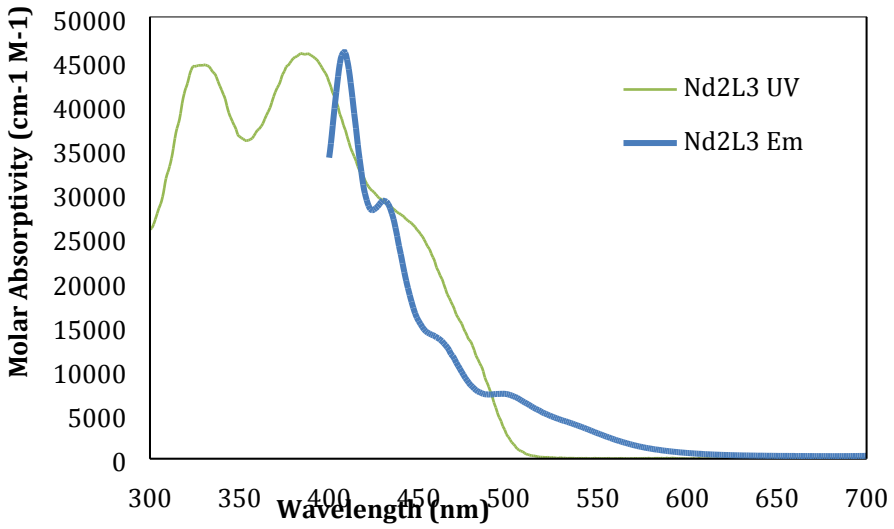

Figure SI15: Solution phase absorbance and emission after 365 nm excitation of Nd_2L_3 (15 µM in $CHCl_3$).

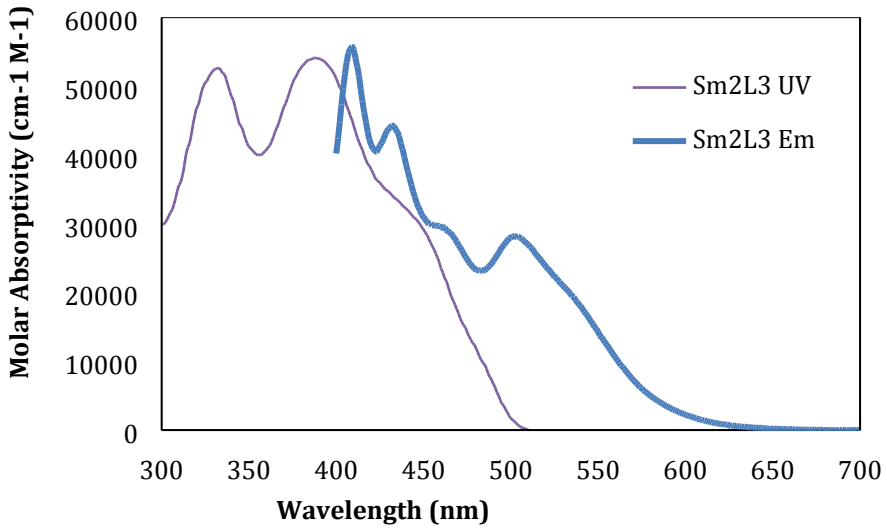

Figure SI16: Solution phase absorbance and emission after 365 nm excitation of Sm_2L_3 (15 µM in $CHCl_3$).

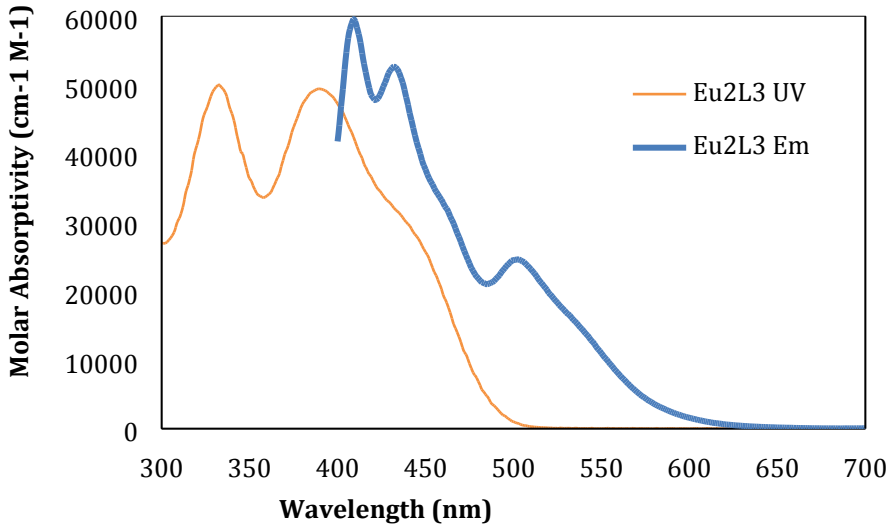

Figure SI17: Solution phase absorbance and emission after 365 nm excitation of Eu_2L_3 (15 µM in $CHCl_3$).

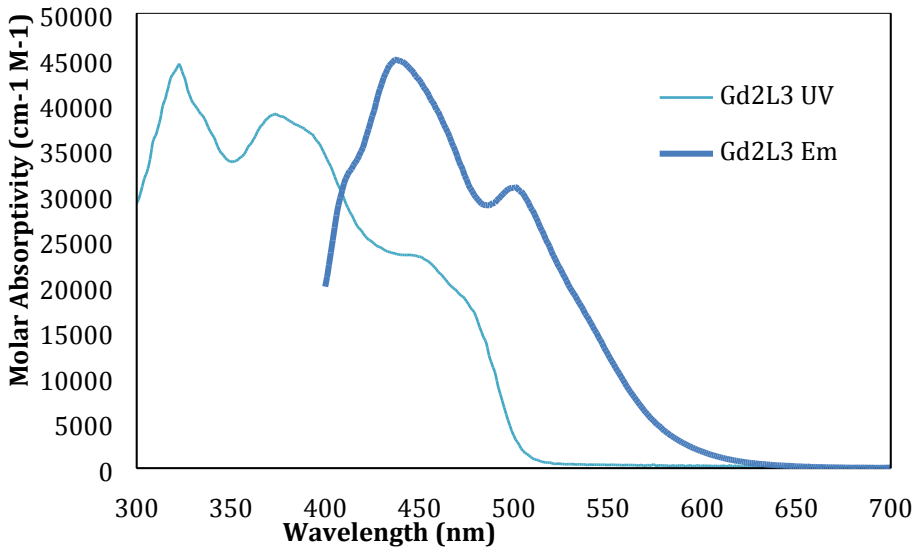

Figure SI18: Solution phase absorbance and emission after 365 nm excitation of Gd_2L_3 (15 µM in $CHCl_3$).

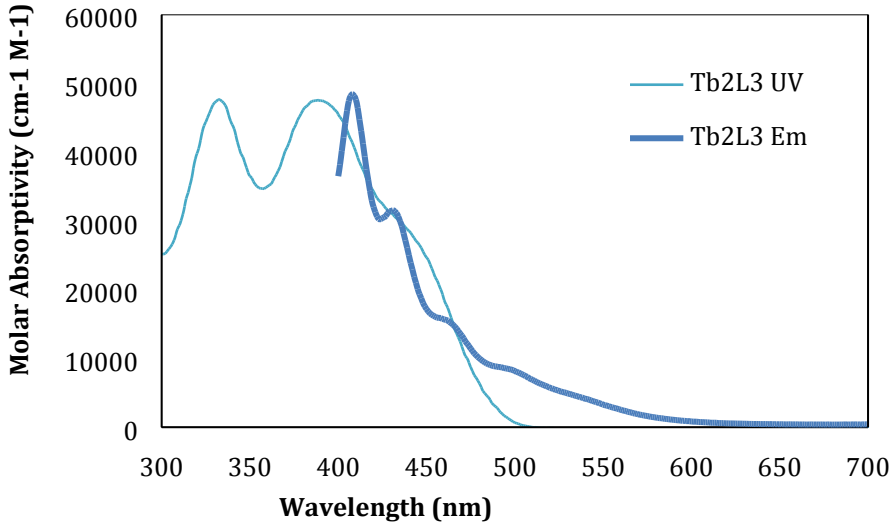

Figure SI19: Solution phase absorbance and emission after 365 nm excitation of Tb_2L_3 (15 µM in $CHCl_3$).

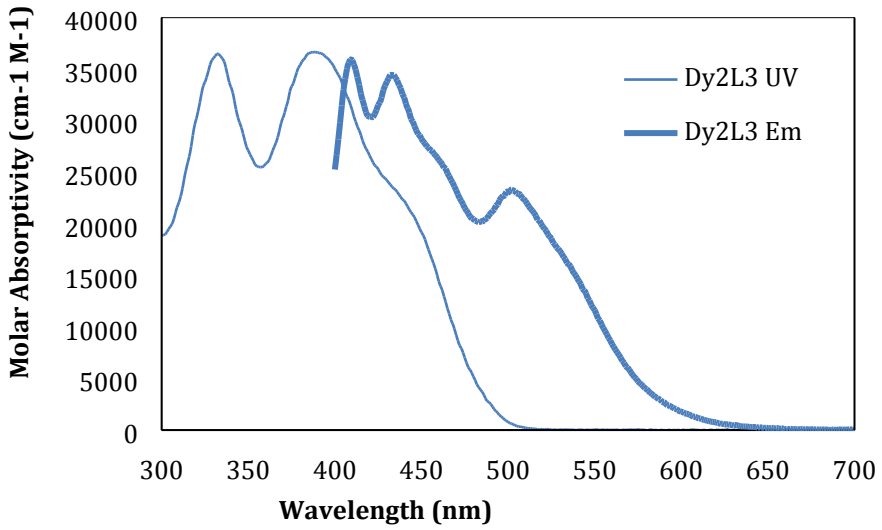

Figure SI20: Solution phase absorbance and emission after 365 nm excitation of Dy_2L_3 (15 µM in $CHCl_3$).

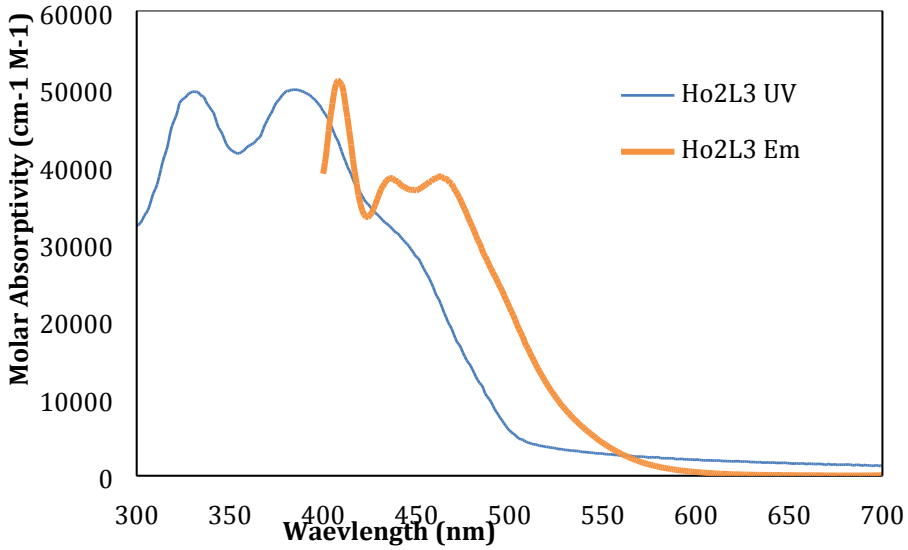

Figure SI21: Solution phase absorbance and emission after 365 nm excitation of Ho_2L_3 (15 µM in $CHCl_3$).

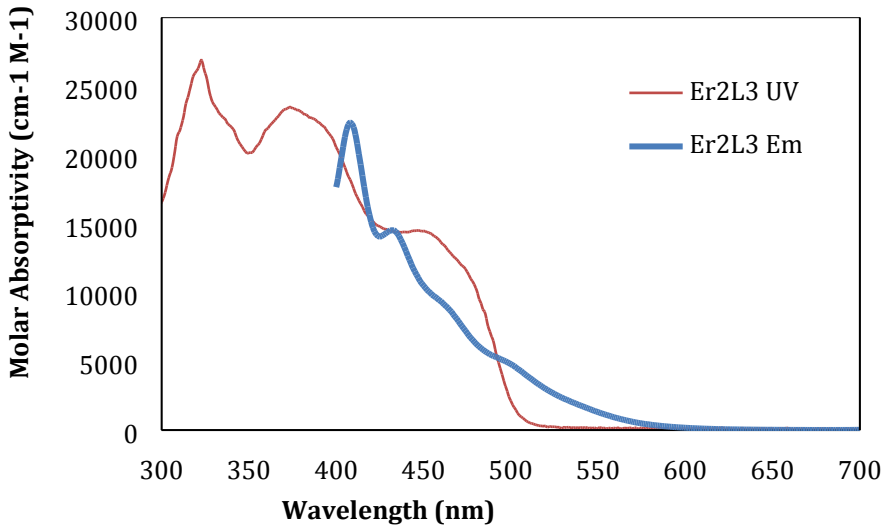

Figure SI22: Solution phase absorbance and emission after 365 nm excitation of Er_2L_3 (15 µM in $CHCl_3$).

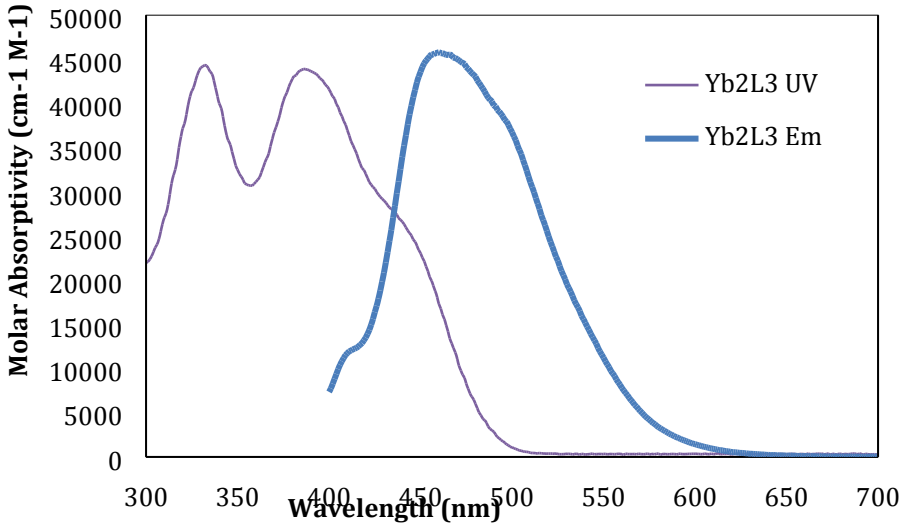

Figure SI23: Solution phase absorbance and emission after 365 nm excitation of Yb_2L_3 (15 µM in $CHCl_3$).

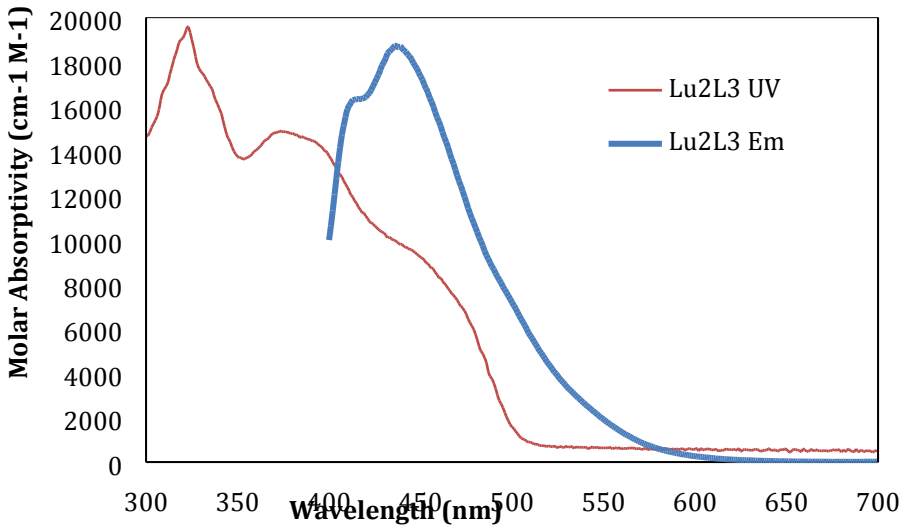

Figure SI24: Solution phase absorbance and emission after 365 nm excitation of Lu_2L_3 (15 µM in $CHCl_3$).

Quantum Yield Calculations

Quantum Yield was calculated via equation 1,

$$\Phi_X = \Phi_{ST}\left(\frac{Slope_X}{Slope_{ST}}\right)\left(\frac{\eta_X^2}{\eta_{ST}^2}\right) \quad (1)$$

Where the subscripts ST and X denote standard and unknown respectively, Φ is the fluorescence quantum yield. Slope is the slope from the plot of fluorescence intensity vs absorbance, and η the refractive index of the solvent. In this case the solvent was held constant, and Φ_{ST} was equal to 24 %.[1] The quantum yields were calculated and tabulated in Table SI2.

Table SI2: Quantum yields of Ln_2L_3 complexes in $CHCl_3$ solution.

Metal Ion	Φ
Dy	0.20%
Eu	0.25%
Gd	0.36%
Ho	1.00%
Lu	2.17%
Er	3.40%
Pr	0.33%
Tb	0.22%
Yb	0.38%

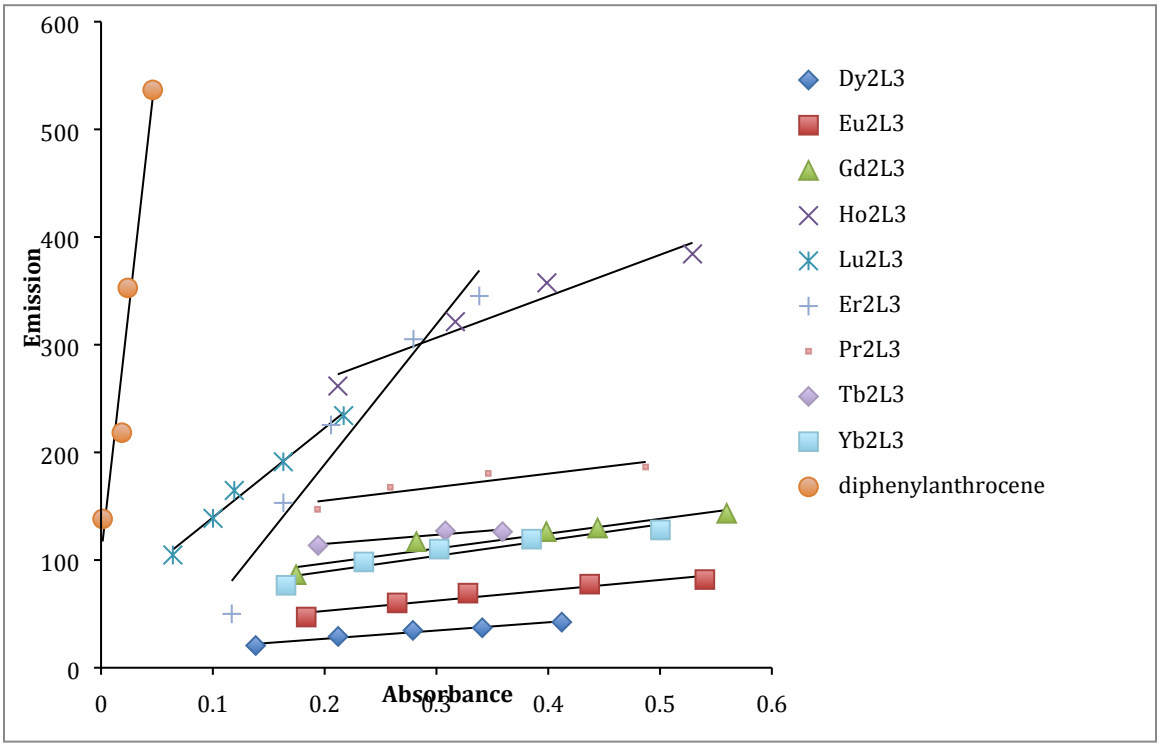

Figure SI25. Quantum Yield Plot

Crystallographic Tables

Gd2L3_FINAL

Table SI3 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Gd2L3_FINAL. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Gd1	13714.93(13)	13048.58(9)	-2942.27(9)	14.34(4)
Gd2	12554.98(14)	10973.24(10)	-2841.57(9)	16.15(4)
O3	13469(2)	11845.5(14)	-2226.1(14)	17.5(5)
O4	13004(2)	12125.7(14)	-3621.9(14)	17.8(5)
N3	12203(2)	13212.1(17)	-1677.5(17)	16.8(5)
N5	11084(3)	11177.8(18)	-1621.6(17)	18.8(6)
N4	11758(2)	13498.8(17)	-3063.3(16)	16.3(5)
N6	10692(2)	11445.9(18)	-3039.1(17)	17.9(6)
C29	13560(3)	11748(2)	-1492.0(19)	16.3(6)
N2	13930(3)	14060.8(18)	-4035.4(17)	18.3(6)
C68	10233(3)	11761(2)	-1683(2)	19.1(7)
O1	15008(2)	13147.4(15)	-2241.6(15)	20.4(5)
O2	15312(2)	12727.8(15)	-3895.5(14)	20.2(5)
N1	13651(3)	14437.2(18)	-2543.4(17)	18.3(6)
C48	11654(3)	13128(2)	-5072(2)	21.9(7)
C71	8610(3)	12912(3)	-1894(3)	28.9(8)
C73	10024(3)	11901(2)	-2425(2)	18.1(6)
C38	12965(3)	12230(2)	-891.4(19)	17.3(6)
C47	11950(3)	12956(2)	-4340.3(19)	17.0(6)
C56	12720(3)	12328(2)	-4284.9(19)	16.9(6)
C46	11368(3)	13392(2)	-3660(2)	18.2(6)
C39	12160(3)	12846(2)	-1023(2)	19.1(7)
C17	13355(3)	14792(2)	-3802(2)	18.7(7)
C66	11758(3)	10217(2)	-757(2)	21.8(7)
C67	10998(3)	10816(2)	-955(2)	21.6(7)
O6	12243(2)	10281.5(16)	-3787.8(16)	24.5(6)
C40	11352(3)	13810(2)	-1714(2)	19.0(7)
O5	12679(3)	9924.6(17)	-2069.2(16)	28.4(6)
C4	14521(3)	13950(2)	-8(2)	24.3(8)
C58	13171(4)	9129(2)	-1080(2)	29.1(9)
C45	11101(3)	13949(2)	-2438(2)	18.8(7)
C37	13076(3)	12076(2)	-106(2)	21.3(7)
C28	15483(3)	12697(2)	-4655(2)	18.6(7)
C12	13220(3)	14996(2)	-3022(2)	19.3(7)
C72	9218(3)	12485(2)	-2519(2)	23.2(7)
C75	10866(3)	10956(2)	-4344(2)	20.1(7)
C82	11765(4)	10057(3)	-5674(2)	30.9(9)
C30	14265(3)	11106(2)	-1317(2)	22.3(7)
C53	12132(3)	12654(2)	-5716(2)	25.3(8)
O7	14481(2)	10551.4(17)	-3394.9(19)	30.5(6)
C77	9626(3)	11701(3)	-5100(2)	26.0(8)

C74	10321(3)	11365(2)	-3655(2)	19.7(7)
C44	10297(3)	14540(2)	-2513(2)	26.8(8)
C19	15005(3)	13258(2)	-5101(2)	19.2(7)
C54	12914(4)	12024(3)	-5636(2)	26.5(8)
C57	12531(3)	9777(2)	-1327(2)	23.2(7)
C32	13775(4)	11425(2)	48(2)	25.0(8)
C20	15153(3)	13142(2)	-5924(2)	22.9(7)
C55	13199(3)	11866(2)	-4949(2)	21.9(7)
C1	14876(3)	13451(2)	-1564(2)	19.7(7)
C84	11773(3)	10400(2)	-4363(2)	21.1(7)
C41	10825(4)	14281(3)	-1090(2)	28.4(8)
C70	8814(4)	12780(3)	-1168(2)	30.1(9)
C76	10441(3)	11100(2)	-5033(2)	20.5(7)
C65	11682(3)	10040(2)	59(2)	23.9(7)
C78	9263(4)	11826(3)	-5768(3)	32.0(9)
C31	14363(4)	10956(2)	-576(2)	27.2(8)
C11	13785(3)	14639(2)	-1875(2)	20.0(7)
C18	14404(3)	13957(2)	-4763(2)	19.9(7)
C13	12597(4)	15689(2)	-2750(2)	25.7(8)
C49	10903(4)	13771(3)	-5171(3)	32.1(9)
C81	10901(4)	10645(2)	-5700(2)	27.5(8)
C79	9700(5)	11361(3)	-6413(3)	41.0(11)
C69	9625(3)	12212(2)	-1062(2)	25.5(8)
C83	12180(4)	9939(2)	-5037(2)	26.5(8)
C26	16363(4)	11974(3)	-5823(2)	27.6(8)
C51	11088(5)	13415(3)	-6505(3)	44.7(13)
C59	13070(4)	8946(2)	-319(3)	31.6(9)
C10	14191(3)	14135(2)	-1326(2)	18.9(7)
C80	10509(5)	10785(3)	-6377(3)	39.0(11)
C60	12334(4)	9394(2)	277(2)	27.6(8)
C25	15808(3)	12481(2)	-6279(2)	24.9(8)
C16	12845(3)	15285(2)	-4285(2)	25.1(8)
C5	14283(4)	14161(3)	779(2)	33.1(9)
C21	14594(4)	13627(3)	-6396(2)	31.1(9)
C61	12262(4)	9218(3)	1071(3)	35.4(10)
C15	12251(4)	15972(2)	-4010(3)	30.4(9)
C2	15477(3)	13076(2)	-1035(2)	24.8(8)
C9	13957(3)	14364(2)	-522(2)	21.7(7)
C27	16215(3)	12081(2)	-5049(2)	25.3(8)
C43	9754(4)	14989(3)	-1883(3)	35.1(10)
C64	11012(4)	10498(3)	664(2)	33.4(9)
C3	15314(4)	13323(2)	-295(2)	28.0(8)
C24	15887(4)	12327(3)	-7067(2)	34.7(10)
C36	12561(4)	12569(3)	520(2)	33.5(9)
C50	10629(5)	13899(3)	-5880(3)	41.6(12)
C8	13141(4)	14956(3)	-209(2)	27.8(8)
C6	13495(4)	14747(3)	1064(2)	35.5(10)
C42	10022(4)	14862(3)	-1177(3)	36.1(10)
C22	14697(5)	13469(3)	-7162(3)	40.9(11)

C14	12128(4)	16172(2)	-3244(3)	29.9(9)
C62	11570(5)	9653(3)	1641(3)	40.0(11)
C63	10950(5)	10305(3)	1432(3)	41.8(12)
C52	11827(4)	12815(3)	-6431(2)	37.3(11)
C33	13883(4)	11272(3)	820(3)	37.8(11)
C35	12691(5)	12406(3)	1257(3)	43.1(12)
C7	12918(4)	15147(3)	564(3)	35.1(10)
Cl4	17991.9(17)	13322.4(13)	-4091.0(9)	78.8(6)
Cl3	17384(2)	14758.5(11)	-3270.3(14)	85.1(6)
C87	16923(5)	13891(3)	-3525(3)	46.6(13)
Cl2	17764(2)	13102.0(16)	-9103.0(12)	96.1(7)
Cl1	19776(2)	12537.6(18)	-8622(2)	114.7(9)
O8	16154(3)	11403.4(17)	-3347.1(18)	28.5(6)
C23	15335(5)	12814(3)	-7502(3)	42.7(12)
C34	13342(5)	11743(3)	1409(3)	45.3(13)
C85	14893(6)	9804(4)	-3681(6)	77(3)
C88A	19015(12)	13414(6)	-9252(6)	55(3)
C86	16731(5)	11473(3)	-2763(3)	40.6(11)
C88B	18398(7)	12422(6)	-8566(6)	36(2)

Table SI4 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Gd2L3_FINAL. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Atom	$\mathbf{U_{11}}$	$\mathbf{U_{22}}$	$\mathbf{U_{33}}$	$\mathbf{U_{12}}$	$\mathbf{U_{13}}$	$\mathbf{U_{23}}$
Gd1	16.29(8)	15.25(8)	11.39(7)	0.34(6)	-3.48(6)	-0.91(5)
Gd2	17.06(8)	16.72(8)	15.22(8)	0.13(6)	-5.30(6)	-0.57(6)
O3	24.6(13)	17.3(12)	11.6(10)	-1.0(9)	-6.7(9)	-0.1(9)
O4	24.9(13)	18.4(12)	12.4(11)	-2.1(10)	-8.8(9)	0.9(9)
N3	16.5(13)	18.4(14)	14.9(13)	1.9(11)	-3.4(11)	-1.9(11)
N5	17.8(14)	20.6(15)	18.7(14)	-1.3(11)	-5.8(11)	0.3(11)
N4	18.3(14)	16.6(13)	13.1(12)	0.5(11)	-2.8(11)	1.1(10)
N6	15.4(13)	19.7(14)	18.1(14)	0.1(11)	-3.6(11)	-0.8(11)
C29	17.6(15)	19.1(16)	13.8(14)	-3.9(12)	-6.3(12)	1.2(12)
N2	20.0(14)	18.1(14)	17.0(13)	0.3(11)	-5.3(11)	-0.1(11)
C68	17.1(16)	22.2(17)	17.4(16)	-0.5(13)	-3.4(13)	1.3(13)
O1	22.1(13)	23.2(13)	17.5(12)	1.3(10)	-8(1)	-5.2(10)
O2	19.6(12)	23.7(13)	15.7(11)	3.9(10)	-2.5(9)	-3.2(10)
N1	22.4(15)	17.0(14)	15.7(13)	1.5(11)	-5.5(11)	-0.6(11)
C48	24.3(18)	26.0(18)	18.2(16)	-10.1(14)	-9.2(14)	5.5(14)
C71	22.9(19)	30(2)	32(2)	6.5(16)	-5.6(16)	-2.0(17)
C73	16.8(16)	20.7(17)	16.4(15)	-0.3(13)	-3.5(12)	-0.2(13)
C38	20.7(16)	19.3(16)	12.8(14)	-3.6(13)	-5.8(12)	4.0(12)
C47	17.4(16)	20.6(16)	14.5(15)	-4.8(13)	-6.5(12)	2.2(12)
C56	18.8(16)	18.7(16)	14.8(15)	-3.9(13)	-6.4(12)	1.6(12)
C46	17.7(16)	18.4(16)	18.8(16)	-0.4(12)	-5.5(13)	2.5(13)
C39	19.7(16)	23.7(17)	13.5(15)	-1.0(13)	-3.1(12)	-2.3(13)
C17	21.4(17)	15.8(16)	18.1(16)	-1.9(13)	-3.2(13)	1.5(12)
C66	22.5(17)	25.5(18)	18.2(16)	-4.7(14)	-6.7(14)	5.9(14)
C67	21.8(17)	26.6(19)	16.7(16)	-4.4(14)	-4.7(13)	2.5(14)
O6	27.2(14)	22.7(13)	26.9(14)	4.8(11)	-14.2(11)	-5.7(11)
C40	18.2(16)	21.2(17)	16.3(15)	1.9(13)	-2.2(13)	-2.3(13)

O5	38.3(16)	24.4(14)	20.7(13)	5.9(12)	-6.4(12)	2.4(11)
C4	30(2)	27.3(19)	17.8(17)	-6.0(15)	-8.2(15)	-2.6(14)
C58	43(2)	18.3(18)	27(2)	2.3(16)	-11.9(18)	0.6(15)
C45	16.2(16)	21.1(17)	17.2(15)	1.1(13)	-1.0(12)	0.2(13)
C37	28.0(19)	25.6(18)	12.0(15)	-6.5(15)	-7.2(13)	3.1(13)
C28	18.1(16)	21.9(17)	15.2(15)	-1.8(13)	-2.1(12)	-3.0(13)
C12	23.7(17)	15.7(16)	18.9(16)	-1.5(13)	-6.1(13)	1.2(13)
C72	21.3(17)	25.7(19)	21.9(17)	1.7(14)	-5.3(14)	-0.1(14)
C75	18.6(16)	21.2(17)	21.5(17)	-2.3(13)	-6.7(13)	-0.7(13)
C82	41(2)	28(2)	25.2(19)	5.0(17)	-10.6(17)	-10.4(16)
C30	27.9(19)	20.3(17)	20.6(17)	1.6(14)	-10.5(15)	1.2(13)
C53	31(2)	34(2)	13.6(16)	-12.0(16)	-8.1(14)	4.6(14)
O7	19.9(13)	23.4(14)	46.7(18)	1.2(11)	-4.8(13)	-10.0(13)
C77	25.0(19)	32(2)	22.9(18)	0.6(15)	-9.8(15)	-2.0(15)
C74	16.2(16)	21.8(17)	21.2(16)	-0.0(13)	-5.1(13)	1.0(13)
C44	24.5(19)	28(2)	27.1(19)	6.6(15)	-6.7(15)	2.0(15)
C19	19.5(16)	23.4(17)	12.5(14)	-4.4(13)	1.3(12)	-0.3(13)
C54	31(2)	33(2)	15.6(16)	-7.3(16)	-4.4(15)	-3.2(15)
C57	28.5(19)	19.8(17)	22.8(18)	-3.9(14)	-9.5(15)	4.9(14)
C32	36(2)	24.9(19)	18.1(17)	-6.6(16)	-13.7(15)	6.8(14)
C20	25.3(18)	28.9(19)	14.4(15)	-8.1(15)	-2.9(13)	-1.0(14)
C55	23.6(18)	23.9(18)	18.4(16)	-4.0(14)	-4.2(14)	-2.9(14)
C1	20.2(17)	22.3(17)	18.3(16)	-4.2(13)	-7.2(13)	-0.2(13)
C84	23.0(18)	20.0(17)	22.8(17)	-4.5(14)	-8.9(14)	-2.9(13)
C41	32(2)	31(2)	18.8(17)	8.1(17)	-1.0(15)	-6.3(15)
C70	26(2)	33(2)	26(2)	5.9(16)	1.5(16)	-6.1(16)
C76	20.6(17)	21.6(17)	20.6(17)	-5.6(13)	-6.1(14)	-0.9(13)
C65	25.5(19)	26.8(19)	21.5(17)	-7.1(15)	-8.8(15)	4.3(14)
C78	33(2)	37(2)	28(2)	-0.3(18)	-14.4(18)	3.4(17)
C31	35(2)	23.5(19)	27.7(19)	1.5(16)	-17.8(17)	4.3(15)
C11	20.7(17)	19.9(17)	19.0(16)	1.2(13)	-4.0(13)	-5.4(13)
C18	20.5(17)	22.3(17)	16.9(15)	-3.8(13)	-4.4(13)	2.5(13)
C13	36(2)	18.8(17)	22.9(18)	2.9(15)	-9.0(16)	-3.2(14)
C49	38(2)	33(2)	28(2)	-2.3(18)	-15.2(18)	8.9(17)
C81	35(2)	25.7(19)	24.6(19)	-0.9(16)	-11.9(16)	-3.8(15)
C79	52(3)	47(3)	30(2)	4(2)	-23(2)	-3(2)
C69	26.0(19)	32(2)	16.8(16)	2.4(16)	-2.4(14)	-3.2(15)
C83	30(2)	21.2(18)	29(2)	4.2(15)	-10.7(16)	-7.2(15)
C26	28(2)	32(2)	20.8(18)	-0.4(16)	-0.8(15)	-11.7(15)
C51	58(3)	61(3)	22(2)	-15(3)	-23(2)	14(2)
C59	48(3)	20.0(19)	31(2)	2.0(17)	-19.0(19)	2.6(16)
C10	20.2(16)	21.2(17)	16.1(15)	-0.7(13)	-5.2(13)	-3.8(13)
C80	58(3)	39(3)	24(2)	4(2)	-18(2)	-9.2(18)
C60	36(2)	27(2)	23.7(18)	-8.1(17)	-14.8(17)	5.3(15)
C25	23.6(18)	34(2)	15.7(16)	-6.8(15)	0.9(14)	-6.8(14)
C16	28.8(19)	26.9(19)	19.5(17)	1.2(15)	-7.1(15)	4.5(14)
C5	41(2)	42(2)	18.3(18)	-6(2)	-9.2(17)	-1.8(17)
C21	34(2)	41(2)	18.3(18)	-1.7(18)	-5.5(16)	-1.1(16)
C61	55(3)	29(2)	28(2)	-4(2)	-21(2)	7.9(17)

C15	35(2)	22.6(19)	34(2)	4.2(16)	-12.2(18)	6.9(16)
C2	26.7(19)	27.6(19)	23.0(18)	2.3(15)	-12.5(15)	-2.2(15)
C9	23.9(18)	24.8(18)	17.8(16)	-3.1(14)	-6.8(14)	-1.7(14)
C27	24.5(19)	29(2)	21.2(18)	4.7(15)	-3.2(15)	-8.6(15)
C43	31(2)	32(2)	38(2)	13.1(18)	-3.9(18)	-2.1(18)
C64	38(2)	41(2)	21.2(19)	2.7(19)	-9.4(17)	4.9(17)
C3	33(2)	30(2)	25.1(19)	0.1(16)	-15.2(17)	-1.5(16)
C24	40(2)	46(3)	16.7(18)	-7(2)	-0.4(17)	-10.1(17)
C36	42(3)	40(2)	17.8(18)	0(2)	-7.9(17)	0.1(17)
C50	50(3)	44(3)	38(3)	-4(2)	-26(2)	18(2)
C8	28(2)	30(2)	25.8(19)	-2.0(16)	-4.7(16)	-7.0(16)
C6	43(3)	44(3)	17.8(18)	-8(2)	-0.7(17)	-10.6(17)
C42	37(2)	33(2)	31(2)	13.0(19)	2.5(18)	-9.3(18)
C22	51(3)	55(3)	18.2(19)	-3(2)	-11.2(19)	1.8(19)
C14	36(2)	17.7(18)	35(2)	4.5(16)	-7.7(18)	-0.5(16)
C62	54(3)	47(3)	23(2)	-7(2)	-17(2)	7.4(19)
C63	48(3)	56(3)	20(2)	3(2)	-7.2(19)	1(2)
C52	48(3)	50(3)	18.2(18)	-12(2)	-14.9(19)	3.7(18)
C33	52(3)	42(3)	23(2)	2(2)	-19(2)	8.3(18)
C35	55(3)	55(3)	18(2)	2(2)	-9(2)	-5(2)
C7	36(2)	41(3)	26(2)	-1.9(19)	-1.3(18)	-11.9(18)
Cl4	88.3(13)	101.4(14)	40.6(8)	56.2(11)	-20.1(8)	-12.9(8)
Cl3	104.8(16)	55.1(10)	107.8(16)	-7.4(10)	-45.6(13)	-20.2(10)
C87	40(3)	48(3)	47(3)	-10(2)	3(2)	-6(2)
Cl2	120.6(19)	106.6(17)	57.1(11)	12.3(15)	-17.5(12)	-16.4(11)
Cl1	65.2(13)	115(2)	161(3)	-5.2(13)	-17.9(15)	-28.6(19)
O8	31.2(15)	23.4(14)	34.1(15)	1.3(12)	-15.1(13)	-0.7(12)
C23	52(3)	60(3)	16.8(19)	-6(2)	-8.3(19)	-6(2)
C34	63(3)	61(3)	15.8(19)	0(3)	-19(2)	5(2)
C85	32(3)	50(4)	142(9)	9(3)	-3(4)	-48(5)
C88A	101(10)	28(5)	26(5)	-16(5)	8(5)	-7(4)
C86	40(3)	46(3)	41(3)	9(2)	-24(2)	-12(2)
C88B	19(4)	44(5)	43(5)	-14(4)	2(3)	-2(4)

Table SI5 Bond Lengths for Gd2L3_FINAL.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Gd1	O3	2.379(2)	C75	C74	1.430(5)
Gd1	O4	2.368(2)	C75	C84	1.414(5)
Gd1	N3	2.562(3)	C75	C76	1.452(5)
Gd1	N4	2.549(3)	C82	C81	1.423(6)
Gd1	N2	2.530(3)	C82	C83	1.355(6)
Gd1	O1	2.275(2)	C30	C31	1.364(5)
Gd1	O2	2.318(2)	C53	C54	1.425(6)
Gd1	N1	2.500(3)	C53	C52	1.422(5)
Gd2	O3	2.386(2)	O7	C85	1.411(7)
Gd2	O4	2.388(2)	C77	C76	1.411(5)
Gd2	N5	2.487(3)	C77	C78	1.373(5)
Gd2	N6	2.493(3)	C44	C43	1.388(6)
Gd2	O6	2.218(3)	C19	C20	1.449(5)

Gd2	O5	2.237(3)	C19	C18	1.436(5)
Gd2	O7	2.419(3)	C54	C55	1.363(5)
O3	C29	1.339(4)	C32	C31	1.413(6)
O4	C56	1.336(4)	C32	C33	1.422(5)
N3	C39	1.290(4)	C20	C25	1.418(6)
N3	C40	1.427(4)	C20	C21	1.421(6)
N5	C68	1.421(5)	C1	C10	1.411(5)
N5	C67	1.299(5)	C1	C2	1.440(5)
N4	C46	1.292(4)	C84	C83	1.426(5)
N4	C45	1.424(4)	C41	C42	1.387(6)
N6	C73	1.420(4)	C70	C69	1.388(6)
N6	C74	1.301(4)	C76	C81	1.420(5)
C29	C38	1.401(5)	C65	C60	1.421(6)
C29	C30	1.426(5)	C65	C64	1.413(6)
N2	C17	1.421(5)	C78	C79	1.396(7)
N2	C18	1.296(5)	C11	C10	1.437(5)
C68	C73	1.413(5)	C13	C14	1.384(6)
C68	C69	1.400(5)	C49	C50	1.387(6)
O1	C1	1.299(4)	C81	C80	1.410(6)
O2	C28	1.317(4)	C79	C80	1.365(7)
N1	C12	1.418(4)	C26	C25	1.419(6)
N1	C11	1.301(4)	C26	C27	1.361(5)
C48	C47	1.448(5)	C51	C50	1.392(8)
C48	C53	1.411(6)	C51	C52	1.352(8)
C48	C49	1.424(6)	C59	C60	1.427(6)
C71	C72	1.383(6)	C10	C9	1.450(5)
C71	C70	1.381(6)	C60	C61	1.413(6)
C73	C72	1.396(5)	C25	C24	1.413(5)
C38	C39	1.452(5)	C16	C15	1.382(6)
C38	C37	1.448(4)	C5	C6	1.369(7)
C47	C56	1.403(5)	C21	C22	1.372(6)
C47	C46	1.451(5)	C61	C62	1.364(7)
C56	C55	1.427(5)	C15	C14	1.386(6)
C17	C12	1.410(5)	C2	C3	1.361(5)
C17	C16	1.406(5)	C9	C8	1.409(6)
C66	C67	1.434(5)	C43	C42	1.380(7)
C66	C57	1.411(6)	C64	C63	1.377(6)
C66	C65	1.451(5)	C24	C23	1.373(7)
O6	C84	1.298(4)	C36	C35	1.374(6)
C40	C45	1.404(5)	C8	C7	1.380(6)
C40	C41	1.396(5)	C6	C7	1.401(7)
O5	C57	1.303(4)	C22	C23	1.393(8)
C4	C5	1.412(5)	C62	C63	1.399(7)
C4	C9	1.418(5)	C33	C34	1.357(7)
C4	C3	1.424(6)	C35	C34	1.402(8)
C58	C57	1.436(5)	Cl4	C87	1.720(6)
C58	C59	1.353(6)	Cl3	C87	1.745(6)
C45	C44	1.395(5)	Cl2	C88A	1.634(14)
C37	C32	1.422(5)	Cl2	C88B	1.740(11)

C37	C36	1.415(6)	Cl1	C88A	2.139(13)
C28	C19	1.410(5)	Cl1	C88B	1.713(9)
C28	C27	1.427(5)	O8	C86	1.410(5)
C12	C13	1.402(5)			

Table SI6 Bond Angles for Gd2L3_FINAL.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4	Gd1	O3	69.21(8)	C3	C4	C9	119.2(3)
N3	Gd1	O3	68.71(9)	C59	C58	C57	121.6(4)
N3	Gd1	O4	103.24(9)	C40	C45	N4	116.1(3)
N4	Gd1	O3	103.88(9)	C44	C45	N4	124.5(3)
N4	Gd1	O4	69.20(9)	C44	C45	C40	119.2(3)
N4	Gd1	N3	63.01(9)	C32	C37	C38	119.3(3)
N2	Gd1	O3	162.36(9)	C36	C37	C38	123.0(4)
N2	Gd1	O4	93.84(9)	C36	C37	C32	117.6(3)
N2	Gd1	N3	122.10(9)	C19	C28	O2	123.1(3)
N2	Gd1	N4	73.08(9)	C27	C28	O2	118.4(3)
O1	Gd1	O3	81.39(9)	C27	C28	C19	118.4(3)
O1	Gd1	O4	141.27(9)	C17	C12	N1	116.3(3)
O1	Gd1	N3	88.17(9)	C13	C12	N1	124.1(3)
O1	Gd1	N4	144.99(9)	C13	C12	C17	119.4(3)
O1	Gd1	N2	111.34(10)	C73	C72	C71	120.8(4)
O2	Gd1	O3	101.11(9)	C84	C75	C74	122.0(3)
O2	Gd1	O4	80.69(9)	C76	C75	C74	118.4(3)
O2	Gd1	N3	166.19(9)	C76	C75	C84	119.6(3)
O2	Gd1	N4	130.11(9)	C83	C82	C81	121.5(4)
O2	Gd1	N2	70.24(9)	C31	C30	C29	121.0(4)
O2	Gd1	O1	80.89(9)	C54	C53	C48	119.2(3)
N1	Gd1	O3	132.77(9)	C52	C53	C48	119.6(4)
N1	Gd1	O4	147.27(9)	C52	C53	C54	121.3(4)
N1	Gd1	N3	72.46(10)	C85	O7	Gd2	126.7(4)
N1	Gd1	N4	80.65(10)	C78	C77	C76	121.8(4)
N1	Gd1	N2	64.54(10)	C75	C74	N6	127.7(3)
N1	Gd1	O1	71.44(9)	C43	C44	C45	120.6(4)
N1	Gd1	O2	111.42(10)	C20	C19	C28	119.5(3)
O4	Gd2	O3	68.77(8)	C18	C19	C28	121.5(3)
N5	Gd2	O3	81.16(9)	C18	C19	C20	119.0(3)
N5	Gd2	O4	115.08(9)	C55	C54	C53	121.2(4)
N6	Gd2	O3	116.69(9)	O5	C57	C66	123.1(3)
N6	Gd2	O4	78.77(9)	C58	C57	C66	118.6(3)
N6	Gd2	N5	65.51(10)	C58	C57	O5	118.3(4)
O6	Gd2	O3	157.93(10)	C31	C32	C37	118.8(3)
O6	Gd2	O4	95.37(9)	C33	C32	C37	119.4(4)
O6	Gd2	N5	120.34(10)	C33	C32	C31	121.7(4)
O6	Gd2	N6	72.75(10)	C25	C20	C19	119.8(4)
O5	Gd2	O3	97.79(10)	C21	C20	C19	123.0(4)
O5	Gd2	O4	161.92(10)	C21	C20	C25	117.0(3)
O5	Gd2	N5	72.81(10)	C54	C55	C56	120.9(4)
O5	Gd2	N6	118.90(11)	C10	C1	O1	123.5(3)

O5	Gd2	O6	93.85(10)	C2	C1	O1	118.1(3)
O7	Gd2	O3	79.76(9)	C2	C1	C10	118.5(3)
O7	Gd2	O4	84.00(10)	C75	C84	O6	122.8(3)
O7	Gd2	N5	145.51(10)	C83	C84	O6	118.3(3)
O7	Gd2	N6	148.95(11)	C83	C84	C75	118.9(3)
O7	Gd2	O6	83.48(10)	C42	C41	C40	120.1(4)
O7	Gd2	O5	81.64(11)	C69	C70	C71	120.0(4)
Gd2	O3	Gd1	110.49(9)	C77	C76	C75	123.8(3)
C29	O3	Gd1	123.9(2)	C81	C76	C75	119.1(3)
C29	O3	Gd2	123.5(2)	C81	C76	C77	117.0(3)
Gd2	O4	Gd1	110.80(9)	C60	C65	C66	119.7(4)
C56	O4	Gd1	120.7(2)	C64	C65	C66	123.3(4)
C56	O4	Gd2	127.3(2)	C64	C65	C60	117.0(4)
C39	N3	Gd1	127.7(2)	C79	C78	C77	120.6(4)
C40	N3	Gd1	114.2(2)	C32	C31	C30	121.7(4)
C40	N3	C39	118.0(3)	C10	C11	N1	126.2(3)
C68	N5	Gd2	114.3(2)	C19	C18	N2	126.6(3)
C67	N5	Gd2	128.3(3)	C14	C13	C12	120.4(4)
C67	N5	C68	117.4(3)	C50	C49	C48	119.8(4)
C46	N4	Gd1	124.9(2)	C76	C81	C82	119.1(4)
C45	N4	Gd1	115.5(2)	C80	C81	C82	121.0(4)
C45	N4	C46	119.4(3)	C80	C81	C76	119.9(4)
C73	N6	Gd2	114.4(2)	C80	C79	C78	119.3(4)
C74	N6	Gd2	127.0(2)	C70	C69	C68	120.7(4)
C74	N6	C73	118.4(3)	C84	C83	C82	121.5(4)
C38	C29	O3	122.8(3)	C27	C26	C25	121.2(4)
C30	C29	O3	118.0(3)	C52	C51	C50	120.0(4)
C30	C29	C38	119.2(3)	C60	C59	C58	121.7(4)
C17	N2	Gd1	113.1(2)	C11	C10	C1	121.2(3)
C18	N2	Gd1	127.4(2)	C9	C10	C1	119.6(3)
C18	N2	C17	119.1(3)	C9	C10	C11	119.1(3)
C73	C68	N5	117.0(3)	C79	C80	C81	121.4(4)
C69	C68	N5	123.9(3)	C59	C60	C65	118.6(4)
C69	C68	C73	119.0(3)	C61	C60	C65	119.9(4)
C1	O1	Gd1	128.4(2)	C61	C60	C59	121.5(4)
C28	O2	Gd1	131.2(2)	C26	C25	C20	118.7(3)
C12	N1	Gd1	114.9(2)	C24	C25	C20	120.3(4)
C11	N1	Gd1	123.7(2)	C24	C25	C26	121.0(4)
C11	N1	C12	120.1(3)	C15	C16	C17	120.8(4)
C53	C48	C47	119.6(4)	C6	C5	C4	121.4(4)
C49	C48	C47	122.2(4)	C22	C21	C20	121.4(4)
C49	C48	C53	118.3(3)	C62	C61	C60	121.5(4)
C70	C71	C72	120.2(4)	C14	C15	C16	120.1(4)
C68	C73	N6	116.6(3)	C3	C2	C1	121.4(4)
C72	C73	N6	124.2(3)	C10	C9	C4	119.4(3)
C72	C73	C68	119.1(3)	C8	C9	C4	117.6(3)
C39	C38	C29	121.5(3)	C8	C9	C10	122.9(3)
C37	C38	C29	119.9(3)	C26	C27	C28	121.8(4)
C37	C38	C39	118.4(3)	C42	C43	C44	120.0(4)

C56	C47	C48	119.5(3)	C63	C64	C65	121.6(4)
C46	C47	C48	119.2(3)	C2	C3	C4	121.1(4)
C46	C47	C56	121.1(3)	C23	C24	C25	120.7(4)
C47	C56	O4	122.4(3)	C35	C36	C37	121.4(4)
C55	C56	O4	118.0(3)	C51	C50	C49	121.2(5)
C55	C56	C47	119.6(3)	C7	C8	C9	121.5(4)
C47	C46	N4	125.2(3)	C7	C6	C5	119.2(4)
C38	C39	N3	124.6(3)	C43	C42	C41	120.4(4)
C12	C17	N2	117.1(3)	C23	C22	C21	121.1(5)
C16	C17	N2	123.7(3)	C15	C14	C13	120.4(4)
C16	C17	C12	118.9(3)	C63	C62	C61	119.0(4)
C57	C66	C67	122.2(3)	C62	C63	C64	120.9(5)
C65	C66	C67	118.1(4)	C51	C52	C53	121.1(5)
C65	C66	C57	119.7(3)	C34	C33	C32	121.0(4)
C66	C67	N5	127.1(4)	C34	C35	C36	120.4(5)
C84	O6	Gd2	137.3(2)	C6	C7	C8	120.6(4)
C45	C40	N3	116.6(3)	Cl3	C87	Cl4	111.8(3)
C41	C40	N3	123.6(3)	C22	C23	C24	119.5(4)
C41	C40	C45	119.7(3)	C35	C34	C33	120.0(4)
C57	O5	Gd2	137.1(3)	Cl1	C88A	Cl2	100.4(5)
C9	C4	C5	119.7(4)	Cl1	C88B	Cl2	115.3(5)
C3	C4	C5	121.0(4)				

Table SI7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Gd2L3_FINAL.

Atom	***x***	***y***	***z***	**U(eq)**
H71	8050(3)	13297(3)	-1964(3)	34.7(10)
H46	10642(3)	13616(2)	-3654(2)	21.9(8)
H39	11558(3)	12991(2)	-597(2)	22.9(8)
H67	10363(3)	10965(2)	-555(2)	26.0(8)
H58	13677(4)	8820(2)	-1460(2)	34.9(10)
H72	9085(3)	12590(2)	-3019(2)	27.8(9)
H82	12057(4)	9741(3)	-6114(2)	37.0(11)
H30	14671(3)	10778(2)	-1723(2)	26.8(9)
H7	15040(12)	10815(16)	-3370(30)	45.7(10)
H77	9321(3)	12028(3)	-4670(2)	31.2(9)
H74	9603(3)	11607(2)	-3645(2)	23.7(8)
H44	10119(3)	14636(2)	-3001(2)	32.2(10)
H54	13243(4)	11707(3)	-6070(2)	31.8(10)
H55	13723(3)	11442(2)	-4912(2)	26.3(8)
H41	11016(4)	14204(3)	-605(2)	34.1(10)
H70	8400(4)	13077(3)	-740(2)	36.1(10)
H78	8708(4)	12233(3)	-5792(3)	38.3(11)
H31	14840(4)	10525(2)	-477(2)	32.6(10)
H11	13596(3)	15171(2)	-1738(2)	24.0(8)
H18	14347(3)	14388(2)	-5107(2)	23.8(8)
H13	12497(4)	15826(2)	-2224(2)	30.9(9)
H49	10590(4)	14111(3)	-4753(3)	38.6(11)
H79	9439(5)	11444(3)	-6872(3)	49.2(14)

H69	9768(3)	12129(2)	-562(2)	30.6(9)
H83	12754(4)	9540(2)	-5039(2)	31.8(10)
H26	16847(4)	11551(3)	-6063(2)	33.1(10)
H51	10881(5)	13507(3)	-6983(3)	53.6(15)
H59	13500(4)	8508(2)	-178(3)	37.9(11)
H80	10813(5)	10473(3)	-6818(3)	46.8(13)
H16	12909(3)	15144(2)	-4807(2)	30.1(9)
H5	14677(4)	13891(3)	1117(2)	39.8(11)
H21	14140(4)	14071(3)	-6177(2)	37.4(11)
H61	12706(4)	8787(3)	1211(3)	42.5(12)
H15	11928(4)	16307(2)	-4346(3)	36.4(10)
H2	15998(3)	12647(2)	-1207(2)	29.8(9)
H27	16609(3)	11737(2)	-4763(2)	30.3(9)
H43	9197(4)	15383(3)	-1937(3)	42.1(12)
H64	10593(4)	10949(3)	537(2)	40.1(11)
H3	15737(4)	13072(2)	37(2)	33.6(10)
H24	16327(4)	11882(3)	-7298(2)	41.6(12)
H36	12118(4)	13021(3)	427(2)	40.2(11)
H50	10119(5)	14324(3)	-5940(3)	50.0(14)
H8	12735(4)	15231(3)	-537(2)	33.4(10)
H6	13341(4)	14881(3)	1596(2)	42.6(12)
H42	9656(4)	15175(3)	-748(3)	43.4(12)
H22	14328(5)	13811(3)	-7467(3)	49.1(14)
H14	11718(4)	16645(2)	-3056(3)	35.8(10)
H62	11509(5)	9516(3)	2173(3)	48.0(13)
H63	10480(5)	10619(3)	1825(3)	50.2(14)
H52	12149(4)	12495(3)	-6863(2)	44.7(13)
H33	14340(4)	10832(3)	925(3)	45.4(13)
H35	12336(5)	12745(3)	1668(3)	51.7(14)
H7a	12369(4)	15553(3)	758(3)	42.2(12)
H87a	16339(5)	14018(3)	-3812(3)	56.0(15)
H87b	16587(5)	13593(3)	-3048(3)	56.0(15)
H8a	15910(40)	11849(4)	-3470(20)	42.7(9)
H23	15387(5)	12705(3)	-8030(3)	51.2(14)
H34	13405(5)	11623(3)	1924(3)	54.4(15)
H85a	15130(70)	9670(50)	-3360(50)	60.9(17)
H85b	15630(60)	9760(40)	-3980(40)	60.9(17)
H85c	14330(60)	9490(40)	-3690(40)	60.9(17)
H86a	16760(60)	11010(40)	-2480(40)	60.9(17)
H86b	16490(50)	11890(40)	-2400(40)	60.9(17)
H86c	17480(60)	11590(40)	-2970(40)	60.9(17)
H88a	19395(12)	13424(6)	-9811(6)	66(4)
H88b	19000(12)	13940(6)	-9038(6)	66(4)
H88c	17984(7)	12451(6)	-8015(6)	43(2)
H88d	18329(7)	11892(6)	-8744(6)	43(2)

Table SI8 Atomic Occupancy for Gd2L3_FINAL.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
C88A	0.500000	C88B	0.500000	H88a	0.500000

H88b 0.500000 H88c 0.500000 H88d 0.500000

Refinement model description

Number of restraints - 3, number of constraints - 126.

Details:

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1. Others
 Fixed Sof: C88A(0.5) C88B(0.5) H88a(0.5) H88b(0.5) H88c(0.5) H88d(0.5)
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Yb2L3

Table SI9 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Yb2L3. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Yb1	7266.79(18)	5570.08(17)	7475.85(16)	17.83(10)
Yb2	7078.7(2)	3998.24(18)	6506.85(17)	20.58(10)
C45	8344(5)	4876(4)	8744(4)	22.0(17)
O4	7843(3)	4893(3)	6779(3)	19.4(11)
O3	6458(3)	4703(3)	7125(3)	21.4(12)
O2	8083(3)	6270(3)	7111(3)	22.3(12)
C47	9185(5)	4947(4)	7175(4)	22.6(17)
O1	6479(3)	5980(3)	6649(3)	29.0(14)
N6	8201(4)	3461(3)	7054(3)	22.4(15)
O6	7719(3)	3662(3)	5729(3)	30.1(14)
C19	9007(5)	6516(4)	8022(4)	23.3(17)
N3	6983(4)	4878(3)	8408(3)	20.7(14)
N2	7754(4)	6277(3)	8386(3)	21.3(14)
N4	8409(4)	5005(3)	8072(3)	20.8(14)
O5	6094(4)	3415(3)	6125(3)	31.7(15)
C30	5094(5)	4642(4)	6844(5)	27.3(19)
C40	7587(5)	4805(4)	8919(4)	24.8(18)
C39	6305(5)	4631(4)	8474(4)	22.0(17)
C73	8152(5)	3302(4)	7720(4)	24.3(18)
C54	9501(5)	5100(5)	5879(5)	33(2)
C55	8747(5)	5055(4)	6020(4)	24.9(18)
C10	5272(5)	6234(4)	7048(4)	24.5(18)
C4	4129(5)	6375(5)	6242(5)	34(2)
N1	6265(4)	6134(3)	7980(3)	21.5(14)
C38	5649(4)	4665(4)	7984(4)	20.0(16)
C46	9032(4)	4845(4)	7836(4)	22.6(17)
C29	5748(4)	4678(4)	7327(4)	19.7(16)
C11	5591(4)	6316(4)	7717(4)	22.4(17)
C28	8785(5)	6439(4)	7350(4)	23.4(17)
C8	3930(5)	6340(5)	7377(5)	31(2)
C56	8583(5)	4968(4)	6669(4)	22.3(17)
C75	9021(5)	3436(4)	6158(4)	23.6(18)
C31	4372(5)	4608(4)	7026(5)	29(2)
C9	4453(5)	6328(4)	6899(4)	25.3(18)
C32	4243(5)	4614(4)	7696(5)	31(2)
C67	6119(5)	3072(4)	7481(4)	23.5(17)
C25	10363(5)	6700(5)	7801(5)	31(2)
C18	8438(5)	6532(4)	8477(4)	24.6(18)
C60	4020(5)	2912(4)	6810(5)	31(2)
C65	4686(5)	2967(4)	7267(4)	26.0(18)
C74	8849(5)	3333(4)	6809(4)	23.6(18)
C27	9355(5)	6557(5)	6912(5)	31(2)
C64	4593(5)	2916(5)	7934(5)	32(2)
C72	8787(5)	3240(5)	8186(4)	30(2)

C66	5426(5)	3102(4)	7034(4)	24.1(18)
C41	7487(6)	4692(5)	9574(4)	33(2)
C81	10007(6)	3392(5)	5386(5)	35(2)
O7	6560(4)	4824(3)	5763(3)	36.5(16)
C12	6451(5)	6265(4)	8652(4)	21.2(17)
N5	6786(4)	3320(4)	7396(3)	22.1(15)
C63	3878(6)	2799(5)	8132(6)	42(3)
C83	8653(6)	3556(6)	4988(5)	41(3)
C51	11511(6)	5129(6)	6712(7)	52(3)
C44	8971(6)	4856(5)	9222(5)	37(2)
C48	9978(5)	4998(4)	7030(5)	27.5(19)
C5	3323(5)	6475(5)	6085(5)	38(2)
C37	4878(5)	4656(4)	8180(5)	27.7(19)
C76	9819(5)	3380(4)	6033(5)	27.3(19)
C71	8685(5)	3109(5)	8824(5)	33(2)
C17	7238(5)	6348(4)	8868(4)	24.2(18)
C13	5916(6)	6295(5)	9106(5)	33(2)
C43	8856(6)	4735(6)	9858(5)	44(3)
C53	10127(5)	5072(4)	6368(5)	31(2)
C57	5467(5)	3225(4)	6362(4)	27.9(19)
C49	10615(5)	5020(5)	7520(6)	39(2)
C68	7407(5)	3239(4)	7897(4)	23.4(17)
C6	2846(5)	6504(5)	6564(6)	40(2)
C2	5389(5)	6181(5)	5888(5)	35(2)
C1	5740(5)	6124(4)	6545(4)	23.8(18)
C69	7315(5)	3120(4)	8549(4)	29(2)
C33	3464(6)	4600(5)	7873(6)	44(3)
C50	11361(6)	5081(6)	7347(7)	52(3)
C84	8441(5)	3558(5)	5648(4)	30(2)
C26	10107(5)	6680(5)	7127(5)	34(2)
C24	11154(5)	6774(5)	8028(6)	41(3)
C58	4779(5)	3136(5)	5926(5)	38(2)
C14	6151(7)	6404(6)	9758(5)	44(3)
C82	9392(6)	3471(6)	4872(5)	45(3)
C59	4091(5)	2983(5)	6137(5)	36(2)
C77	10442(6)	3332(5)	6527(5)	40(2)
C3	4632(6)	6303(6)	5742(5)	42(3)
C16	7477(6)	6442(5)	9526(4)	37(2)
C42	8116(7)	4646(6)	10043(5)	45(3)
C20	9814(5)	6618(4)	8257(5)	28.0(19)
C52	10915(6)	5128(5)	6229(6)	44(3)
C61	3291(5)	2779(5)	7045(6)	40(2)
C62	3223(6)	2714(5)	7688(6)	47(3)
C36	4725(6)	4709(5)	8834(5)	37(2)
C7	3147(5)	6429(5)	7212(5)	36(2)
C70	7945(6)	3052(5)	9008(5)	37(2)
C34	3354(6)	4644(6)	8516(7)	54(3)
Cl1	5733(2)	1928(2)	4641.8(19)	82.6(12)
Cl2	6420(3)	1397(3)	5860(2)	110.0(18)

Cl4	9367(3)	6302(3)	10625(3)	123(2)
Cl3	8650(6)	6574(6)	11752(4)	201(4)
C21	10091(5)	6624(5)	8926(5)	35(2)
C35	3971(7)	4702(6)	8990(6)	52(3)
C22	10869(6)	6712(5)	9124(6)	48(3)
C80	10785(7)	3343(7)	5258(6)	55(3)
C79	11372(6)	3296(7)	5745(6)	58(3)
C23	11407(6)	6781(6)	8681(6)	48(3)
C78	11194(6)	3295(6)	6386(6)	50(3)
C15	6938(7)	6473(6)	9971(5)	47(3)
C85	6647(10)	4978(7)	5109(6)	73(4)
C87	9001(10)	6904(9)	11056(11)	113(8)
C86	6386(10)	2070(8)	5338(8)	84(5)

Table SI10 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Yb2L3. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Yb1	13.51(16)	22.65(18)	17.51(17)	0.48(13)	2.49(12)	1.55(13)
Yb2	17.15(18)	25.62(19)	19.00(18)	-4.08(14)	2.16(13)	-0.78(14)
C45	20(4)	25(4)	19(4)	4(3)	-5(3)	2(3)
O4	12(3)	25(3)	21(3)	-4(2)	3(2)	-4(2)
O3	15(3)	29(3)	21(3)	-2(2)	7(2)	0(2)
O2	19(3)	27(3)	22(3)	-6(2)	4(2)	2(2)
C47	21(4)	18(4)	29(4)	-1(3)	6(3)	-7(3)
O1	20(3)	41(4)	27(3)	3(3)	8(2)	8(3)
N6	21(3)	23(4)	24(4)	-5(3)	5(3)	1(3)
O6	22(3)	48(4)	20(3)	-1(3)	2(2)	-7(3)
C19	19(4)	20(4)	30(4)	-2(3)	1(3)	2(3)
N3	17(3)	26(4)	19(3)	6(3)	4(3)	-1(3)
N2	23(4)	22(4)	19(3)	2(3)	4(3)	1(3)
N4	16(3)	26(4)	20(3)	2(3)	0(3)	1(3)
O5	30(3)	43(4)	22(3)	-17(3)	6(3)	-2(3)
C30	22(4)	25(4)	34(5)	-6(4)	3(4)	1(4)
C40	30(5)	18(4)	26(4)	7(3)	2(4)	-1(3)
C39	26(4)	19(4)	22(4)	3(3)	11(3)	1(3)
C73	23(4)	27(4)	23(4)	4(3)	2(3)	0(3)
C54	31(5)	40(5)	30(5)	-4(4)	16(4)	-4(4)
C55	22(4)	28(5)	26(4)	-6(3)	8(3)	-2(4)
C10	23(4)	18(4)	33(5)	2(3)	6(4)	6(3)
C4	27(5)	36(5)	39(5)	3(4)	4(4)	15(4)
N1	25(4)	18(3)	22(3)	1(3)	7(3)	3(3)
C38	15(4)	18(4)	27(4)	1(3)	7(3)	5(3)
C46	11(4)	23(4)	34(5)	-1(3)	-3(3)	-3(4)
C29	15(4)	12(4)	33(5)	-2(3)	8(3)	2(3)
C11	11(4)	21(4)	35(5)	-1(3)	5(3)	6(3)
C28	20(4)	23(4)	29(4)	-5(3)	7(3)	1(3)
C8	23(4)	31(5)	41(5)	7(4)	6(4)	-2(4)
C56	17(4)	15(4)	36(5)	-1(3)	9(3)	-7(3)
C75	24(4)	22(4)	26(4)	1(3)	8(3)	-5(3)
C31	11(4)	24(5)	52(6)	0(3)	4(4)	3(4)

C9	21(4)	18(4)	38(5)	4(3)	6(4)	6(4)
C32	23(5)	21(4)	50(6)	3(3)	16(4)	7(4)
C67	29(4)	15(4)	28(4)	1(3)	7(4)	2(3)
C25	21(4)	28(5)	43(5)	-2(4)	6(4)	5(4)
C18	22(4)	28(5)	23(4)	-1(3)	-3(3)	-1(3)
C60	23(4)	23(5)	49(6)	-3(4)	9(4)	-2(4)
C65	26(4)	17(4)	37(5)	-1(3)	9(4)	-1(4)
C74	19(4)	21(4)	32(5)	1(3)	7(3)	-2(3)
C27	35(5)	32(5)	28(5)	-3(4)	8(4)	3(4)
C64	27(5)	28(5)	43(6)	-4(4)	7(4)	3(4)
C72	27(5)	32(5)	32(5)	-1(4)	7(4)	3(4)
C66	22(4)	12(4)	38(5)	-3(3)	4(4)	-2(3)
C41	42(6)	36(5)	22(4)	5(4)	4(4)	6(4)
C81	32(5)	33(5)	41(6)	4(4)	17(4)	0(4)
O7	43(4)	41(4)	26(3)	4(3)	2(3)	5(3)
C12	16(4)	24(4)	25(4)	2(3)	9(3)	0(3)
N5	15(3)	29(4)	23(4)	-1(3)	4(3)	3(3)
C63	44(6)	41(6)	47(6)	4(5)	26(5)	7(5)
C83	37(6)	60(7)	27(5)	-1(5)	7(4)	-16(5)
C51	19(5)	55(7)	86(9)	-2(5)	20(5)	2(7)
C44	33(5)	46(6)	31(5)	5(4)	-2(4)	4(4)
C48	18(4)	20(4)	45(5)	3(3)	8(4)	-3(4)
C5	25(5)	43(6)	44(6)	7(4)	-7(4)	5(5)
C37	20(4)	24(4)	41(5)	2(3)	12(4)	7(4)
C76	23(4)	24(4)	38(5)	3(3)	15(4)	0(4)
C71	23(5)	43(6)	33(5)	3(4)	-2(4)	-1(4)
C17	32(5)	20(4)	22(4)	0(3)	8(3)	-4(3)
C13	31(5)	35(5)	36(5)	6(4)	13(4)	7(4)
C43	37(6)	60(7)	33(5)	7(5)	-11(4)	5(5)
C53	25(5)	25(5)	47(6)	-7(4)	14(4)	-3(4)
C57	24(4)	26(5)	34(5)	-7(4)	4(4)	-3(4)
C49	17(4)	46(6)	53(6)	-3(4)	9(4)	-6(5)
C68	23(4)	23(4)	25(4)	3(3)	4(3)	2(3)
C6	13(4)	41(6)	65(7)	5(4)	7(4)	3(5)
C2	25(5)	52(6)	29(5)	11(4)	6(4)	20(4)
C1	15(4)	28(5)	28(4)	4(3)	3(3)	11(4)
C69	26(5)	30(5)	31(5)	-6(4)	2(4)	8(4)
C33	19(5)	39(6)	75(8)	0(4)	14(5)	9(5)
C50	13(5)	60(8)	81(9)	-1(5)	-1(5)	1(6)
C84	29(5)	31(5)	31(5)	-3(4)	12(4)	-10(4)
C26	24(5)	29(5)	52(6)	-5(4)	17(4)	6(4)
C24	22(5)	27(5)	73(8)	-4(4)	8(5)	-1(5)
C58	29(5)	50(6)	33(5)	-14(4)	-1(4)	-4(5)
C14	49(6)	55(7)	32(5)	8(5)	19(5)	4(5)
C82	50(7)	54(7)	32(5)	3(5)	16(5)	-12(5)
C59	19(4)	43(6)	43(6)	-12(4)	-1(4)	-3(5)
C77	27(5)	51(6)	43(6)	9(5)	10(4)	7(5)
C3	37(6)	56(7)	34(5)	12(5)	3(4)	20(5)
C16	32(5)	55(7)	25(5)	-2(5)	4(4)	0(4)

C42	60(7)	49(7)	24(5)	9(5)	-2(5)	7(4)
C20	24(4)	22(4)	37(5)	2(3)	-1(4)	-2(4)
C52	27(5)	36(6)	75(8)	1(4)	30(5)	2(5)
C61	18(4)	33(5)	68(7)	-6(4)	7(5)	-5(5)
C62	31(6)	39(6)	75(8)	-1(5)	25(5)	0(6)
C36	31(5)	40(6)	45(6)	-4(4)	22(4)	6(5)
C7	23(5)	39(6)	48(6)	3(4)	9(4)	-1(5)
C70	51(6)	31(5)	29(5)	-6(4)	6(4)	8(4)
C34	26(6)	57(7)	83(9)	8(5)	26(6)	11(7)
Cl1	76(2)	116(3)	60(2)	-6(2)	27.6(19)	4(2)
Cl2	64(3)	177(5)	91(3)	2(3)	15(2)	49(3)
Cl4	91(3)	160(5)	115(4)	23(3)	-8(3)	-48(4)
Cl3	216(9)	295(12)	104(5)	40(8)	68(6)	23(6)
C21	27(5)	44(6)	33(5)	-1(4)	-5(4)	4(4)
C35	45(7)	52(7)	67(8)	11(5)	43(6)	8(6)
C22	42(6)	43(6)	53(7)	2(5)	-22(5)	3(5)
C80	48(7)	74(9)	50(7)	8(6)	33(6)	1(6)
C79	25(5)	92(10)	60(8)	17(6)	24(5)	18(7)
C23	22(5)	45(6)	75(8)	0(4)	-7(5)	3(6)
C78	23(5)	70(8)	59(7)	5(5)	12(5)	14(6)
C15	54(7)	68(8)	22(5)	4(6)	15(5)	-5(5)
C85	121(13)	55(8)	43(7)	11(8)	15(8)	5(6)
C87	76(12)	69(11)	180(20)	23(9)	-25(13)	-40(13)
C86	83(11)	73(10)	98(12)	-16(9)	24(9)	-30(9)

Table SI11 Bond Lengths for Yb2L3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Yb1	O4	2.303(5)	C32	C33	1.443(12)
Yb1	O3	2.328(6)	C67	C66	1.438(12)
Yb1	O2	2.206(5)	C67	N5	1.296(11)
Yb1	O1	2.234(6)	C25	C26	1.416(14)
Yb1	N3	2.481(7)	C25	C24	1.413(13)
Yb1	N2	2.447(7)	C25	C20	1.423(13)
Yb1	N4	2.504(6)	C60	C65	1.417(13)
Yb1	N1	2.419(7)	C60	C59	1.416(14)
Yb2	O4	2.294(5)	C60	C61	1.433(12)
Yb2	O3	2.274(6)	C65	C64	1.408(13)
Yb2	N6	2.413(7)	C65	C66	1.450(12)
Yb2	O6	2.165(6)	C27	C26	1.360(13)
Yb2	O5	2.165(6)	C64	C63	1.372(13)
Yb2	O7	2.392(7)	C72	C71	1.374(13)
Yb2	N5	2.400(7)	C66	C57	1.422(13)
C45	N4	1.430(10)	C41	C42	1.384(14)
C45	C40	1.410(12)	C81	C76	1.412(13)
C45	C44	1.390(12)	C81	C82	1.432(15)
O4	C56	1.340(9)	C81	C80	1.412(14)
O3	C29	1.347(9)	O7	C85	1.411(13)
O2	C28	1.313(10)	C12	C17	1.403(12)
C47	C46	1.434(12)	C12	C13	1.393(12)

C47	C56	1.398(12)	N5	C68	1.422(11)
C47	C48	1.449(11)	C63	C62	1.394(16)
O1	C1	1.315(10)	C83	C84	1.450(13)
N6	C73	1.424(11)	C83	C82	1.346(14)
N6	C74	1.312(10)	C51	C50	1.368(18)
O6	C84	1.302(11)	C51	C52	1.358(17)
C19	C28	1.409(12)	C44	C43	1.374(14)
C19	C18	1.439(12)	C48	C53	1.426(13)
C19	C20	1.450(12)	C48	C49	1.419(13)
N3	C40	1.415(10)	C5	C6	1.361(14)
N3	C39	1.304(11)	C37	C36	1.409(13)
N2	C18	1.294(11)	C76	C77	1.410(14)
N2	C17	1.419(10)	C71	C70	1.387(14)
N4	C46	1.278(10)	C17	C16	1.391(12)
O5	C57	1.302(10)	C13	C14	1.381(14)
C30	C29	1.432(12)	C43	C42	1.395(16)
C30	C31	1.352(12)	C53	C52	1.436(12)
C40	C41	1.402(12)	C57	C58	1.430(12)
C39	C38	1.444(11)	C49	C50	1.390(13)
C73	C72	1.391(12)	C68	C69	1.395(12)
C73	C68	1.392(12)	C6	C7	1.391(15)
C54	C55	1.378(12)	C2	C1	1.432(12)
C54	C53	1.404(14)	C2	C3	1.342(13)
C55	C56	1.413(12)	C69	C70	1.377(13)
C10	C11	1.442(12)	C33	C34	1.367(17)
C10	C9	1.438(12)	C24	C23	1.372(16)
C10	C1	1.408(12)	C58	C59	1.355(13)
C4	C9	1.416(13)	C14	C15	1.398(16)
C4	C5	1.419(13)	C77	C78	1.374(13)
C4	C3	1.432(14)	C16	C15	1.385(14)
N1	C11	1.291(10)	C20	C21	1.412(13)
N1	C12	1.416(11)	C61	C62	1.354(16)
C38	C29	1.387(12)	C36	C35	1.386(13)
C38	C37	1.442(11)	C34	C35	1.377(18)
C28	C27	1.435(12)	Cl1	C86	1.757(17)
C8	C9	1.414(12)	Cl2	C86	1.745(18)
C8	C7	1.381(13)	Cl4	C87	1.683(18)
C75	C74	1.425(12)	Cl3	C87	1.76(2)
C75	C76	1.444(11)	C21	C22	1.384(14)
C75	C84	1.401(13)	C22	C23	1.385(17)
C31	C32	1.427(14)	C80	C79	1.355(17)
C32	C37	1.411(13)	C79	C78	1.393(16)

Table SI12 Bond Angles for Yb2L3.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O3	Yb1	O4	68.82(18)	C55	C56	O4	118.2(8)
O2	Yb1	O4	80.5(2)	C55	C56	C47	120.0(7)
O2	Yb1	O3	140.9(2)	C76	C75	C74	117.5(8)
O1	Yb1	O4	91.1(2)	C84	C75	C74	121.9(8)

O1	Yb1	O3	75.3(2)	C84	C75	C76	120.6(8)
O1	Yb1	O2	81.9(2)	C32	C31	C30	121.2(9)
N3	Yb1	O4	106.3(2)	C4	C9	C10	119.8(8)
N3	Yb1	O3	69.2(2)	C8	C9	C10	123.4(8)
N3	Yb1	O2	145.6(2)	C8	C9	C4	116.7(8)
N3	Yb1	O1	130.5(2)	C37	C32	C31	119.7(8)
N2	Yb1	O4	134.1(2)	C33	C32	C31	119.8(9)
N2	Yb1	O3	146.6(2)	C33	C32	C37	120.5(9)
N2	Yb1	O2	72.5(2)	N5	C67	C66	126.7(8)
N2	Yb1	O1	119.9(2)	C24	C25	C26	121.3(9)
N2	Yb1	N3	79.7(2)	C20	C25	C26	119.1(8)
N4	Yb1	O4	69.8(2)	C20	C25	C24	119.6(9)
N4	Yb1	O3	103.0(2)	N2	C18	C19	125.7(8)
N4	Yb1	O2	87.7(2)	C59	C60	C65	119.6(8)
N4	Yb1	O1	159.6(2)	C61	C60	C65	118.6(9)
N4	Yb1	N3	64.6(2)	C61	C60	C59	121.8(9)
N4	Yb1	N2	72.8(2)	C64	C65	C60	118.2(8)
N1	Yb1	O4	159.8(2)	C66	C65	C60	119.0(8)
N1	Yb1	O3	93.2(2)	C66	C65	C64	122.7(8)
N1	Yb1	O2	111.1(2)	C75	C74	N6	127.8(8)
N1	Yb1	O1	74.9(2)	C26	C27	C28	122.1(9)
N1	Yb1	N3	73.9(2)	C63	C64	C65	120.7(9)
N1	Yb1	N2	66.0(2)	C71	C72	C73	120.4(8)
N1	Yb1	N4	125.4(2)	C65	C66	C67	119.5(8)
O3	Yb2	O4	69.91(19)	C57	C66	C67	120.4(8)
N6	Yb2	O4	80.2(2)	C57	C66	C65	120.0(8)
N6	Yb2	O3	115.8(2)	C42	C41	C40	121.0(10)
O6	Yb2	O4	95.9(2)	C82	C81	C76	118.2(8)
O6	Yb2	O3	158.8(2)	C80	C81	C76	120.1(10)
O6	Yb2	N6	75.3(2)	C80	C81	C82	121.7(10)
O5	Yb2	O4	160.5(2)	C85	O7	Yb2	134.4(7)
O5	Yb2	O3	98.4(2)	C17	C12	N1	116.4(7)
O5	Yb2	N6	119.3(2)	C13	C12	N1	124.7(8)
O5	Yb2	O6	90.4(2)	C13	C12	C17	118.8(8)
O7	Yb2	O4	76.3(2)	C67	N5	Yb2	126.7(6)
O7	Yb2	O3	75.2(2)	C68	N5	Yb2	114.6(5)
O7	Yb2	N6	148.4(2)	C68	N5	C67	118.5(7)
O7	Yb2	O6	86.3(2)	C62	C63	C64	121.8(10)
O7	Yb2	O5	85.7(2)	C82	C83	C84	121.0(10)
N5	Yb2	O4	116.0(2)	C52	C51	C50	119.6(9)
N5	Yb2	O3	77.4(2)	C43	C44	C45	119.9(9)
N5	Yb2	N6	66.9(2)	C53	C48	C47	118.9(8)
N5	Yb2	O6	123.7(2)	C49	C48	C47	122.8(9)
N5	Yb2	O5	74.6(2)	C49	C48	C53	118.1(8)
N5	Yb2	O7	143.3(2)	C6	C5	C4	120.5(9)
C40	C45	N4	116.4(7)	C32	C37	C38	118.8(8)
C44	C45	N4	123.7(8)	C36	C37	C38	123.2(9)
C44	C45	C40	119.9(8)	C36	C37	C32	117.9(8)
Yb2	O4	Yb1	110.5(2)	C81	C76	C75	119.6(9)

C56	O4	Yb1	122.0(5)	C77	C76	C75	123.7(8)
C56	O4	Yb2	126.2(5)	C77	C76	C81	116.6(8)
Yb2	O3	Yb1	110.4(2)	C70	C71	C72	120.1(9)
C29	O3	Yb1	118.4(5)	C12	C17	N2	115.8(7)
C29	O3	Yb2	131.2(5)	C16	C17	N2	123.8(8)
C28	O2	Yb1	130.4(5)	C16	C17	C12	120.2(8)
C56	C47	C46	121.0(7)	C14	C13	C12	121.0(9)
C48	C47	C46	119.2(8)	C42	C43	C44	121.4(9)
C48	C47	C56	119.8(8)	C48	C53	C54	119.0(8)
C1	O1	Yb1	135.8(5)	C52	C53	C54	122.3(9)
C73	N6	Yb2	115.1(5)	C52	C53	C48	118.6(9)
C74	N6	Yb2	126.6(6)	C66	C57	O5	123.6(8)
C74	N6	C73	118.2(7)	C58	C57	O5	118.7(8)
C84	O6	Yb2	136.8(6)	C58	C57	C66	117.7(8)
C18	C19	C28	120.8(7)	C50	C49	C48	119.9(10)
C20	C19	C28	119.9(8)	N5	C68	C73	116.9(7)
C20	C19	C18	119.3(8)	C69	C68	C73	118.7(8)
C40	N3	Yb1	116.4(5)	C69	C68	N5	124.4(8)
C39	N3	Yb1	124.1(5)	C7	C6	C5	119.9(9)
C39	N3	C40	119.2(7)	C3	C2	C1	122.2(9)
C18	N2	Yb1	125.8(6)	C10	C1	O1	123.4(8)
C17	N2	Yb1	114.0(5)	C2	C1	O1	118.7(8)
C17	N2	C18	119.9(7)	C2	C1	C10	117.8(8)
C45	N4	Yb1	114.8(5)	C70	C69	C68	121.1(9)
C46	N4	Yb1	126.2(6)	C34	C33	C32	118.7(10)
C46	N4	C45	119.0(7)	C49	C50	C51	122.3(11)
C57	O5	Yb2	133.6(6)	C75	C84	O6	123.9(8)
C31	C30	C29	120.2(9)	C83	C84	O6	118.0(9)
N3	C40	C45	115.9(7)	C83	C84	C75	118.0(8)
C41	C40	C45	118.8(8)	C27	C26	C25	121.0(9)
C41	C40	N3	125.3(8)	C23	C24	C25	121.5(10)
C38	C39	N3	124.3(7)	C59	C58	C57	122.4(9)
C72	C73	N6	124.3(8)	C15	C14	C13	119.9(9)
C68	C73	N6	115.6(7)	C83	C82	C81	122.2(10)
C68	C73	C72	120.1(8)	C58	C59	C60	121.0(9)
C53	C54	C55	121.8(9)	C78	C77	C76	121.7(10)
C56	C55	C54	120.3(8)	C2	C3	C4	121.4(9)
C9	C10	C11	117.4(8)	C15	C16	C17	120.3(9)
C1	C10	C11	122.1(8)	C43	C42	C41	118.9(9)
C1	C10	C9	120.2(8)	C25	C20	C19	119.4(8)
C5	C4	C9	120.6(9)	C21	C20	C19	122.9(9)
C3	C4	C9	118.2(8)	C21	C20	C25	117.6(8)
C3	C4	C5	121.2(9)	C53	C52	C51	121.4(11)
C11	N1	Yb1	128.2(6)	C62	C61	C60	121.8(10)
C12	N1	Yb1	114.4(5)	C61	C62	C63	118.8(9)
C12	N1	C11	117.3(7)	C35	C36	C37	120.4(11)
C29	C38	C39	120.9(7)	C6	C7	C8	120.7(9)
C37	C38	C39	119.4(8)	C69	C70	C71	119.7(9)
C37	C38	C29	119.7(8)	C35	C34	C33	121.1(10)

N4	C46	C47	125.4(8)	C22	C21	C20	120.6(10)
C30	C29	O3	118.1(7)	C34	C35	C36	121.3(11)
C38	C29	O3	121.4(7)	C23	C22	C21	121.8(10)
C38	C29	C30	120.4(7)	C79	C80	C81	121.8(10)
N1	C11	C10	127.5(8)	C78	C79	C80	118.5(10)
C19	C28	O2	123.0(7)	C22	C23	C24	118.8(10)
C27	C28	O2	119.0(8)	C79	C78	C77	121.2(11)
C27	C28	C19	118.0(8)	C16	C15	C14	119.8(9)
C7	C8	C9	121.4(9)	Cl3	C87	Cl4	109.9(11)
C47	C56	O4	121.7(8)	Cl2	C86	Cl1	110.5(9)

Table SI13 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Yb2L3.

Atom	*x*	*y*	*z*	U(eq)
H30	5167(5)	4642(4)	6395(5)	33(2)
H39	6240(5)	4414(4)	8871(4)	26(2)
H54	9601(5)	5150(5)	5439(5)	39(3)
H55	8336(5)	5083(4)	5679(4)	30(2)
H46	9426(4)	4642(4)	8122(4)	27(2)
H11	5270(4)	6528(4)	7996(4)	27(2)
H8	4123(5)	6286(5)	7822(5)	38(2)
H31	3942(5)	4579(4)	6701(5)	35(2)
H67	6085(5)	2846(4)	7879(4)	28(2)
H18	8576(5)	6748(4)	8880(4)	30(2)
H74	9253(5)	3150(4)	7100(4)	28(2)
H27	9201(5)	6549(5)	6456(5)	38(2)
H64	5029(5)	2962(5)	8249(5)	39(2)
H72	9295(5)	3288(5)	8064(4)	36(2)
H41	6980(6)	4647(5)	9698(4)	40(3)
H7	6440(50)	5188(16)	5950(10)	55(2)
H63	3828(6)	2775(5)	8585(6)	51(3)
H83	8264(6)	3615(6)	4633(5)	50(3)
H51	12028(6)	5163(6)	6610(7)	63(4)
H44	9479(6)	4926(5)	9108(5)	44(3)
H5	3116(5)	6523(5)	5643(5)	46(3)
H71	9121(5)	3057(5)	9138(5)	40(3)
H13	5382(6)	6239(5)	8966(5)	40(3)
H43	9290(6)	4711(6)	10179(5)	53(3)
H49	10531(5)	4992(5)	7966(6)	46(3)
H6	2308(5)	6576(5)	6456(6)	48(3)
H2	5703(5)	6131(5)	5542(5)	42(3)
H69	6809(5)	3085(4)	8678(4)	35(2)
H33	3036(6)	4562(5)	7548(6)	52(3)
H50	11782(6)	5089(6)	7681(7)	62(4)
H26	10467(5)	6754(5)	6820(5)	41(3)
H24	11519(5)	6821(5)	7722(6)	49(3)
H58	4805(5)	3185(5)	5471(5)	45(3)
H14	5779(7)	6433(6)	10060(5)	53(3)
H82	9510(6)	3464(6)	4434(5)	54(3)
H59	3650(5)	2923(5)	5830(5)	43(3)

H77	10339(6)	3325(5)	6970(5)	48(3)
H3	4426(6)	6342(6)	5299(5)	51(3)
H16	8011(6)	6484(5)	9671(4)	44(3)
H42	8045(7)	4556(6)	10483(5)	54(3)
H52	11022(6)	5166(5)	5789(6)	53(3)
H61	2844(5)	2735(5)	6741(6)	48(3)
H62	2738(6)	2613(5)	7834(6)	56(3)
H36	5141(6)	4750(5)	9170(5)	45(3)
H7a	2810(5)	6439(5)	7544(5)	43(3)
H70	7873(6)	2966(5)	9450(5)	44(3)
H34	2844(6)	4633(6)	8639(7)	65(4)
H21	9739(5)	6568(5)	9242(5)	42(3)
H35	3878(7)	4738(6)	9434(6)	62(4)
H22	11040(6)	6724(5)	9576(6)	58(3)
H80	10901(7)	3342(7)	4820(6)	66(4)
H79	11893(6)	3265(7)	5650(6)	69(4)
H23	11940(6)	6832(6)	8827(6)	58(3)
H78	11600(6)	3268(6)	6731(6)	60(4)
H15	7102(7)	6541(6)	10420(5)	57(3)
H85a	6136(10)	5030(50)	4864(13)	109(7)
H85b	6940(60)	5390(30)	5093(7)	109(7)
H85c	6930(60)	4620(30)	4917(17)	109(7)
H87a	9408(10)	7231(9)	11187(11)	135(9)
H87b	8576(10)	7126(9)	10783(11)	135(9)
H86a	6907(10)	2154(8)	5207(8)	100(6)
H86b	6223(10)	2463(8)	5568(8)	100(6)

Refinement model description

Number of restraints - 3, number of constraints - 119.

Details:

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1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups
 At 1.5 times of:
  All C(H,H,H) groups, All O(H) groups
2. Restrained distances
 O7-H7
 0.87 with sigma of 0.01
 C85-H7
 1.886919 with sigma of 0.02
 Yb2-H7
 2.888526 with sigma of 0.02
3.a Secondary CH2 refined with riding coordinates:
 C87(H87a,H87b), C86(H86a,H86b)
3.b Aromatic/amide H refined with riding coordinates:
 C30(H30), C39(H39), C54(H54), C55(H55), C46(H46), C11(H11), C8(H8), C31(H31),
 C67(H67), C18(H18), C74(H74), C27(H27), C64(H64), C72(H72), C41(H41), C63(H63),
  C83(H83), C51(H51), C44(H44), C5(H5), C71(H71), C13(H13), C43(H43), C49(H49),
 C6(H6), C2(H2), C69(H69), C33(H33), C50(H50), C26(H26), C24(H24), C58(H58),
 C14(H14), C82(H82), C59(H59), C77(H77), C3(H3), C16(H16), C42(H42), C52(H52),
 C61(H61), C62(H62), C36(H36), C7(H7a), C70(H70), C34(H34), C21(H21), C35(H35),
 C22(H22), C80(H80), C79(H79), C23(H23), C78(H78), C15(H15)
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3.c Idealised Me refined as rotating group:
C85(H85a,H85b,H85c)

Ho2L3

Table SI14 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Ho2L3. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ho1	2619.07(10)	7771.32(6)	2630.58(6)	14.39(3)
Ho2	6073.49(11)	7857.42(6)	1753.80(6)	15.40(3)
O4	4341.5(17)	8515.7(9)	2378.6(9)	16.3(3)
O3	4313.6(17)	7143.9(9)	1945.2(9)	15.6(3)
N4	3616(2)	7984.6(11)	3765.2(11)	15.8(4)
N5	7139(2)	6663.8(12)	2388.1(12)	18.3(4)
N3	3705(2)	6581.1(11)	3367.4(11)	16.6(4)
C47	4130(2)	9281.8(13)	3346.0(13)	15.6(5)
N6	7103(2)	8050.6(12)	2832.0(11)	17.2(4)
C56	4321(2)	9195.5(13)	2616.3(13)	15.6(4)
O2	1829.3(19)	8594.2(10)	1718.6(10)	22.8(4)
C38	4296(2)	5804.8(14)	2391.8(14)	17.3(5)
O1	1554.8(18)	6961.6(11)	2133.6(10)	20.5(4)
C29	4330(2)	6408.8(13)	1830.9(13)	16.2(5)
C55	4551(2)	9846.8(14)	2113.3(14)	19.5(5)
C46	4045(2)	8614.5(14)	3873.1(13)	16.8(5)
C40	3682(2)	6622.9(14)	4112.7(13)	17.7(5)
N2	1191(2)	8810.2(12)	3133.9(12)	17.9(4)
C81	7968(3)	10747.0(15)	2314.2(17)	25.0(6)
C75	7600(2)	9372.5(14)	2498.3(14)	18.9(5)
C45	3641(2)	7362.6(14)	4324.8(13)	16.8(5)
N1	922(2)	7316.7(12)	3509.3(11)	16.5(4)
O7	4913(2)	8513.5(12)	762.6(11)	28.8(4)
C68	7160(2)	6681.3(14)	3135.2(14)	17.8(5)
C84	7562(3)	9378.7(15)	1752.4(15)	20.7(5)
C30	4419(3)	6232.0(15)	1115.7(14)	21.8(5)
O5	7037(2)	7178.6(11)	933.4(10)	24.4(4)
C37	4374(3)	5015.3(14)	2236.6(15)	21.6(5)
C72	7049(3)	7470.2(16)	4104.2(14)	22.3(5)
C48	4127(2)	10037.3(14)	3571.8(15)	19.7(5)
C74	7536(2)	8675.5(14)	2973.8(14)	18.4(5)
C67	7604(3)	6022.3(15)	2131.0(15)	21.9(5)
C39	4221(2)	5949.0(14)	3129.7(14)	18.0(5)
C4	579(3)	4766.1(15)	2793.3(15)	24.4(6)
C66	7639(3)	5869.1(15)	1405.8(15)	21.6(5)
C53	4374(3)	10668.8(14)	3060.1(16)	21.8(5)
C54	4579(3)	10552.5(15)	2328.1(16)	23.3(5)
C18	989(3)	9529.3(15)	2852.0(15)	20.6(5)
C12	496(2)	7825.8(14)	4028.2(13)	16.7(5)
C1	1203(2)	6286.0(15)	2365.1(15)	20.3(5)
C17	662(2)	8605.3(14)	3833.5(13)	17.5(5)
C28	1667(3)	9338.2(15)	1600.1(14)	20.8(5)
O6	7275.6(19)	8798.7(11)	1456.6(10)	23.5(4)
C73	7119(2)	7412.4(14)	3373.6(13)	17.0(5)

C9	448(3)	5306.1(15)	3298.1(15)	21.7(5)
C32	4470(3)	4865.0(15)	1514.1(16)	24.7(6)
C10	746(2)	6085.0(14)	3074.2(14)	18.0(5)
C13	-8(3)	7593.8(16)	4714.0(14)	23.8(5)
C20	1372(3)	10656.1(15)	1977.8(15)	21.3(5)
C76	7757(2)	10076.4(15)	2788.7(15)	21.2(5)
C44	3579(3)	7448.2(16)	5052.2(14)	24.2(5)
C11	449(2)	6661.9(14)	3555.1(14)	17.9(5)
C65	7962(3)	5075.1(16)	1252.0(17)	27.1(6)
C69	7149(3)	6029.5(15)	3643.6(15)	24.1(5)
C31	4480(3)	5491.6(16)	964.5(16)	25.3(6)
C57	7432(3)	6465.2(16)	838.0(15)	22.9(5)
C71	7050(3)	6816.9(17)	4598.1(15)	26.8(6)
C83	7864(3)	10053.4(17)	1295.1(16)	27.4(6)
C41	3655(3)	5987.2(16)	4633.5(15)	27.1(6)
C43	3589(3)	6810.0(17)	5559.7(15)	29.8(6)
C36	4294(4)	4383.5(16)	2773.3(17)	35.4(7)
C6	-179(4)	3781.6(18)	3683.0(19)	46.8(10)
C16	335(3)	9123.8(16)	4338.9(16)	30.1(6)
C60	8208(3)	4923.2(18)	532.7(18)	33.8(7)
C82	8060(3)	10703.0(17)	1566.4(17)	28.8(6)
C19	1375(2)	9827.5(14)	2144.8(14)	19.7(5)
C77	7651(3)	10146.8(17)	3526.8(16)	27.4(6)
C70	7100(3)	6097.7(17)	4365.1(16)	28.9(6)
C42	3624(3)	6078.8(17)	5350.0(16)	32.8(7)
C78	7786(3)	10829.4(18)	3779.2(19)	34.3(7)
C21	1314(3)	11159.0(16)	2506.2(17)	27.9(6)
C52	4369(3)	11408.8(16)	3276.7(19)	31.8(7)
C22	1369(3)	11939.7(17)	2332.3(18)	33.7(7)
C2	1259(3)	5729.5(17)	1866.6(15)	26.0(6)
C58	7671(3)	6285.4(19)	121.3(17)	35.1(7)
C3	975(3)	5004.6(17)	2073.3(16)	28.4(6)
C8	22(3)	5043.6(17)	4001.6(16)	33.1(7)
C27	1728(3)	9700.3(17)	872.5(16)	27.4(6)
C26	1640(3)	10476.4(17)	713.7(16)	31.4(7)
C15	-189(4)	8884.8(18)	5006.5(17)	35.3(7)
C25	1512(3)	10979.4(16)	1258.7(16)	26.8(6)
C49	3841(3)	10182.5(17)	4288.5(16)	29.7(6)
C62	8650(4)	3555(2)	905(2)	51.9(11)
C5	280(4)	4005.7(17)	3004.5(18)	36.1(7)
C59	8055(4)	5548(2)	-16.3(18)	41.0(8)
C80	8085(3)	11440.8(17)	2592(2)	36.5(7)
C14	-365(3)	8120.8(17)	5195.3(15)	29.2(6)
C24	1556(3)	11781.6(18)	1095.5(18)	35.3(7)
C33	4505(4)	4095.1(17)	1356.2(18)	36.2(7)
C23	1485(3)	12253.4(17)	1617.6(19)	36.9(7)
C63	8352(4)	3694.0(19)	1606(2)	49.5(10)
C79	8004(3)	11485.6(19)	3312(2)	40.6(8)
C7	-318(4)	4310.9(19)	4184.9(18)	43.2(9)

C50	3838(4)	10913.5(18)	4478.4(19)	36.9(7)
C51	4110(3)	11528.8(17)	3975(2)	38.3(8)
C64	7999(4)	4435.7(17)	1779(2)	38.3(8)
C35	4332(5)	3642.5(18)	2597(2)	51.9(11)
C85	5477(5)	8943(3)	163(2)	57.6(12)
C61	8557(4)	4154(2)	381(2)	47.5(9)
O9	1309(2)	7347.0(14)	698.7(12)	38.3(5)
O8	3186(2)	8053.6(15)	3.0(13)	41.1(6)
C86	3838(4)	7628(2)	-532(2)	46.7(9)
C34	4442(4)	3497.9(18)	1887(2)	48.9(10)
C87	82(5)	7821(3)	659(3)	77.6(16)

Table SI15 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Ho2L3. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ho1	15.58(5)	11.24(5)	16.81(6)	-2.06(4)	-0.36(4)	-3.23(4)
Ho2	17.05(6)	13.05(5)	16.53(6)	-3.12(4)	0.53(4)	-2.83(4)
O4	18.6(8)	12.4(8)	19.2(9)	-4.0(6)	1.7(7)	-5.7(6)
O3	18.4(8)	10.3(7)	18.9(8)	-4.3(6)	2.3(7)	-4.0(6)
N4	17.7(10)	11.6(9)	18(1)	-1.0(7)	-0.7(8)	-2.2(7)
N5	18.1(10)	16(1)	21.4(11)	-1.5(8)	-2.6(8)	-5.0(8)
N3	18.8(10)	12.6(9)	18.9(10)	-3.6(8)	-0.3(8)	-2.7(8)
C47	16.8(11)	10.4(10)	20.3(12)	-1.3(8)	-1.9(9)	-5.1(9)
N6	19.1(10)	12.9(9)	19.2(10)	-1.4(8)	-1.3(8)	-1.6(8)
C56	13.9(11)	12.6(10)	21.1(12)	-3.2(8)	-1.0(9)	-3.8(9)
O2	29.8(10)	16.7(9)	21.4(9)	0.3(7)	-5.6(8)	-1.8(7)
C38	17.9(11)	11.4(10)	23.1(12)	-1.3(9)	1.0(9)	-4.9(9)
O1	20.2(9)	22.5(9)	20.9(9)	-8.8(7)	2.1(7)	-6.4(7)
C29	15.5(11)	12.1(10)	21.5(12)	-2.0(8)	1.7(9)	-5.2(9)
C55	19.3(12)	15.5(11)	22.8(13)	-2.9(9)	1.4(10)	0.1(9)
C46	18.1(11)	15.8(11)	17.5(11)	-2.8(9)	-0.9(9)	-5.3(9)
C40	20.5(12)	13.9(11)	18.6(12)	-2.9(9)	0.8(9)	-1.5(9)
N2	18.3(10)	14.8(9)	20.5(10)	-0.7(8)	-2.1(8)	-2.7(8)
C81	19.6(13)	16.9(12)	39.2(16)	-3.8(10)	-0.9(11)	-4.8(11)
C75	16.6(11)	15.6(11)	25.4(13)	-4.7(9)	-1.7(10)	-3.1(10)
C45	18.5(11)	14.3(11)	17.5(11)	-3.2(9)	-1.1(9)	-0.4(9)
N1	16.3(10)	13.8(9)	20.3(10)	-1.5(7)	-1.3(8)	-5.2(8)
O7	30.8(11)	32.0(11)	22.4(10)	-4.0(9)	-4.0(8)	2.8(8)
C68	16.8(11)	14.9(11)	21.3(12)	-0.9(9)	-2.0(9)	-1.5(9)
C84	18.1(12)	18.9(12)	26.0(13)	-6.7(9)	-0.4(10)	-2.3(10)
C30	25.1(13)	19.9(12)	20.8(13)	-3.9(10)	2.4(10)	-4.4(10)
O5	30.8(11)	19.9(9)	22.5(10)	-3.0(8)	5.7(8)	-5.5(7)
C37	25.1(13)	11.5(11)	28.7(14)	-1.1(9)	-0.1(11)	-6.2(10)
C72	22.5(13)	21.5(12)	22.7(13)	-0.6(10)	-0.4(10)	-4.9(10)
C48	18.8(12)	14.1(11)	27.8(13)	-2.7(9)	-1.2(10)	-7.9(10)
C74	16.7(11)	17.4(11)	21.5(12)	-0.2(9)	-2.7(9)	-4.5(9)
C67	21.1(13)	17.2(12)	27.5(14)	0.9(10)	-3.7(10)	-4.8(10)
C39	19.9(12)	11.5(10)	22.9(12)	-4.4(9)	-0.9(10)	-1.0(9)
C4	27.9(14)	19.0(12)	28.1(14)	-1.2(10)	-6.6(11)	-9.1(11)
C66	17.3(12)	20.1(12)	28.2(14)	0.7(9)	-0.4(10)	-9.2(10)

C53	19.9(12)	12.2(11)	34.5(15)	-2.6(9)	-0.5(11)	-6.5(10)
C54	23.5(13)	13.1(11)	32.2(15)	-3.2(10)	0.6(11)	0.8(10)
C18	18.2(12)	18.0(12)	25.2(13)	0.6(9)	-1.6(10)	-3.3(10)
C12	16.3(11)	16.0(11)	18.6(12)	-1.0(9)	-1.5(9)	-6.0(9)
C1	15.7(11)	21.4(12)	26.0(13)	-4.2(9)	-2(1)	-8.7(10)
C17	18.9(12)	14.4(11)	19.5(12)	-1.1(9)	-1.4(9)	-3.8(9)
C28	20.8(12)	19.0(12)	22.3(13)	-0.6(10)	-5.7(10)	-0.4(10)
O6	28.4(10)	21.8(9)	22.3(9)	-11.1(8)	1.1(8)	-3.9(7)
C73	15.9(11)	16.1(11)	18.7(12)	-1.9(9)	-1.2(9)	-0.8(9)
C9	25.8(13)	16.4(11)	23.6(13)	-1.2(10)	-5.7(10)	-4.6(10)
C32	27.9(14)	17.0(12)	31.2(15)	-2.7(10)	0.6(11)	-11.6(11)
C10	18.7(12)	14.7(11)	21.7(12)	-2.4(9)	-0.7(9)	-6.5(9)
C13	32.8(15)	19.2(12)	19.7(13)	-4.4(11)	2.0(11)	-3.8(10)
C20	18.2(12)	15.9(11)	28.9(14)	-0.8(9)	-2.7(10)	0.6(10)
C76	16.5(12)	16.4(11)	31.6(14)	-1.7(9)	-3.4(10)	-5.8(10)
C44	32.0(15)	21.0(13)	20.3(13)	-4.5(11)	0.4(11)	-4.4(10)
C11	18.0(11)	16.8(11)	19.2(12)	-2.8(9)	0.2(9)	-3.4(9)
C65	22.7(13)	22.2(13)	39.1(16)	1.3(10)	-9.3(12)	-14.2(12)
C69	26.4(14)	16.2(12)	29.2(14)	-3.8(10)	-0.9(11)	0.3(10)
C31	28.4(14)	22.8(13)	26.4(14)	-3.7(11)	1.7(11)	-11.1(11)
C57	21.2(13)	22.8(13)	26.1(14)	-4.8(10)	4.9(10)	-9.0(11)
C71	30.3(15)	30.8(15)	18.0(13)	-2.8(12)	-0.3(11)	0.3(11)
C83	32.5(15)	25.1(14)	25.2(14)	-11.0(12)	2.3(12)	0.1(11)
C41	38.6(16)	17.0(12)	25.5(14)	-7.7(11)	3.2(12)	-0.6(10)
C43	41.8(17)	30.5(15)	16.5(13)	-5.8(13)	1.4(12)	-0.7(11)
C36	62(2)	14.7(12)	29.9(16)	-4.5(13)	-2.9(15)	-3.6(11)
C6	89(3)	17.4(14)	36.8(19)	-13.4(16)	-13.7(19)	0.1(13)
C16	46.5(18)	15.6(12)	29.0(15)	-1.9(12)	-0.4(13)	-8.1(11)
C60	31.3(16)	30.9(15)	42.4(19)	2.4(12)	-4.1(14)	-21.7(14)
C82	30.1(15)	21.8(13)	34.9(16)	-9.8(11)	-0.9(12)	2.1(12)
C19	17.3(12)	16.6(11)	23.9(13)	1.7(9)	-4.2(10)	-0.1(10)
C77	28.0(14)	23.0(13)	32.7(15)	-3.2(11)	-3.1(12)	-8.1(11)
C70	32.4(15)	23.7(14)	28.8(15)	-4.7(12)	-0.9(12)	4.6(11)
C42	52(2)	23.7(14)	20.5(14)	-8.9(13)	4.0(13)	5.6(11)
C78	34.9(17)	32.7(16)	39.5(18)	-7.2(13)	-0.5(14)	-18.5(14)
C21	30.9(15)	19.9(13)	31.0(15)	1.0(11)	-0.2(12)	-0.5(11)
C52	34.5(16)	13.1(12)	49.2(19)	-4.7(11)	-2.1(14)	-7.4(12)
C22	41.0(18)	17.3(13)	41.8(18)	-0.5(12)	-2.1(14)	-3.0(12)
C2	27.0(14)	30.6(14)	24.0(14)	-11.1(11)	6.1(11)	-13.0(11)
C58	47.3(19)	32.5(16)	26.0(15)	-7.4(14)	9.5(14)	-8.6(13)
C3	30.6(15)	28.1(14)	30.4(15)	-7.0(12)	1.9(12)	-17.0(12)
C8	56(2)	19.3(13)	25.9(15)	-6.4(13)	-6.2(14)	-3.9(11)
C27	34.3(16)	23.4(13)	23.6(14)	-0.7(11)	-5.1(12)	-0.7(11)
C26	41.8(18)	26.6(14)	23.5(14)	-1.0(13)	-6.0(13)	5.2(11)
C15	56(2)	24.1(14)	26.4(15)	-1.0(14)	4.1(14)	-14.4(12)
C25	27.4(14)	20.0(13)	31.3(15)	-1.4(11)	-5.5(12)	3.6(11)
C49	39.3(17)	21.8(13)	30.2(15)	-6.6(12)	2.7(13)	-11.3(11)
C62	58(2)	28.4(17)	74(3)	11.8(16)	-26(2)	-31.4(18)
C5	58(2)	17.0(13)	35.9(17)	-2.8(13)	-11.5(15)	-8.2(12)

C59	53(2)	40.4(19)	31.3(17)	-3.1(16)	8.0(15)	-19.9(15)
C80	39.4(18)	18.9(13)	53(2)	-8.7(12)	0.0(15)	-8.1(13)
C14	40.9(17)	26.8(14)	20.1(13)	-2.0(12)	2.9(12)	-7.9(11)
C24	46.2(19)	23.0(14)	34.0(17)	-3.5(13)	-5.8(14)	8.1(12)
C33	53(2)	20.7(14)	37.5(18)	-4.3(13)	0.2(15)	-14.9(13)
C23	44.0(19)	16.0(13)	49(2)	-2.8(12)	-7.1(15)	3.4(13)
C63	65(3)	21.3(15)	66(3)	5.2(15)	-28(2)	-13.9(16)
C79	41.8(19)	26.6(15)	59(2)	-11.4(14)	0.9(16)	-20.4(15)
C7	78(3)	24.7(15)	28.3(16)	-13.8(16)	-7.0(17)	2.7(13)
C50	49(2)	27.6(15)	38.0(18)	-6.1(14)	3.1(15)	-19.4(13)
C51	47(2)	18.8(14)	53(2)	-4.8(13)	-3.0(16)	-20.0(14)
C64	51(2)	20.1(14)	47(2)	3.0(13)	-17.6(16)	-12.3(13)
C35	96(3)	12.9(14)	46(2)	-7.4(17)	-4(2)	-2.4(14)
C85	69(3)	67(3)	38(2)	-35(2)	-17.0(19)	20.1(19)
C61	50(2)	40(2)	56(2)	6.3(16)	-9.1(18)	-32.3(18)
O9	46.3(14)	44.9(14)	26.9(11)	-10.9(11)	-5.7(10)	-8.9(10)
O8	39.9(14)	47.9(14)	37.7(13)	-9.7(11)	-2.7(11)	-8.3(11)
C86	52(2)	52(2)	35.7(19)	1.1(18)	-4.8(16)	-9.7(17)
C34	85(3)	15.3(14)	49(2)	-6.9(16)	0(2)	-13.0(14)
C87	59(3)	103(4)	78(4)	-13(3)	-39(3)	-19(3)

Table SI16 Bond Lengths for Ho2L3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O4	C56	1.328(3)	C12	C17	1.405(3)
O3	C29	1.337(3)	C12	C13	1.397(4)
N4	C46	1.292(3)	C1	C10	1.410(4)
N4	C45	1.422(3)	C1	C2	1.437(4)
N5	C68	1.419(3)	C17	C16	1.400(4)
N5	C67	1.307(3)	C28	C19	1.418(4)
N3	C40	1.420(3)	C28	C27	1.442(4)
N3	C39	1.290(3)	C9	C10	1.450(4)
C47	C56	1.406(3)	C9	C8	1.414(4)
C47	C46	1.449(3)	C32	C31	1.417(4)
C47	C48	1.447(3)	C32	C33	1.420(4)
N6	C74	1.305(3)	C10	C11	1.438(3)
N6	C73	1.420(3)	C13	C14	1.381(4)
C56	C55	1.429(3)	C20	C19	1.452(3)
O2	C28	1.291(3)	C20	C21	1.410(4)
C38	C29	1.406(3)	C20	C25	1.412(4)
C38	C37	1.447(3)	C76	C77	1.413(4)
C38	C39	1.445(4)	C44	C43	1.381(4)
O1	C1	1.304(3)	C65	C60	1.420(4)
C29	C30	1.421(4)	C65	C64	1.404(5)
C55	C54	1.360(4)	C69	C70	1.382(4)
C40	C45	1.405(3)	C57	C58	1.429(4)
C40	C41	1.396(4)	C71	C70	1.386(4)
N2	C18	1.305(3)	C83	C82	1.355(4)
N2	C17	1.420(3)	C41	C42	1.383(4)
C81	C76	1.421(4)	C43	C42	1.390(4)
C81	C82	1.423(4)	C36	C35	1.381(4)
C81	C80	1.412(4)	C6	C5	1.367(5)
C75	C84	1.413(4)	C6	C7	1.401(5)
C75	C74	1.433(4)	C16	C15	1.378(4)
C75	C76	1.450(3)	C60	C59	1.413(5)
C45	C44	1.400(4)	C60	C61	1.415(4)
N1	C12	1.422(3)	C77	C78	1.375(4)
N1	C11	1.302(3)	C78	C79	1.396(5)
O7	C85	1.417(4)	C21	C22	1.380(4)
C68	C73	1.411(3)	C52	C51	1.368(5)
C68	C69	1.401(4)	C22	C23	1.398(5)
C84	O6	1.300(3)	C2	C3	1.351(4)
C84	C83	1.434(4)	C58	C59	1.360(4)
C30	C31	1.362(4)	C8	C7	1.377(4)
O5	C57	1.299(3)	C27	C26	1.353(4)
C37	C32	1.420(4)	C26	C25	1.431(4)
C37	C36	1.414(4)	C15	C14	1.380(4)
C72	C73	1.395(4)	C25	C24	1.413(4)
C72	C71	1.387(4)	C49	C50	1.379(4)
C48	C53	1.416(4)	C62	C63	1.386(6)
C48	C49	1.416(4)	C62	C61	1.351(6)

C67	C66	1.428(4)	C80	C79	1.371(5)
C4	C9	1.419(4)	C24	C23	1.361(5)
C4	C3	1.423(4)	C33	C34	1.363(5)
C4	C5	1.416(4)	C63	C64	1.383(4)
C66	C65	1.455(4)	C50	C51	1.393(5)
C66	C57	1.409(4)	C35	C34	1.394(5)
C53	C54	1.423(4)	O9	C87	1.426(5)
C53	C52	1.414(4)	O8	C86	1.417(4)
C18	C19	1.425(4)			

Table SI17 Bond Angles for Ho2L3.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O3	Ho1	O4	68.85(6)	C5	C4	C3	120.8(3)
N4	Ho1	O4	68.89(6)	C65	C66	C67	118.5(3)
N4	Ho1	O3	106.11(6)	C57	C66	C67	122.0(2)
N3	Ho1	O4	101.82(6)	C57	C66	C65	119.4(3)
N3	Ho1	O3	69.95(6)	C54	C53	C48	119.2(2)
N3	Ho1	N4	63.32(6)	C52	C53	C48	119.9(3)
O2	Ho1	O4	79.99(7)	C52	C53	C54	120.9(3)
O2	Ho1	O3	95.14(7)	C53	C54	C55	121.2(2)
O2	Ho1	N4	131.80(6)	C19	C18	N2	126.3(2)
O2	Ho1	N3	162.62(7)	C17	C12	N1	116.3(2)
O1	Ho1	O4	140.73(6)	C13	C12	N1	124.4(2)
O1	Ho1	O3	78.58(6)	C13	C12	C17	119.2(2)
O1	Ho1	N4	144.05(7)	C10	C1	O1	123.1(2)
O1	Ho1	N3	86.41(7)	C2	C1	O1	118.1(2)
O1	Ho1	O2	81.74(7)	C2	C1	C10	118.8(2)
N2	Ho1	O4	93.12(6)	C12	C17	N2	117.1(2)
N2	Ho1	O3	160.09(6)	C16	C17	N2	124.2(2)
N2	Ho1	N4	73.30(7)	C16	C17	C12	118.7(2)
N2	Ho1	N3	124.13(7)	C19	C28	O2	123.7(2)
N2	Ho1	O2	72.65(7)	C27	C28	O2	118.8(2)
N2	Ho1	O1	114.00(7)	C27	C28	C19	117.4(2)
N1	Ho1	O4	147.55(6)	C68	C73	N6	115.9(2)
N1	Ho1	O3	133.90(6)	C72	C73	N6	124.6(2)
N1	Ho1	N4	80.99(7)	C72	C73	C68	119.5(2)
N1	Ho1	N3	73.71(7)	C10	C9	C4	119.4(2)
N1	Ho1	O2	113.98(7)	C8	C9	C4	117.0(2)
N1	Ho1	O1	71.70(7)	C8	C9	C10	123.6(2)
N1	Ho1	N2	66.00(7)	C31	C32	C37	119.1(2)
O3	Ho2	O4	69.20(6)	C33	C32	C37	119.5(3)
N5	Ho2	O4	116.15(7)	C33	C32	C31	121.3(3)
N5	Ho2	O3	80.13(7)	C9	C10	C1	119.5(2)
N6	Ho2	O4	78.21(6)	C11	C10	C1	120.7(2)
N6	Ho2	O3	115.16(6)	C11	C10	C9	119.6(2)
N6	Ho2	N5	66.30(7)	C14	C13	C12	121.0(3)
O7	Ho2	O4	81.27(7)	C21	C20	C19	123.0(3)
O7	Ho2	O3	84.50(7)	C25	C20	C19	119.5(2)
O7	Ho2	N5	150.11(7)	C25	C20	C21	117.4(2)

O7	Ho2	N6	143.52(7)	C75	C76	C81	119.2(3)
O5	Ho2	O4	157.23(7)	C77	C76	C81	117.3(2)
O5	Ho2	O3	93.96(7)	C77	C76	C75	123.4(2)
O5	Ho2	N5	73.77(7)	C43	C44	C45	120.4(3)
O5	Ho2	N6	123.92(7)	C10	C11	N1	126.5(2)
O5	Ho2	O7	81.95(7)	C60	C65	C66	119.3(3)
O6	Ho2	O4	99.48(6)	C64	C65	C66	123.4(3)
O6	Ho2	O3	162.94(7)	C64	C65	C60	117.2(3)
O6	Ho2	N5	116.80(7)	C70	C69	C68	120.9(3)
O6	Ho2	N6	73.03(7)	C32	C31	C30	121.4(3)
O6	Ho2	O7	81.08(7)	C66	C57	O5	123.0(2)
O6	Ho2	O5	93.00(7)	C58	C57	O5	117.9(3)
C45	N4	C46	119.1(2)	C58	C57	C66	119.1(3)
C67	N5	C68	118.1(2)	C70	C71	C72	119.7(3)
C39	N3	C40	118.5(2)	C82	C83	C84	121.2(3)
C46	C47	C56	120.6(2)	C42	C41	C40	120.6(3)
C48	C47	C56	119.2(2)	C42	C43	C44	120.0(3)
C48	C47	C46	120.0(2)	C35	C36	C37	120.8(3)
C73	N6	C74	118.4(2)	C7	C6	C5	119.1(3)
C47	C56	O4	121.9(2)	C15	C16	C17	121.0(3)
C55	C56	O4	118.4(2)	C59	C60	C65	118.7(3)
C55	C56	C47	119.7(2)	C61	C60	C65	119.6(3)
C37	C38	C29	120.0(2)	C61	C60	C59	121.7(3)
C39	C38	C29	121.5(2)	C83	C82	C81	121.6(3)
C39	C38	C37	118.5(2)	C28	C19	C18	121.2(2)
C38	C29	O3	122.4(2)	C20	C19	C18	118.5(2)
C30	C29	O3	118.6(2)	C20	C19	C28	120.2(2)
C30	C29	C38	119.0(2)	C78	C77	C76	121.5(3)
C54	C55	C56	121.0(2)	C71	C70	C69	120.3(3)
C47	C46	N4	125.3(2)	C43	C42	C41	120.2(3)
C45	C40	N3	116.5(2)	C79	C78	C77	121.0(3)
C41	C40	N3	124.3(2)	C22	C21	C20	121.7(3)
C41	C40	C45	119.2(2)	C51	C52	C53	120.9(3)
C17	N2	C18	118.7(2)	C23	C22	C21	120.2(3)
C82	C81	C76	119.1(2)	C3	C2	C1	121.6(3)
C80	C81	C76	119.6(3)	C59	C58	C57	120.9(3)
C80	C81	C82	121.3(3)	C2	C3	C4	121.2(3)
C74	C75	C84	121.2(2)	C7	C8	C9	121.9(3)
C76	C75	C84	119.6(2)	C26	C27	C28	121.7(3)
C76	C75	C74	119.1(2)	C25	C26	C27	121.8(3)
C40	C45	N4	116.0(2)	C14	C15	C16	120.3(3)
C44	C45	N4	124.5(2)	C26	C25	C20	118.6(3)
C44	C45	C40	119.5(2)	C24	C25	C20	119.7(3)
C11	N1	C12	118.8(2)	C24	C25	C26	121.7(3)
C73	C68	N5	117.0(2)	C50	C49	C48	120.5(3)
C69	C68	N5	124.2(2)	C61	C62	C63	119.3(3)
C69	C68	C73	118.7(2)	C6	C5	C4	121.5(3)
O6	C84	C75	123.2(2)	C58	C59	C60	122.2(3)
C83	C84	C75	118.7(2)	C79	C80	C81	121.6(3)

C83	C84	O6	118.0(2)	C15	C14	C13	119.7(3)
C31	C30	C29	121.4(3)	C23	C24	C25	121.5(3)
C32	C37	C38	119.1(2)	C34	C33	C32	121.1(3)
C36	C37	C38	123.0(3)	C24	C23	C22	119.5(3)
C36	C37	C32	117.9(2)	C64	C63	C62	121.1(4)
C71	C72	C73	120.8(3)	C80	C79	C78	118.9(3)
C53	C48	C47	119.6(2)	C8	C7	C6	120.6(3)
C49	C48	C47	122.5(2)	C51	C50	C49	121.3(3)
C49	C48	C53	117.8(2)	C50	C51	C52	119.4(3)
C75	C74	N6	126.4(2)	C63	C64	C65	121.1(3)
C66	C67	N5	127.4(3)	C34	C35	C36	120.9(3)
C38	C39	N3	125.5(2)	C62	C61	C60	121.5(3)
C3	C4	C9	119.3(2)	C35	C34	C33	119.7(3)
C5	C4	C9	119.9(3)				

Table SI18 Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Ho2L3.

Atom	***x***	***y***	***z***	**U(eq)**
H55	4685(2)	9786.0(14)	1620.9(14)	23.4(6)
H46	4328(2)	8642.6(14)	4335.6(13)	20.1(6)
H7	4250(20)	8341(16)	608(12)	43.2(7)
H30	4436(3)	6638.8(15)	734.9(14)	26.2(6)
H72	7001(3)	7963.3(16)	4265.2(14)	26.7(6)
H74	7838(2)	8667.1(14)	3438.4(14)	22.1(6)
H67	7959(3)	5610.7(15)	2464.5(15)	26.3(6)
H39	4583(2)	5544.3(14)	3467.9(14)	21.6(6)
H54	4739(3)	10975.7(15)	1983.3(16)	27.9(7)
H18	541(3)	9888.3(15)	3146.6(15)	24.7(6)
H13	-105(3)	7065.4(16)	4851.1(14)	28.6(7)
H44	3530(3)	7948.6(16)	5197.9(14)	29.1(7)
H11	-153(2)	6554.4(14)	3945.0(14)	21.4(6)
H69	7175(3)	5534.0(15)	3490.4(15)	29.0(7)
H31	4530(3)	5393.3(16)	480.5(16)	30.3(7)
H71	7016(3)	6862.0(17)	5094.3(15)	32.2(7)
H83	7927(3)	10044.8(17)	792.8(16)	32.8(7)
H41	3658(3)	5487.0(16)	4494.6(15)	32.5(7)
H43	3571(3)	6871.0(17)	6052.2(15)	35.8(8)
H36	4212(4)	4469.7(16)	3260.8(17)	42.5(9)
H6	-401(4)	3273.9(18)	3812.4(19)	56.2(12)
H16	476(3)	9648.3(16)	4220.1(16)	36.1(8)
H82	8263(3)	11139.5(17)	1249.7(17)	34.6(7)
H77	7484(3)	9712.5(17)	3856.2(16)	32.9(7)
H70	7101(3)	5649.5(17)	4702.9(16)	34.7(7)
H42	3627(3)	5640.6(17)	5699.7(16)	39.4(8)
H78	7729(3)	10854.9(18)	4279.1(19)	41.1(8)
H21	1234(3)	10954.8(16)	2994.5(17)	33.5(7)
H52	4549(3)	11828.5(16)	2932.4(19)	38.1(8)
H22	1328(3)	12264.9(17)	2699.4(18)	40.4(8)
H2	1503(3)	5874.7(17)	1380.0(15)	31.2(7)
H58	7561(3)	6686.8(19)	-264.0(17)	42.1(9)

H3	1039(3)	4647.8(17)	1731.8(16)	34.1(7)
H8	-31(3)	5382.2(17)	4358.3(16)	39.8(8)
H27	1833(3)	9385.8(17)	495.0(16)	32.8(7)
H26	1663(3)	10693.1(17)	227.4(16)	37.7(8)
H15	-429(4)	9247.6(18)	5338.1(17)	42.4(9)
H49	3649(3)	9772.8(17)	4641.3(16)	35.6(8)
H62	8916(4)	3045(2)	795(2)	62.2(13)
H5	401(4)	3643.1(17)	2667.1(18)	43.4(9)
H59	8227(4)	5448(2)	-497.8(18)	49.2(10)
H80	8223(3)	11887.5(17)	2272(2)	43.8(9)
H14	-731(3)	7958.1(17)	5654.8(15)	35.0(7)
H24	1638(3)	11996.7(18)	610.4(18)	42.4(9)
H33	4572(4)	3994.5(17)	872.6(18)	43.5(9)
H23	1513(3)	12791.7(17)	1497.0(19)	44.3(9)
H63	8390(4)	3272.0(19)	1974(2)	59.4(12)
H79	8096(3)	11955.5(19)	3490(2)	48.7(10)
H7a	-649(4)	4163.4(19)	4655.8(18)	51.9(11)
H50	3646(4)	10999.4(18)	4962.1(19)	44.3(9)
H51	4115(3)	12027.5(17)	4116(2)	46.0(9)
H64	7778(4)	4513.9(17)	2262(2)	46.0(9)
H35	4283(5)	3225.4(18)	2966(2)	62.3(13)
H85a	6090(20)	8595(4)	-103(10)	86.4(18)
H85b	4787(5)	9199(15)	-147(9)	86.4(18)
H85c	5950(30)	9333(12)	324(2)	86.4(18)
H61	8731(4)	4056(2)	-101(2)	57.0(11)
H86a	3810(20)	7951(6)	-994(3)	70.1(13)
H86b	4749(8)	7470(14)	-414(8)	70.1(13)
H86c	3409(17)	7169(9)	-557(10)	70.1(13)
H34	4474(4)	2985.3(18)	1773(2)	58.7(12)
H8a	2580(30)	7820(13)	202(16)	61.7(8)
H9	1500(20)	7230(20)	1127.9(17)	57.5(8)
H87a	78(14)	8180(15)	218(11)	116(2)
H87b	-616(6)	7495(4)	660(20)	116(2)
H87c	-59(18)	8113(17)	1071(11)	116(2)

Refinement model description

Number of restraints - 3, number of constraints - 125.

Details:

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1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
 At 1.5 times of:
  All C(H,H,H) groups, All O(H) groups
2. Restrained distances
 O7-H7
 0.87 with sigma of 0.01
 C85-H7
 1.863295 with sigma of 0.02
 Ho2-H7
```

2.957705 with sigma of 0.02
3.a Aromatic/amide H refined with riding coordinates:
C55(H55), C46(H46), C30(H30), C72(H72), C74(H74), C67(H67), C39(H39),
C54(H54), C18(H18), C13(H13), C44(H44), C11(H11), C69(H69), C31(H31), C71(H71),
C83(H83), C41(H41), C43(H43), C36(H36), C6(H6), C16(H16), C82(H82), C77(H77),
C70(H70), C42(H42), C78(H78), C21(H21), C52(H52), C22(H22), C2(H2), C58(H58),
C3(H3), C8(H8), C27(H27), C26(H26), C15(H15), C49(H49), C62(H62), C5(H5),
C59(H59), C80(H80), C14(H14), C24(H24), C33(H33), C23(H23), C63(H63), C79(H79),
C7(H7a), C50(H50), C51(H51), C64(H64), C35(H35), C61(H61), C34(H34)
3.b Idealised Me refined as rotating group:
C85(H85a,H85b,H85c), C86(H86a,H86b,H86c), C87(H87a,H87b,H87c)
3.c Idealised tetrahedral OH refined as rotating group:
O9(H9), O8(H8a)

Nd2L3

Table SI19 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Nd2L3_Final. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Nd2	1397.7(6)	1180.48(15)	3016.2(4)	49.1(3)
Nd1	4768.5(6)	1298.81(15)	1934.3(3)	46.7(3)
O3	2754(6)	984.2(17)	1935(4)	44.3(17)
O1	5727(7)	901.1(17)	1226(5)	53.2(19)
O4	3328(6)	1516.6(17)	2897(4)	47.1(18)
C73	17(9)	1346(2)	1248(6)	37(2)
N1	6402(8)	1525(2)	964(5)	42(2)
O5	403(7)	764(2)	3596(4)	60(2)
O6	594(8)	1658(2)	3452(4)	60(2)
C1	5941(10)	863(3)	493(7)	48(3)
N6	398(8)	1524(2)	1890(5)	41(2)
C68	-398(9)	1036(3)	1366(6)	41(2)
C56	3684(9)	1784(3)	3214(7)	48(3)
N5	-441(8)	930(2)	2144(5)	43(2)
C29	2557(9)	756(3)	1438(6)	43(3)
N4	3810(8)	1850(2)	1498(5)	47(2)
N2	6605(7)	1656.0(19)	2508(5)	38.7(19)
C39	2896(11)	1108(3)	293(6)	49(3)
C17	6884(10)	1904(3)	2000(6)	46(3)
N3	3477(8)	1337(2)	631(5)	44(2)
C46	3605(9)	2077(3)	1984(6)	47(3)
C41	3361(12)	1667(3)	-552(7)	57(3)
C45	3592(10)	1905(2)	699(6)	45(3)
C47	3841(11)	2057(3)	2805(6)	48(3)
C57	-569(11)	563(3)	3593(6)	57(3)
C67	-1392(9)	732(2)	2297(6)	41(2)
C16	7178(10)	2210(3)	2227(7)	53(3)
C31	1779(11)	220(2)	1199(7)	51(3)
C32	1926(10)	249(3)	383(7)	50(3)
C3	6038(11)	489(3)	-558(7)	56(3)
C58	-695(10)	357(3)	4250(7)	52(3)
C43	3309(12)	2232(3)	-424(7)	64(3)
C10	6353(10)	1106(3)	19(6)	47(3)
C66	-1504(10)	552(3)	2992(7)	53(3)
C40	3465(10)	1632(2)	228(6)	43(2)
C33	1589(11)	10(3)	-135(7)	58(3)
C64	-3632(10)	309(3)	2481(7)	51(3)
C69	-680(9)	840(2)	741(5)	39(2)
C4	6457(11)	733(3)	-1049(7)	57(3)
C13	6986(11)	2084(3)	673(7)	56(3)
C49	4353(12)	2642(3)	2815(7)	60(3)
C53	4312(12)	2351(3)	3994(8)	65(3)
C74	251(10)	1827(3)	1859(7)	50(3)
C44	3492(11)	2200(3)	353(7)	54(3)

C35	2273(12)	324(3)	-1198(6)	55(3)
C60	-2647(11)	120(3)	3676(7)	55(3)
C70	-506(10)	945(3)	3(6)	46(3)
C63	-4600(11)	88(3)	2553(7)	59(3)
C36	2620(12)	564(3)	-695(7)	56(3)
C9	6611(10)	1047(3)	-789(6)	49(3)
C12	6799(10)	1845(2)	1188(6)	44(3)
C50	4604(15)	2921(3)	3206(9)	78(4)
C81	846(12)	2609(3)	2850(8)	63(3)
C38	2702(9)	797(3)	638(6)	45(3)
C62	-4620(13)	-122(3)	3163(8)	71(4)
C71	-95(10)	1253(2)	-121(7)	47(3)
C2	5790(11)	550(3)	190(7)	56(3)
C7	7324(13)	1197(3)	-2048(7)	64(3)
C15	7379(12)	2453(3)	1700(8)	64(3)
C48	4158(11)	2352(3)	3192(7)	53(3)
C8	7022(12)	1276(3)	-1319(7)	61(3)
C65	-2590(10)	327(2)	3034(7)	47(3)
C84	659(11)	1953(3)	3236(7)	54(3)
C14	7254(11)	2383(3)	914(7)	57(3)
C59	-1676(11)	150(3)	4281(7)	60(3)
C30	2067(10)	463(2)	1698(7)	48(3)
C72	196(10)	1454(3)	485(7)	50(3)
C37	2392(10)	541(3)	108(7)	49(3)
C75	567(10)	2049(2)	2471(7)	47(3)
C61	-3670(10)	-103(3)	3722(8)	64(3)
C5	6750(13)	655(3)	-1819(7)	63(3)
C42	3250(13)	1968(3)	-902(8)	67(3)
C34	1778(11)	42(3)	-909(7)	56(3)
C78	982(14)	2809(3)	1319(10)	81(4)
C55	3863(11)	1785(3)	4028(7)	60(3)
C77	785(12)	2494(3)	1512(9)	67(4)
C54	4138(13)	2066(4)	4414(7)	74(4)
C6	7193(15)	885(3)	-2311(8)	76(4)
C76	704(11)	2380(3)	2276(8)	58(3)
C52	4614(15)	2640(4)	4394(9)	82(5)
C80	970(15)	2935(4)	2687(11)	86(5)
C83	824(11)	2196(4)	3810(8)	72(4)
C51	4725(18)	2915(4)	4002(10)	102(6)
C82	887(12)	2512(3)	3636(9)	75(4)
C79	1002(15)	3025(4)	1940(12)	90(5)
O2	5692(7)	1073.5(18)	3093(4)	51.3(19)
O7	3326(7)	864(2)	3617(5)	64(2)
O8	1486(9)	1282(2)	4492(4)	67(2)
C28	6370(11)	1147(3)	3705(6)	50(3)
C19	7076(10)	1425(3)	3784(6)	44(3)
C18	7247(10)	1651(3)	3152(6)	48(3)
C11	6741(10)	1412(3)	317(6)	50(3)
C26	7127(13)	976(3)	4952(8)	65(3)

C20	7702(10)	1498(3)	4523(6)	46(3)
C27	6488(12)	923(3)	4291(7)	61(3)
C25	7741(12)	1271(3)	5127(8)	60(3)
C22	8914(13)	1849(3)	5424(7)	67(3)
C24	8371(13)	1337(3)	5826(7)	66(4)
C21	8322(11)	1797(3)	4692(7)	59(3)
C85	3335(14)	560(3)	3965(8)	77(4)
C23	8948(14)	1618(4)	5976(8)	76(4)
C86	1359(17)	1070(4)	5132(9)	94(5)

Table SI20 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Nd2L3_Final. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Nd2	43.2(4)	58.2(5)	45.9(4)	-2.9(3)	-1.1(3)	0.1(3)
Nd1	40.3(4)	52.9(4)	46.9(4)	-0.5(3)	-1.0(3)	-0.2(3)
O3	39(4)	56(5)	38(4)	-11(3)	-1(3)	-3(4)
O1	54(5)	46(4)	60(5)	7(4)	3(4)	14(4)
O4	31(4)	53(5)	58(5)	-5(3)	8(3)	-5(4)
C73	34(5)	41(6)	34(6)	3(4)	-6(4)	-4(4)
N1	35(4)	51(5)	42(5)	-8(4)	8(4)	12(4)
O5	45(4)	83(6)	51(5)	-13(4)	-14(4)	12(4)
O6	54(5)	77(6)	48(5)	-8(4)	5(4)	2(4)
C1	30(5)	63(8)	51(7)	1(5)	-12(5)	8(6)
N6	42(5)	42(5)	38(5)	7(4)	-15(4)	8(4)
C68	33(5)	52(7)	37(6)	-1(5)	-6(4)	5(5)
C56	29(5)	56(7)	58(7)	-9(5)	-3(5)	-18(6)
N5	45(5)	43(5)	39(5)	-8(4)	-14(4)	-1(4)
C29	33(5)	47(6)	50(7)	1(5)	-3(5)	-3(5)
N4	48(5)	41(5)	51(6)	7(4)	-8(4)	9(4)
N2	30(4)	43(5)	42(5)	-12(4)	-9(4)	2(4)
C39	50(6)	71(8)	25(5)	-2(6)	-20(5)	-2(5)
C17	41(6)	51(7)	45(6)	-10(5)	-5(5)	-9(5)
N3	38(5)	63(6)	31(5)	3(4)	-8(4)	5(4)
C46	33(6)	47(7)	60(7)	3(5)	5(5)	3(6)
C41	64(7)	51(7)	53(7)	-3(6)	-14(6)	-9(6)
C45	43(6)	40(6)	52(7)	-5(5)	-9(5)	2(5)
C47	49(6)	42(6)	51(7)	0(5)	-3(5)	-9(5)
C57	44(7)	83(9)	44(7)	2(6)	-4(5)	19(6)
C67	35(5)	47(6)	41(6)	-3(5)	-9(4)	6(5)
C16	37(6)	61(8)	60(7)	-7(5)	0(5)	14(6)
C31	52(7)	33(6)	68(8)	-3(5)	9(6)	-6(5)
C32	46(6)	48(7)	57(7)	7(5)	-7(5)	4(6)
C3	61(7)	44(7)	63(8)	0(5)	3(6)	-5(6)
C58	40(6)	65(7)	53(7)	3(5)	4(5)	22(6)
C43	72(8)	54(8)	64(8)	-13(6)	-12(7)	8(6)
C10	37(6)	55(7)	49(7)	3(5)	-1(5)	3(5)
C66	43(6)	62(7)	52(7)	5(5)	-2(5)	11(6)
C40	41(6)	45(6)	42(6)	6(5)	-9(5)	9(5)
C33	58(7)	42(6)	73(9)	-9(5)	9(6)	-16(6)

C64	42(6)	44(6)	69(8)	-1(5)	-5(6)	8(6)
C69	33(5)	46(6)	38(6)	1(4)	-9(4)	2(5)
C4	56(7)	56(7)	58(8)	10(6)	-4(6)	-3(6)
C13	46(6)	78(9)	45(7)	1(6)	3(5)	23(6)
C49	66(8)	54(8)	60(8)	-5(6)	3(6)	-7(6)
C53	56(7)	70(9)	67(9)	-18(6)	-5(6)	3(7)
C74	35(6)	58(8)	56(7)	4(5)	3(5)	11(6)
C44	61(7)	44(7)	58(8)	0(5)	6(6)	-4(6)
C35	74(8)	53(7)	38(6)	-14(6)	-6(6)	-11(5)
C60	46(6)	48(7)	70(8)	8(5)	3(6)	15(6)
C70	40(6)	62(7)	36(6)	6(5)	-8(5)	-2(5)
C63	49(7)	64(8)	65(8)	-9(6)	-9(6)	16(6)
C36	65(8)	50(7)	54(7)	-5(6)	-3(6)	-3(6)
C9	48(6)	60(7)	38(6)	12(5)	-8(5)	-2(5)
C12	38(6)	47(6)	48(6)	5(5)	-7(5)	2(5)
C50	101(11)	50(8)	84(11)	-19(7)	18(8)	-25(7)
C81	64(8)	50(8)	76(9)	-9(6)	5(7)	-16(7)
C38	33(5)	53(7)	48(7)	3(5)	-4(5)	-17(5)
C62	64(8)	56(8)	95(10)	-14(6)	6(8)	2(7)
C71	43(6)	46(7)	51(7)	2(5)	2(5)	6(5)
C2	55(7)	68(8)	46(7)	14(6)	0(5)	5(6)
C7	87(9)	66(8)	40(7)	5(7)	4(6)	-2(6)
C15	63(8)	45(7)	84(10)	-5(6)	3(7)	-5(7)
C48	42(6)	63(8)	55(7)	1(5)	-7(5)	-15(6)
C8	70(8)	70(9)	43(7)	14(7)	1(6)	4(6)
C65	37(6)	41(6)	63(7)	4(5)	6(5)	11(5)
C84	43(6)	66(8)	53(7)	2(6)	0(5)	-14(6)
C14	53(7)	49(7)	68(8)	-7(5)	-12(6)	0(6)
C59	55(7)	77(9)	48(7)	9(6)	8(6)	16(6)
C30	45(6)	46(7)	55(7)	-4(5)	11(5)	8(5)
C72	38(6)	43(6)	69(8)	-16(5)	-3(5)	-6(6)
C37	40(6)	52(7)	55(7)	2(5)	2(5)	-1(5)
C75	34(6)	37(6)	70(8)	1(4)	-3(5)	-10(5)
C61	34(6)	69(8)	88(10)	-15(6)	4(6)	13(7)
C5	75(8)	64(8)	52(7)	4(7)	4(6)	-13(6)
C42	78(9)	64(9)	59(8)	-10(7)	2(7)	12(7)
C34	61(7)	45(7)	61(8)	-4(6)	2(6)	-14(6)
C78	84(10)	49(8)	109(12)	-4(7)	-11(9)	26(8)
C55	50(7)	78(9)	51(7)	-5(6)	-5(6)	-7(6)
C77	52(7)	50(8)	98(11)	3(6)	-14(7)	-5(7)
C54	68(8)	111(12)	43(7)	-8(8)	8(6)	-25(8)
C6	97(11)	78(10)	52(8)	-3(8)	5(7)	3(7)
C76	42(6)	52(7)	80(9)	-1(5)	-7(6)	-11(7)
C52	94(11)	75(10)	77(10)	-27(8)	8(8)	-42(9)
C80	84(10)	66(10)	108(13)	-10(8)	15(9)	-37(9)
C83	46(7)	98(12)	73(9)	-13(7)	13(6)	-40(8)
C51	136(15)	80(12)	89(12)	-27(10)	-3(11)	-44(10)
C82	58(8)	70(10)	97(12)	-9(7)	25(8)	-32(8)
C79	72(10)	69(10)	129(15)	-2(8)	1(10)	-21(11)

O2	43(4)	60(5)	50(5)	4(4)	-15(4)	7(4)
O7	52(5)	77(6)	62(5)	-3(4)	-2(4)	36(4)
O8	95(7)	86(6)	20(4)	-3(5)	0(4)	-10(4)
C28	49(7)	54(7)	47(7)	7(5)	-4(5)	8(5)
C19	51(6)	46(6)	36(6)	3(5)	9(5)	2(5)
C18	37(6)	55(7)	51(7)	2(5)	2(5)	4(5)
C11	34(6)	74(8)	44(7)	11(5)	17(5)	12(6)
C26	69(8)	60(8)	66(9)	13(6)	7(7)	17(7)
C20	41(6)	63(7)	33(6)	12(5)	4(5)	1(5)
C27	55(7)	79(9)	49(7)	-11(6)	-7(6)	9(6)
C25	52(7)	66(8)	63(8)	7(6)	-7(6)	8(6)
C22	77(9)	74(9)	49(7)	-11(7)	-8(6)	-2(7)
C24	67(8)	86(10)	43(7)	3(7)	-7(6)	12(6)
C21	48(7)	65(8)	63(8)	-1(6)	-6(6)	-2(6)
C23	83(10)	91(11)	55(8)	-17(8)	-15(7)	3(8)

Table SI21 Bond Lengths for Nd2L3_Final.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Nd2	O3	2.512(7)	C43	C42	1.394(18)
Nd2	O4	2.456(7)	C10	C9	1.459(15)
Nd2	O5	2.288(8)	C10	C11	1.450(17)
Nd2	O6	2.322(9)	C66	C65	1.470(15)
Nd2	N6	2.629(7)	C33	C34	1.373(17)
Nd2	N5	2.617(8)	C64	C63	1.375(16)
Nd2	O7	2.590(8)	C64	C65	1.422(15)
Nd2	O8	2.602(7)	C69	C70	1.376(14)
Nd1	O3	2.462(6)	C4	C9	1.417(17)
Nd1	O1	2.324(8)	C4	C5	1.420(16)
Nd1	O4	2.445(7)	C13	C12	1.370(15)
Nd1	N1	2.595(8)	C13	C14	1.359(17)
Nd1	C56	3.251(11)	C49	C50	1.387(17)
Nd1	N4	2.642(8)	C49	C48	1.409(17)
Nd1	N2	2.598(7)	C53	C48	1.400(17)
Nd1	N3	2.601(8)	C53	C54	1.425(19)
Nd1	O2	2.402(7)	C53	C52	1.438(18)
O3	C29	1.310(12)	C74	C75	1.452(16)
O1	C1	1.309(13)	C35	C36	1.385(15)
O4	C56	1.310(12)	C35	C34	1.399(16)
C73	N6	1.394(12)	C60	C65	1.426(15)
C73	C68	1.401(14)	C60	C59	1.436(17)
C73	C72	1.419(15)	C60	C61	1.417(16)
N1	C12	1.468(14)	C70	C71	1.392(15)
N1	C11	1.279(13)	C63	C62	1.385(17)
O5	C57	1.312(14)	C36	C37	1.425(16)
O6	C84	1.310(15)	C9	C8	1.411(17)
C1	C10	1.394(16)	C50	C51	1.39(2)
C1	C2	1.435(17)	C81	C76	1.397(17)
N6	C74	1.295(14)	C81	C80	1.42(2)
C68	N5	1.428(13)	C81	C82	1.43(2)

C68	C69	1.391(14)	C38	C37	1.455(15)
C56	C47	1.368(16)	C62	C61	1.361(18)
C56	C55	1.423(16)	C71	C72	1.383(15)
N5	C67	1.319(13)	C7	C8	1.356(17)
C29	C38	1.415(15)	C7	C6	1.404(18)
C29	C30	1.419(15)	C15	C14	1.402(18)
N4	C46	1.301(14)	C84	C75	1.391(16)
N4	C45	1.421(14)	C84	C83	1.440(17)
N2	C17	1.408(13)	C75	C76	1.455(16)
N2	C18	1.285(13)	C5	C6	1.384(18)
C39	N3	1.275(14)	C78	C77	1.392(18)
C39	C38	1.465(16)	C78	C79	1.42(2)
C17	C16	1.387(16)	C55	C54	1.394(18)
C17	C12	1.436(15)	C77	C76	1.420(19)
N3	C40	1.432(13)	C52	C51	1.36(2)
C46	C47	1.446(15)	C80	C79	1.36(2)
C41	C40	1.366(15)	C83	C82	1.38(2)
C41	C42	1.417(17)	O2	C28	1.296(13)
C45	C40	1.423(15)	O7	C85	1.425(15)
C45	C44	1.393(15)	O8	C86	1.438(17)
C47	C48	1.456(15)	C28	C19	1.389(16)
C57	C58	1.448(15)	C28	C27	1.397(16)
C57	C66	1.401(16)	C19	C18	1.472(15)
C67	C66	1.438(15)	C19	C20	1.455(15)
C16	C15	1.398(16)	C26	C27	1.327(17)
C31	C32	1.436(16)	C26	C25	1.430(18)
C31	C30	1.373(15)	C20	C25	1.424(16)
C32	C33	1.394(16)	C20	C21	1.444(16)
C32	C37	1.417(16)	C25	C24	1.391(17)
C3	C4	1.415(17)	C22	C21	1.413(16)
C3	C2	1.357(16)	C22	C23	1.372(18)
C58	C59	1.338(16)	C24	C23	1.353(19)
C43	C44	1.366(17)			

Table SI22 Bond Angles for Nd2L3_Final.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O4	Nd2	O3	70.4(2)	C58	C57	O5	118.3(10)
O5	Nd2	O3	109.7(3)	C66	C57	O5	122.1(10)
O5	Nd2	O4	148.9(2)	C66	C57	C58	119.6(11)
O6	Nd2	O3	138.0(3)	C66	C67	N5	125.8(9)
O6	Nd2	O4	79.4(3)	C15	C16	C17	122.6(12)
O6	Nd2	O5	111.3(3)	C30	C31	C32	122.4(10)
N6	Nd2	O3	80.7(3)	C33	C32	C31	123.2(11)
N6	Nd2	O4	85.2(3)	C37	C32	C31	116.9(10)
N6	Nd2	O5	125.9(3)	C37	C32	C33	119.9(11)
N6	Nd2	O6	68.0(3)	C2	C3	C4	120.5(11)
N5	Nd2	O3	80.6(2)	C59	C58	C57	120.8(11)
N5	Nd2	O4	139.4(3)	C42	C43	C44	120.9(12)
N5	Nd2	O5	67.5(3)	C9	C10	C1	120.6(11)

N5	Nd2	O6	106.7(3)	C11	C10	C1	122.5(10)
N5	Nd2	N6	62.1(3)	C11	C10	C9	116.2(10)
O7	Nd2	O3	72.4(2)	C67	C66	C57	122.7(10)
O7	Nd2	O4	74.0(2)	C65	C66	C57	119.4(10)
O7	Nd2	O5	76.5(3)	C65	C66	C67	117.7(10)
O7	Nd2	O6	126.5(3)	C41	C40	N3	125.6(10)
O7	Nd2	N6	150.2(3)	C45	C40	N3	115.4(9)
O7	Nd2	N5	123.7(3)	C45	C40	C41	119.1(10)
O8	Nd2	O3	142.0(3)	C34	C33	C32	121.5(11)
O8	Nd2	O4	88.9(3)	C65	C64	C63	120.5(11)
O8	Nd2	O5	72.4(3)	C70	C69	C68	120.3(10)
O8	Nd2	O6	62.4(3)	C9	C4	C3	121.9(11)
O8	Nd2	N6	130.3(3)	C5	C4	C3	118.3(11)
O8	Nd2	N5	130.2(3)	C5	C4	C9	119.7(12)
O8	Nd2	O7	71.4(3)	C14	C13	C12	121.3(12)
O1	Nd1	O3	88.5(3)	C48	C49	C50	123.0(12)
O4	Nd1	O3	71.4(2)	C54	C53	C48	120.1(12)
O4	Nd1	O1	155.5(2)	C52	C53	C48	119.7(13)
N1	Nd1	O3	139.3(2)	C52	C53	C54	120.2(13)
N1	Nd1	O1	68.4(3)	C75	C74	N6	126.1(10)
N1	Nd1	O4	136.0(3)	C43	C44	C45	121.5(11)
C56	Nd1	O3	92.3(2)	C34	C35	C36	119.5(11)
C56	Nd1	O1	168.8(3)	C59	C60	C65	118.4(10)
C56	Nd1	O4	21.1(2)	C61	C60	C65	120.2(11)
C56	Nd1	N1	116.8(3)	C61	C60	C59	121.4(11)
N4	Nd1	O3	100.0(3)	C71	C70	C69	119.8(10)
N4	Nd1	O1	130.6(3)	C62	C63	C64	122.4(11)
N4	Nd1	O4	68.6(3)	C37	C36	C35	121.5(11)
N4	Nd1	N1	74.2(3)	C4	C9	C10	116.6(11)
N4	Nd1	C56	60.2(3)	C8	C9	C10	125.3(11)
N2	Nd1	O3	156.6(2)	C8	C9	C4	118.2(11)
N2	Nd1	O1	108.3(3)	C17	C12	N1	115.6(9)
N2	Nd1	O4	87.9(2)	C13	C12	N1	123.7(10)
N2	Nd1	N1	63.8(3)	C13	C12	C17	120.5(11)
N2	Nd1	C56	68.0(3)	C51	C50	C49	119.0(14)
N2	Nd1	N4	81.6(3)	C80	C81	C76	122.8(14)
N3	Nd1	O3	68.0(2)	C82	C81	C76	118.9(12)
N3	Nd1	O1	78.3(3)	C82	C81	C80	118.3(13)
N3	Nd1	O4	105.6(3)	C39	C38	C29	122.2(9)
N3	Nd1	N1	74.5(3)	C37	C38	C29	120.3(10)
N3	Nd1	C56	112.4(3)	C37	C38	C39	116.3(9)
N3	Nd1	N4	61.1(3)	C61	C62	C63	118.9(12)
N3	Nd1	N2	130.3(3)	C72	C71	C70	121.3(10)
O2	Nd1	O3	95.5(2)	C3	C2	C1	120.4(12)
O2	Nd1	O1	89.6(3)	C6	C7	C8	121.0(13)
O2	Nd1	O4	78.9(3)	C14	C15	C16	118.1(11)
O2	Nd1	N1	116.4(3)	C49	C48	C47	124.7(11)
O2	Nd1	C56	79.2(3)	C53	C48	C47	118.3(11)
O2	Nd1	N4	136.8(3)	C53	C48	C49	117.0(11)

O2	Nd1	N2	69.1(3)	C7	C8	C9	121.4(12)
O2	Nd1	N3	159.5(3)	C64	C65	C66	124.0(10)
Nd1	O3	Nd2	107.7(3)	C60	C65	C66	119.1(10)
C29	O3	Nd2	131.3(6)	C60	C65	C64	116.8(10)
C29	O3	Nd1	121.0(6)	C75	C84	O6	123.4(10)
C1	O1	Nd1	133.7(7)	C83	C84	O6	119.4(12)
Nd1	O4	Nd2	110.0(3)	C83	C84	C75	117.3(12)
C56	O4	Nd2	133.2(6)	C15	C14	C13	120.7(12)
C56	O4	Nd1	116.6(6)	C60	C59	C58	122.5(11)
C68	C73	N6	118.1(9)	C31	C30	C29	121.8(11)
C72	C73	N6	122.2(9)	C71	C72	C73	118.9(10)
C72	C73	C68	119.1(9)	C36	C37	C32	117.2(10)
C12	N1	Nd1	110.4(6)	C38	C37	C32	120.6(10)
C11	N1	Nd1	129.1(8)	C38	C37	C36	122.0(10)
C11	N1	C12	119.8(9)	C84	C75	C74	121.4(10)
C57	O5	Nd2	148.0(7)	C76	C75	C74	118.5(11)
C84	O6	Nd2	136.0(7)	C76	C75	C84	120.0(11)
C10	C1	O1	123.0(11)	C62	C61	C60	121.1(12)
C2	C1	O1	117.0(10)	C6	C5	C4	120.0(12)
C2	C1	C10	120.0(11)	C43	C42	C41	117.7(12)
C73	N6	Nd2	113.1(6)	C35	C34	C33	120.0(11)
C74	N6	Nd2	128.6(7)	C79	C78	C77	115.9(15)
C74	N6	C73	118.3(9)	C54	C55	C56	119.9(13)
N5	C68	C73	116.9(9)	C76	C77	C78	124.4(14)
C69	C68	C73	120.3(9)	C55	C54	C53	120.4(12)
C69	C68	N5	122.7(9)	C5	C6	C7	119.7(12)
O4	C56	Nd1	42.2(5)	C75	C76	C81	120.9(12)
C47	C56	Nd1	97.6(7)	C77	C76	C81	115.2(12)
C47	C56	O4	123.3(10)	C77	C76	C75	123.8(11)
C55	C56	Nd1	130.2(8)	C51	C52	C53	120.7(14)
C55	C56	O4	116.5(11)	C79	C80	C81	118.3(14)
C55	C56	C47	120.1(10)	C82	C83	C84	123.3(14)
C68	N5	Nd2	112.4(6)	C52	C51	C50	120.6(13)
C67	N5	Nd2	131.9(7)	C83	C82	C81	119.5(13)
C67	N5	C68	115.7(8)	C80	C79	C78	123.1(15)
C38	C29	O3	122.6(10)	C28	O2	Nd1	141.7(7)
C30	C29	O3	119.1(10)	C85	O7	Nd2	129.6(7)
C30	C29	C38	118.0(10)	C86	O8	Nd2	131.3(8)
C46	N4	Nd1	122.3(7)	C19	C28	O2	123.7(10)
C45	N4	Nd1	118.2(7)	C27	C28	O2	118.0(11)
C45	N4	C46	119.4(9)	C27	C28	C19	118.1(10)
C17	N2	Nd1	110.7(6)	C18	C19	C28	123.5(10)
C18	N2	Nd1	132.5(7)	C20	C19	C28	119.0(10)
C18	N2	C17	116.7(8)	C20	C19	C18	117.5(10)
C38	C39	N3	124.5(9)	C19	C18	N2	126.3(10)
C16	C17	N2	124.6(10)	C10	C11	N1	124.6(10)
C12	C17	N2	118.5(9)	C25	C26	C27	122.5(12)
C12	C17	C16	116.8(10)	C25	C20	C19	120.7(11)
C39	N3	Nd1	125.1(7)	C21	C20	C19	123.2(10)

C40	N3	Nd1	118.6(6)	C21	C20	C25	116.0(10)
C40	N3	C39	116.2(8)	C26	C27	C28	123.3(13)
C47	C46	N4	124.8(10)	C20	C25	C26	115.5(11)
C42	C41	C40	121.9(11)	C24	C25	C26	123.7(12)
C40	C45	N4	116.2(9)	C24	C25	C20	120.8(12)
C44	C45	N4	125.2(10)	C23	C22	C21	121.4(13)
C44	C45	C40	118.6(10)	C23	C24	C25	122.5(13)
C46	C47	C56	123.0(10)	C22	C21	C20	119.9(12)
C48	C47	C56	121.1(10)	C24	C23	C22	119.4(12)
C48	C47	C46	115.7(10)				

Table SI23 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Nd2L3_Final.

Atom	*x*	*y*	*z*	U(eq)
H39	2566(11)	1142(3)	-216(6)	58(3)
H46	3275(9)	2271(3)	1783(6)	56(3)
H41	3363(12)	1485(3)	-869(7)	68(4)
H67	-2061(9)	707(2)	1914(6)	49(3)
H16	7247(10)	2256(3)	2761(7)	63(4)
H31	1472(11)	27(2)	1401(7)	61(3)
H3	5930(11)	281(3)	-754(7)	67(4)
H58	-74(10)	368(3)	4663(7)	63(3)
H43	3220(12)	2436(3)	-641(7)	76(4)
H33	1221(11)	-180(3)	53(7)	69(4)
H64	-3660(10)	451(3)	2058(7)	62(3)
H69	-993(9)	632(2)	826(5)	47(3)
H13	6926(11)	2041(3)	138(7)	68(4)
H49	4312(12)	2646(3)	2269(7)	72(4)
H74	-96(10)	1912(3)	1392(7)	60(3)
H44	3553(11)	2384(3)	665(7)	65(3)
H35	2370(12)	350(3)	-1736(6)	66(4)
H70	-667(10)	808(3)	-421(6)	56(3)
H63	-5279(11)	79(3)	2172(7)	71(4)
H36	3019(12)	749(3)	-889(7)	67(4)
H50	4692(15)	3114(3)	2933(9)	94(5)
H62	-5286(13)	-277(3)	3190(8)	86(4)
H71	-12(10)	1327(2)	-633(7)	56(3)
H2	5514(11)	384(3)	515(7)	68(4)
H15	7593(12)	2660(3)	1870(8)	77(4)
H14	7359(11)	2545(3)	545(7)	68(4)
H59	-1731(11)	18(3)	4720(7)	72(4)
H30	1935(10)	434(2)	2232(7)	58(3)
H72	510(10)	1661(3)	393(7)	60(3)
H61	-3692(10)	-242(3)	4150(8)	77(4)
H5	6644(13)	444(3)	-1997(7)	76(4)
H42	3139(13)	1990(3)	-1444(8)	80(4)
H34	1573(11)	-128(3)	-1249(7)	67(4)
H78	1097(14)	2875(3)	803(10)	97(5)
H55	3796(11)	1594(3)	4309(7)	71(4)

H77	698(12)	2346(3)	1104(9)	80(4)
H54	4210(13)	2068(4)	4959(7)	88(5)
H6	7406(15)	833(3)	-2823(8)	91(5)
H52	4736(15)	2638(4)	4937(9)	99(5)
H80	1029(15)	3086(4)	3090(11)	103(6)
H83	893(11)	2134(4)	4335(8)	86(5)
H51	4886(18)	3106(4)	4276(10)	122(7)
H82	957(12)	2664(3)	4036(9)	90(5)
H79	1040(15)	3244(4)	1828(12)	108(6)
H18	7895(10)	1809(3)	3228(6)	57(3)
H11	7286(10)	1539(3)	9(6)	60(3)
H26	7179(13)	812(3)	5322(8)	78(4)
H27	6091(12)	723(3)	4213(7)	74(4)
H22	9296(13)	2048(3)	5535(7)	80(4)
H24	8396(13)	1179(3)	6214(7)	79(4)
H21	8333(11)	1957(3)	4312(7)	71(4)
H23	9374(14)	1655(4)	6459(8)	92(5)
H85a	4225(14)	506(3)	4136(8)	116(6)
H85b	2766(14)	560(3)	4408(8)	116(6)
H85c	3022(14)	403(3)	3590(8)	116(6)
H86a	1444(17)	1189(4)	5614(9)	141(7)
H86b	504(17)	968(4)	5102(9)	141(7)
H86c	2044(17)	910(4)	5118(9)	141(7)
H8	7089(12)	1490(3)	-1162(7)	73(4)
H7	7629(13)	1355(3)	-2387(7)	77(4)
H7a	4127(8)	914(14)	3510(50)	96(3)
H8a	1320(110)	1472(5)	4654(12)	101(4)

Table SI24 Solvent masks information for Nd2L3_Final.

Number	X	Y	Z	Volume	Electron count	Content
1	-0.122	0.000	0.500	685.2	209.3	5DCM
2	-0.129	0.500	0.000	685.2	209.3	5DCM

Refinement model description

Number of restraints - 6, number of constraints - 118.

Dy2L3_Final

Table SI25 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Dy2L3_Final. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Dy1	2906.80(18)	6036.87(17)	3535.16(16)	19.23(10)
Dy2	2741.09(18)	4440.98(16)	2554.43(15)	16.03(10)
O1	1910(3)	3720(2)	2914(2)	21.5(11)
O6	3900(3)	6647(3)	3898(2)	30.4(13)
N6	3186(3)	6722(3)	2619(3)	18.7(13)
O5	2233(3)	6380(3)	4307(2)	30.7(13)
O2	3565(3)	4039(3)	3384(2)	28.7(13)
N1	2260(3)	3729(3)	1631(3)	19.8(13)
O3	2131(2)	5126(2)	3249(2)	20.1(11)
N4	3009(3)	5145(3)	1600(3)	16.9(13)
O4	3550(3)	5328(2)	2903(2)	20.5(11)
C85	3316(8)	4967(8)	4933(7)	109(5)
N5	1769(3)	6576(3)	2974(3)	20.0(13)
N2	3755(3)	3869(3)	2038(3)	19.3(13)
N3	1589(3)	5018(3)	1931(3)	21.7(14)
C40	1657(4)	5138(4)	1258(3)	23.1(17)
C45	2408(4)	5214(3)	1090(3)	22.3(17)
C84	4524(4)	6821(3)	3646(4)	24.9(18)
C83	5218(5)	6914(4)	4072(4)	36(2)
C82	5895(4)	7055(4)	3848(4)	34(2)
C81	5955(4)	7110(4)	3170(4)	29.9(19)
C80	6667(4)	7235(4)	2928(5)	36(2)
C79	6722(5)	7291(4)	2276(5)	46(2)
C78	6066(5)	7213(4)	1838(5)	41(2)
C77	5361(5)	7099(4)	2052(4)	34(2)
C76	5278(4)	7060(3)	2727(4)	23.9(17)
C75	4550(4)	6939(3)	2977(3)	22.2(17)
C74	3856(4)	6965(3)	2533(4)	22.8(17)
C73	2564(4)	6797(3)	2122(3)	19.6(16)
C68	1817(4)	6732(4)	2303(4)	26.0(18)
C67	1129(4)	6699(3)	3208(4)	23.4(17)
C66	937(4)	6582(3)	3859(3)	22.2(17)
C57	1513(4)	6473(4)	4380(4)	26.9(18)
C58	1281(5)	6464(4)	5026(4)	38(2)
C59	542(5)	6533(4)	5136(4)	41(2)
C60	-56(5)	6617(4)	4624(4)	34(2)
C65	135(4)	6640(4)	3973(4)	26.3(18)
C64	-478(4)	6684(4)	3475(4)	34(2)
C63	-1232(5)	6724(5)	3594(5)	49(3)
C62	-1406(5)	6719(5)	4236(5)	58(3)
C61	-836(5)	6654(5)	4733(5)	48(2)
C69	1186(4)	6785(4)	1826(4)	27.1(18)
C70	1283(5)	6911(4)	1185(4)	33(2)
C71	2022(5)	6971(4)	1003(4)	34(2)

C72	2644(4)	6906(4)	1463(4)	26.9(18)
C18	4432(4)	3701(3)	2300(4)	22.0(17)
C19	4760(4)	3779(3)	2964(3)	18.9(16)
C20	5582(4)	3691(3)	3112(4)	24.1(17)
C25	5912(4)	3643(4)	3770(4)	30.0(19)
C24	6715(4)	3549(4)	3913(4)	38(2)
C23	7182(4)	3523(4)	3433(4)	39(2)
C22	6868(4)	3595(4)	2782(4)	36(2)
C21	6091(4)	3679(4)	2631(4)	29.6(19)
C26	5429(5)	3706(5)	4274(4)	42(2)
C27	4659(4)	3838(4)	4131(4)	36(2)
C28	4303(4)	3893(4)	3472(4)	26.3(18)
C17	3554(4)	3739(3)	1362(3)	19.2(16)
C12	2775(4)	3660(3)	1150(3)	21.5(17)
C11	1579(4)	3466(3)	1536(3)	20.3(16)
C10	1007(4)	3492(3)	1982(4)	21.5(17)
C1	1213(4)	3568(3)	2658(3)	20.9(16)
C2	628(4)	3464(4)	3083(4)	26.5(18)
C3	-116(4)	3347(4)	2849(4)	29.7(19)
C4	-357(4)	3326(4)	2173(4)	26.7(18)
C9	204(4)	3391(4)	1734(4)	25.2(17)
C8	-53(5)	3377(4)	1060(4)	36(2)
C7	-824(5)	3299(4)	847(5)	45(2)
C6	-1370(5)	3246(4)	1289(5)	43(2)
C5	-1142(4)	3259(4)	1934(4)	37(2)
C13	2546(4)	3565(4)	485(4)	29.1(19)
C14	3077(5)	3543(5)	43(4)	42(2)
C15	3850(5)	3621(4)	252(4)	36(2)
C16	4090(5)	3722(4)	903(4)	28.9(19)
C39	968(4)	5182(3)	2166(4)	21.3(17)
C38	807(4)	5078(4)	2830(4)	22.6(17)
C29	1394(4)	5055(4)	3343(4)	22.3(17)
C30	1203(4)	4960(4)	3991(4)	27.5(18)
C31	464(4)	4911(4)	4117(4)	33(2)
C32	-153(4)	4947(4)	3615(4)	32(2)
C37	6(4)	5026(4)	2961(4)	27.1(18)
C36	-618(4)	5013(4)	2462(5)	38(2)
C35	-1361(5)	4942(5)	2613(5)	52(3)
C34	-1520(5)	4893(4)	3258(5)	48(3)
C33	-930(5)	4883(4)	3751(5)	46(2)
C46	3680(4)	5391(3)	1541(3)	21.5(17)
C47	4345(4)	5356(3)	2032(3)	18.5(16)
C56	4247(4)	5353(3)	2696(3)	18.3(16)
C55	4905(4)	5398(3)	3162(4)	22.8(17)
C54	5631(4)	5425(4)	2985(4)	30.7(19)
C53	5754(4)	5402(3)	2316(4)	29.5(19)
C52	6504(5)	5411(4)	2119(5)	43(2)
C51	6624(5)	5362(5)	1485(5)	54(3)
C50	5993(5)	5299(5)	1009(5)	51(3)

C49	5251(5)	5294(4)	1168(4)	33(2)
C48	5106(4)	5359(3)	1828(4)	23.7(18)
C44	2510(5)	5319(4)	432(4)	30.6(19)
C43	1886(5)	5352(4)	-38(4)	42(2)
C42	1151(5)	5262(5)	135(4)	46(2)
C41	1033(5)	5150(4)	777(4)	35(2)
O7	3453(3)	5195(3)	4282(2)	39.0(14)

Table SI26 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Dy2L3_Final. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Dy1	14.73(18)	26.6(2)	16.55(18)	-4.48(15)	2.64(13)	-2.37(15)
Dy2	10.01(17)	23.27(19)	14.92(17)	0.33(14)	1.88(12)	1.19(15)
O6	20(3)	47(4)	24(3)	-16(3)	5(2)	0(3)
N6	7(3)	21(3)	27(3)	-2(3)	0(3)	-4(3)
O5	24(3)	47(4)	22(3)	1(3)	6(2)	-7(3)
O2	12(3)	52(4)	22(3)	4(2)	3(2)	10(3)
N1	18(3)	22(3)	19(3)	1(3)	4(3)	3(3)
O3	13(3)	26(3)	22(3)	-4(2)	4(2)	-2(2)
N4	5(3)	22(3)	24(3)	1(3)	3(2)	0(3)
O4	14(3)	29(3)	19(3)	-2(2)	3(2)	-2(2)
N5	17(3)	23(3)	21(3)	-1(3)	8(3)	-1(3)
N2	16(3)	17(3)	25(3)	-3(3)	4(3)	5(3)
N3	17(3)	22(3)	26(3)	-1(3)	2(3)	-2(3)
C40	19(4)	31(5)	18(4)	4(3)	-4(3)	5(3)
C45	26(4)	14(4)	27(4)	5(3)	4(3)	4(3)
C84	24(4)	13(4)	36(5)	-9(3)	0(4)	-7(3)
C83	37(5)	40(5)	29(5)	-14(4)	0(4)	-2(4)
C82	20(4)	33(5)	45(5)	-7(4)	-7(4)	-2(4)
C81	25(4)	18(4)	47(5)	-8(3)	6(4)	-3(4)
C80	19(4)	24(5)	63(6)	-1(4)	3(4)	-2(4)
C79	31(5)	38(6)	74(7)	1(4)	25(5)	10(5)
C78	31(5)	42(5)	54(6)	2(4)	24(4)	9(5)
C77	32(5)	28(5)	42(5)	-2(4)	7(4)	-2(4)
C76	24(4)	14(4)	35(5)	-4(3)	10(3)	-1(3)
C75	22(4)	17(4)	27(4)	-6(3)	1(3)	-2(3)
C74	22(4)	22(4)	25(4)	2(3)	6(3)	-1(3)
C73	23(4)	16(4)	21(4)	0(3)	4(3)	1(3)
C68	24(4)	28(5)	28(4)	3(3)	8(3)	-3(3)
C67	25(4)	18(4)	27(4)	4(3)	-2(3)	0(3)
C66	22(4)	20(4)	26(4)	1(3)	10(3)	-7(3)
C57	28(5)	28(5)	26(4)	-3(4)	10(4)	-5(3)
C58	33(5)	55(6)	28(5)	-2(4)	10(4)	-11(4)
C59	44(6)	54(6)	27(5)	-1(5)	12(4)	-12(4)
C60	31(5)	37(5)	39(5)	2(4)	18(4)	-5(4)
C65	22(4)	22(4)	37(5)	2(3)	14(4)	1(4)
C64	24(4)	42(5)	37(5)	9(4)	10(4)	7(4)
C63	36(5)	64(7)	48(6)	10(5)	8(4)	17(5)
C62	27(5)	81(8)	70(7)	16(5)	26(5)	13(6)

C61	40(6)	64(7)	45(6)	1(5)	24(5)	-3(5)
C69	19(4)	34(5)	28(4)	0(3)	2(3)	0(4)
C70	30(5)	39(5)	27(5)	3(4)	-4(4)	7(4)
C71	36(5)	46(5)	22(4)	0(4)	8(4)	1(4)
C72	21(4)	32(5)	29(4)	-6(3)	4(3)	8(4)
C18	18(4)	14(4)	36(5)	2(3)	11(3)	2(3)
C19	17(4)	15(4)	24(4)	1(3)	1(3)	7(3)
C20	18(4)	17(4)	38(5)	0(3)	8(3)	11(3)
C25	22(4)	30(5)	39(5)	3(4)	4(4)	14(4)
C24	21(4)	46(6)	43(5)	0(4)	-7(4)	13(4)
C23	10(4)	44(6)	62(6)	1(4)	0(4)	5(5)
C22	20(4)	43(5)	46(5)	-2(4)	11(4)	1(4)
C21	19(4)	30(5)	39(5)	1(3)	3(4)	3(4)
C26	37(5)	61(6)	27(5)	6(5)	-3(4)	22(4)
C27	26(4)	60(6)	23(4)	14(4)	5(3)	17(4)
C28	22(4)	26(4)	31(4)	0(3)	4(3)	12(4)
C17	24(4)	15(4)	18(4)	-1(3)	2(3)	3(3)
C12	26(4)	18(4)	21(4)	6(3)	6(3)	4(3)
C11	21(4)	23(4)	17(4)	5(3)	0(3)	-1(3)
C10	16(4)	17(4)	31(4)	-1(3)	3(3)	2(3)
C2	32(5)	28(4)	21(4)	-1(4)	9(3)	5(3)
C3	18(4)	29(5)	46(5)	-2(3)	20(4)	2(4)
C4	18(4)	22(4)	40(5)	-1(3)	4(4)	0(4)
C9	25(4)	21(4)	28(4)	2(3)	-3(3)	0(3)
C8	26(5)	37(5)	42(5)	-4(4)	-9(4)	7(4)
C7	42(6)	42(6)	47(6)	2(4)	-12(5)	3(5)
C6	16(4)	42(6)	66(7)	0(4)	-19(4)	4(5)
C5	20(4)	34(5)	57(6)	-6(4)	7(4)	-1(4)
C13	27(4)	35(5)	25(4)	0(4)	1(4)	-3(4)
C14	46(6)	57(6)	22(5)	0(5)	7(4)	-2(4)
C15	43(5)	36(5)	33(5)	11(4)	21(4)	5(4)
C16	31(5)	29(5)	29(5)	10(4)	15(4)	7(4)
C39	8(4)	18(4)	36(5)	0(3)	-3(3)	-1(3)
C38	16(4)	23(4)	30(4)	4(3)	8(3)	-3(3)
C29	13(4)	25(4)	31(4)	-3(3)	9(3)	-8(3)
C30	21(4)	32(5)	31(5)	-4(4)	12(3)	-4(4)
C31	31(5)	33(5)	40(5)	-6(4)	20(4)	-4(4)
C32	22(4)	21(4)	55(6)	-1(3)	18(4)	-6(4)
C37	17(4)	21(4)	44(5)	2(3)	6(4)	-6(4)
C36	22(5)	37(5)	56(6)	0(4)	7(4)	-3(4)
C35	10(4)	61(7)	84(8)	1(4)	4(5)	-8(6)
C34	16(5)	44(6)	85(8)	1(4)	18(5)	1(5)
C33	33(5)	41(6)	69(7)	-4(4)	27(5)	4(5)
C46	33(5)	15(4)	19(4)	9(3)	11(3)	-1(3)
C47	15(4)	11(4)	32(4)	-2(3)	10(3)	2(3)
C56	10(4)	16(4)	29(4)	-2(3)	6(3)	3(3)
C55	15(4)	22(4)	32(4)	-2(3)	4(3)	5(3)
C54	16(4)	27(5)	48(5)	1(3)	-2(4)	0(4)
C53	19(4)	15(4)	56(6)	0(3)	12(4)	0(4)

C52	20(5)	36(5)	75(7)	6(4)	15(5)	9(5)
C51	27(5)	59(7)	83(8)	8(5)	34(5)	16(6)
C50	45(6)	56(6)	61(7)	10(5)	40(5)	13(5)
C49	35(5)	28(5)	39(5)	3(4)	16(4)	3(4)
C48	18(4)	12(4)	43(5)	2(3)	13(4)	6(3)
C44	30(5)	35(5)	27(4)	10(4)	4(4)	8(4)
C43	59(6)	50(6)	15(4)	11(5)	-1(4)	6(4)
C42	42(6)	52(6)	38(5)	10(5)	-16(4)	9(5)
C41	29(5)	41(5)	33(5)	4(4)	-1(4)	0(4)
O7	38(3)	54(4)	24(3)	4(3)	-2(3)	10(3)

Table SI27 Bond Lengths for Dy2L3_Final.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Dy1	O6	2.202(5)	C63	C62	1.389(13)
Dy1	N6	2.446(6)	C62	C61	1.353(13)
Dy1	O5	2.197(5)	C69	C70	1.375(10)
Dy1	O3	2.343(5)	C70	C71	1.389(11)
Dy1	O4	2.324(5)	C71	C72	1.366(10)
Dy1	N5	2.448(6)	C18	C19	1.431(10)
Dy1	O7	2.434(5)	C19	C20	1.445(10)
Dy2	O1	2.255(5)	C19	C28	1.405(10)
Dy2	O2	2.263(5)	C20	C25	1.417(11)
Dy2	N1	2.469(6)	C20	C21	1.405(10)
Dy2	O3	2.345(5)	C25	C24	1.415(10)
Dy2	N4	2.525(6)	C25	C26	1.415(11)
Dy2	O4	2.365(5)	C24	C23	1.353(12)
Dy2	N2	2.464(6)	C23	C22	1.398(12)
Dy2	N3	2.554(6)	C22	C21	1.370(10)
O1	C1	1.309(8)	C26	C27	1.371(11)
O6	C84	1.308(8)	C27	C28	1.433(10)
N6	C74	1.302(9)	C17	C12	1.391(10)
N6	C73	1.415(9)	C17	C16	1.404(10)
O5	C57	1.298(9)	C12	C13	1.398(10)
O2	C28	1.316(8)	C11	C10	1.432(10)
N1	C12	1.417(9)	C10	C1	1.409(10)
N1	C11	1.301(9)	C10	C9	1.453(10)
O3	C29	1.331(8)	C1	C2	1.433(10)
N4	C45	1.407(9)	C2	C3	1.356(10)
N4	C46	1.295(9)	C3	C4	1.409(11)
O4	C56	1.335(8)	C4	C9	1.414(10)
C85	O7	1.465(14)	C4	C5	1.412(10)
N5	C68	1.430(9)	C9	C8	1.410(11)
N5	C67	1.291(9)	C8	C7	1.378(11)
N2	C18	1.290(9)	C7	C6	1.396(13)
N2	C17	1.423(9)	C6	C5	1.344(12)
N3	C40	1.425(9)	C13	C14	1.371(11)
N3	C39	1.282(9)	C14	C15	1.381(12)
C40	C45	1.402(10)	C15	C16	1.375(11)
C40	C41	1.389(10)	C39	C38	1.442(10)

C45	C44	1.403(10)	C38	C29	1.389(10)
C84	C83	1.428(10)	C38	C37	1.459(10)
C84	C75	1.405(10)	C29	C30	1.426(10)
C83	C82	1.349(11)	C30	C31	1.350(10)
C82	C81	1.416(11)	C31	C32	1.411(11)
C81	C80	1.415(11)	C32	C37	1.415(11)
C81	C76	1.414(11)	C32	C33	1.423(11)
C80	C79	1.363(12)	C37	C36	1.412(11)
C79	C78	1.386(12)	C36	C35	1.376(11)
C78	C77	1.374(11)	C35	C34	1.392(13)
C77	C76	1.418(11)	C34	C33	1.365(13)
C76	C75	1.445(10)	C46	C47	1.454(10)
C75	C74	1.436(10)	C47	C56	1.398(10)
C73	C68	1.405(10)	C47	C48	1.439(9)
C73	C72	1.398(10)	C56	C55	1.416(10)
C68	C69	1.395(10)	C55	C54	1.360(10)
C67	C66	1.439(10)	C54	C53	1.418(11)
C66	C57	1.405(10)	C53	C52	1.415(11)
C66	C65	1.451(10)	C53	C48	1.429(11)
C57	C58	1.435(11)	C52	C51	1.349(13)
C58	C59	1.344(11)	C51	C50	1.398(14)
C59	C60	1.410(12)	C50	C49	1.372(11)
C60	C65	1.418(11)	C49	C48	1.417(11)
C60	C61	1.408(11)	C44	C43	1.376(11)
C65	C64	1.401(11)	C43	C42	1.383(12)
C64	C63	1.370(11)	C42	C41	1.380(12)

Table SI28 Bond Angles for Dy2L3_Final.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N6	Dy1	O6	73.62(18)	C65	C66	C57	120.7(6)
O5	Dy1	O6	92.19(19)	C66	C57	O5	123.8(6)
O5	Dy1	N6	122.98(19)	C58	C57	O5	119.0(7)
O3	Dy1	O6	161.84(18)	C58	C57	C66	117.2(7)
O3	Dy1	N6	115.03(17)	C59	C58	C57	122.2(8)
O3	Dy1	O5	95.45(17)	C60	C59	C58	122.2(8)
O4	Dy1	O6	97.64(17)	C65	C60	C59	118.5(7)
O4	Dy1	N6	77.02(17)	C61	C60	C59	122.5(8)
O4	Dy1	O5	159.69(18)	C61	C60	C65	119.0(8)
O4	Dy1	O3	70.37(15)	C60	C65	C66	119.1(7)
N5	Dy1	O6	118.2(2)	C64	C65	C66	124.0(7)
N5	Dy1	N6	66.32(18)	C64	C65	C60	116.9(7)
N5	Dy1	O5	74.02(18)	C63	C64	C65	123.0(8)
N5	Dy1	O3	79.85(17)	C62	C63	C64	119.2(9)
N5	Dy1	O4	115.84(17)	C61	C62	C63	120.0(8)
O7	Dy1	O6	87.10(19)	C62	C61	C60	121.9(8)
O7	Dy1	N6	142.81(18)	C70	C69	C68	121.2(7)
O7	Dy1	O5	88.50(19)	C71	C70	C69	119.7(7)
O7	Dy1	O3	76.67(18)	C72	C71	C70	119.7(7)
O7	Dy1	O4	74.37(17)	C71	C72	C73	122.0(7)

O7	Dy1	N5	149.14(18)	C19	C18	N2	128.4(7)
O2	Dy2	O1	83.80(17)	C20	C19	C18	118.0(6)
N1	Dy2	O1	71.95(17)	C28	C19	C18	122.0(6)
N1	Dy2	O2	119.95(19)	C28	C19	C20	119.9(6)
O3	Dy2	O1	80.65(16)	C25	C20	C19	119.9(7)
O3	Dy2	O2	92.98(17)	C21	C20	C19	123.2(7)
O3	Dy2	N1	133.25(17)	C21	C20	C25	116.9(7)
N4	Dy2	O1	144.41(17)	C24	C25	C20	119.8(7)
N4	Dy2	O2	129.67(17)	C26	C25	C20	118.9(7)
N4	Dy2	N1	79.32(18)	C26	C25	C24	121.3(7)
N4	Dy2	O3	105.63(17)	C23	C24	C25	121.2(8)
O4	Dy2	O1	142.11(16)	C22	C23	C24	119.6(7)
O4	Dy2	O2	75.08(18)	C21	C22	C23	120.2(8)
O4	Dy2	N1	145.94(17)	C22	C21	C20	122.2(8)
O4	Dy2	O3	69.64(15)	C27	C26	C25	120.8(7)
O4	Dy2	N4	68.91(16)	C28	C27	C26	122.1(7)
N2	Dy2	O1	110.59(17)	C19	C28	O2	124.4(7)
N2	Dy2	O2	74.05(18)	C27	C28	O2	117.6(7)
N2	Dy2	N1	65.48(18)	C27	C28	C19	118.0(7)
N2	Dy2	O3	161.25(17)	C12	C17	N2	117.0(6)
N2	Dy2	N4	74.36(17)	C16	C17	N2	123.5(6)
N2	Dy2	O4	93.56(17)	C16	C17	C12	119.4(7)
N3	Dy2	O1	88.18(17)	C17	C12	N1	116.4(6)
N3	Dy2	O2	161.36(18)	C13	C12	N1	124.4(7)
N3	Dy2	N1	72.86(18)	C13	C12	C17	119.0(6)
N3	Dy2	O3	69.06(17)	C10	C11	N1	125.6(6)
N3	Dy2	N4	63.13(17)	C1	C10	C11	121.2(6)
N3	Dy2	O4	101.98(17)	C9	C10	C11	119.1(6)
N3	Dy2	N2	124.58(18)	C9	C10	C1	119.6(6)
C1	O1	Dy2	128.9(4)	C10	C1	O1	123.2(6)
C84	O6	Dy1	132.8(4)	C2	C1	O1	118.9(6)
C74	N6	Dy1	125.7(5)	C2	C1	C10	117.8(6)
C73	N6	Dy1	114.6(4)	C3	C2	C1	122.0(7)
C73	N6	C74	119.3(6)	C4	C3	C2	121.7(7)
C57	O5	Dy1	137.4(5)	C9	C4	C3	118.5(7)
C28	O2	Dy2	135.8(4)	C5	C4	C3	121.3(7)
C12	N1	Dy2	114.2(4)	C5	C4	C9	120.1(7)
C11	N1	Dy2	125.9(5)	C4	C9	C10	120.0(7)
C11	N1	C12	119.7(6)	C8	C9	C10	122.5(7)
Dy2	O3	Dy1	109.89(17)	C8	C9	C4	117.5(7)
C29	O3	Dy1	126.3(4)	C7	C8	C9	120.6(8)
C29	O3	Dy2	122.5(4)	C6	C7	C8	121.1(8)
C45	N4	Dy2	116.8(4)	C5	C6	C7	119.7(8)
C46	N4	Dy2	123.0(5)	C6	C5	C4	121.1(8)
C46	N4	C45	119.9(6)	C14	C13	C12	120.9(7)
Dy2	O4	Dy1	109.88(18)	C15	C14	C13	120.1(8)
C56	O4	Dy1	132.1(4)	C16	C15	C14	120.1(7)
C56	O4	Dy2	117.9(4)	C15	C16	C17	120.4(7)
C68	N5	Dy1	115.2(4)	C38	C39	N3	125.7(7)

C67	N5	Dy1	127.1(5)	C29	C38	C39	121.3(6)
C67	N5	C68	117.6(6)	C37	C38	C39	118.7(6)
C18	N2	Dy2	128.0(5)	C37	C38	C29	120.0(7)
C17	N2	Dy2	113.6(4)	C38	C29	O3	122.0(6)
C17	N2	C18	118.4(6)	C30	C29	O3	118.9(6)
C40	N3	Dy2	114.9(4)	C30	C29	C38	119.1(6)
C39	N3	Dy2	125.7(5)	C31	C30	C29	121.3(7)
C39	N3	C40	119.3(6)	C32	C31	C30	121.6(7)
C45	C40	N3	116.3(6)	C37	C32	C31	119.3(7)
C41	C40	N3	123.5(7)	C33	C32	C31	121.2(8)
C41	C40	C45	120.2(7)	C33	C32	C37	119.5(8)
C40	C45	N4	116.4(6)	C32	C37	C38	118.6(7)
C44	C45	N4	124.8(6)	C36	C37	C38	123.1(7)
C44	C45	C40	118.7(7)	C36	C37	C32	118.3(7)
C83	C84	O6	118.7(7)	C35	C36	C37	120.5(9)
C75	C84	O6	123.9(6)	C34	C35	C36	121.2(9)
C75	C84	C83	117.4(7)	C33	C34	C35	119.8(8)
C82	C83	C84	122.4(8)	C34	C33	C32	120.6(9)
C81	C82	C83	121.3(7)	C47	C46	N4	125.2(6)
C80	C81	C82	121.8(7)	C56	C47	C46	120.3(6)
C76	C81	C82	118.7(7)	C48	C47	C46	119.3(6)
C76	C81	C80	119.4(8)	C48	C47	C56	120.3(6)
C79	C80	C81	121.6(8)	C47	C56	O4	121.9(6)
C78	C79	C80	119.2(8)	C55	C56	O4	119.1(6)
C77	C78	C79	121.1(8)	C55	C56	C47	119.0(6)
C76	C77	C78	121.3(8)	C54	C55	C56	122.1(7)
C77	C76	C81	117.3(7)	C53	C54	C55	120.5(7)
C75	C76	C81	119.3(7)	C52	C53	C54	121.6(8)
C75	C76	C77	123.4(7)	C48	C53	C54	119.3(7)
C76	C75	C84	120.4(6)	C48	C53	C52	119.0(8)
C74	C75	C84	120.8(6)	C51	C52	C53	121.7(9)
C74	C75	C76	118.8(7)	C50	C51	C52	119.3(8)
C75	C74	N6	127.4(7)	C49	C50	C51	121.7(9)
C68	C73	N6	117.3(6)	C48	C49	C50	120.2(8)
C72	C73	N6	124.6(6)	C53	C48	C47	118.7(7)
C72	C73	C68	118.0(7)	C49	C48	C47	123.3(7)
C73	C68	N5	115.8(6)	C49	C48	C53	117.9(7)
C69	C68	N5	124.8(6)	C43	C44	C45	120.8(8)
C69	C68	C73	119.3(7)	C42	C43	C44	119.7(8)
C66	C67	N5	128.2(7)	C41	C42	C43	120.8(8)
C57	C66	C67	121.1(6)	C42	C41	C40	119.8(8)
C65	C66	C67	118.0(7)				

Table SI29 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Dy2L3_Final.

Atom	*x*	*y*	*z*	U(eq)
H85a	2890(40)	5220(40)	5080(20)	163(7)
H85b	3180(60)	4503(15)	4912(12)	163(7)
H85c	3780(20)	5030(50)	5237(13)	163(7)
H83	5202(5)	6875(4)	4530(4)	43(2)

H82	6340(4)	7119(4)	4150(4)	41(2)
H80	7118(4)	7282(4)	3228(5)	43(3)
H79	7204(5)	7381(4)	2123(5)	55(3)
H78	6104(5)	7240(4)	1382(5)	49(3)
H77	4922(5)	7044(4)	1741(4)	41(2)
H74	3889(4)	7184(3)	2131(4)	27(2)
H67	736(4)	6891(3)	2913(4)	28(2)
H58	1663(5)	6407(4)	5388(4)	46(3)
H59	418(5)	6524(4)	5573(4)	49(3)
H64	-365(4)	6686(4)	3034(4)	41(2)
H63	-1631(5)	6756(5)	3243(5)	59(3)
H62	-1925(5)	6761(5)	4325(5)	70(3)
H61	-966(5)	6632(5)	5168(5)	58(3)
H69	681(4)	6732(4)	1947(4)	33(2)
H70	848(5)	6958(4)	869(4)	39(2)
H71	2094(5)	7057(4)	561(4)	41(2)
H72	3146(4)	6935(4)	1331(4)	32(2)
H18	4753(4)	3499(3)	2016(4)	26(2)
H24	6931(4)	3503(4)	4355(4)	45(3)
H23	7720(4)	3457(4)	3537(4)	47(3)
H22	7195(4)	3585(4)	2443(4)	43(2)
H21	5890(4)	3731(4)	2186(4)	35(2)
H26	5640(5)	3657(5)	4717(4)	50(3)
H27	4353(4)	3894(4)	4479(4)	43(3)
H11	1451(4)	3237(3)	1138(3)	24(2)
H2	766(4)	3478(4)	3542(4)	32(2)
H3	-483(4)	3278(4)	3149(4)	36(2)
H8	308(5)	3421(4)	751(4)	43(3)
H7	-986(5)	3282(4)	391(5)	54(3)
H6	-1901(5)	3201(4)	1135(5)	52(3)
H5	-1516(4)	3222(4)	2234(4)	44(3)
H13	2014(4)	3515(4)	336(4)	35(2)
H14	2913(5)	3475(5)	-407(4)	50(3)
H15	4217(5)	3604(4)	-54(4)	43(3)
H16	4622(5)	3781(4)	1044(4)	35(2)
H39	581(4)	5390(3)	1879(4)	26(2)
H30	1605(4)	4930(4)	4342(4)	33(2)
H31	357(4)	4850(4)	4555(4)	40(2)
H36	-524(4)	5055(4)	2018(5)	46(3)
H35	-1772(5)	4925(5)	2270(5)	62(3)
H34	-2038(5)	4868(4)	3354(5)	57(3)
H33	-1039(5)	4833(4)	4190(5)	55(3)
H46	3743(4)	5611(3)	1144(3)	26(2)
H55	4837(4)	5410(3)	3613(4)	27(2)
H54	6058(4)	5459(4)	3311(4)	37(2)
H52	6934(5)	5453(4)	2441(5)	52(3)
H51	7132(5)	5370(5)	1364(5)	65(3)
H50	6079(5)	5258(5)	564(5)	62(3)
H49	4833(5)	5247(4)	834(4)	40(2)

H44	3015(5)	5367(4)	310(4)	37(2)
H43	1960(5)	5435(4)	-480(4)	50(3)
H42	723(5)	5279(5)	-191(4)	55(3)
H41	527(5)	5080(4)	889(4)	41(2)
H7a	3501(3)	4835(3)	4067(2)	59(2)

Table SI30 Solvent masks information for Dy2L3_Final.

Number	X	Y	Z	Volume	Electron count	Content
1	0.347	0.204	0.465	322.5	105.0	2DCM/1H2O
2	0.347	0.296	0.965	322.5	101.1	2DCM/1H2O
3	-0.347	0.704	0.035	322.5	102.0	2DCM/1H2O
4	-0.347	0.796	0.535	322.5	98.2	2DCM/1H2O

Refinement model description

Number of restraints - 0, number of constraints - 114.

Tb2L3_final

Table SI31 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Tb2L3_final. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Tb1	2254.28(13)	4429.63(12)	2434.26(11)	20.82(6)
Tb2	2083.24(13)	6030.80(12)	1446.19(11)	22.83(7)
C40	3356(2)	5132(2)	3720(2)	17.3(9)
C68	3170(3)	6724(2)	2683(2)	23.5(10)
N3	3406(2)	5014(2)	3053.0(19)	22.6(9)
N5	3224(2)	6575(2)	2012(2)	22.4(8)
O1	3100.1(19)	3703.5(18)	2085.2(17)	26.5(8)
C29	3602(3)	5042(2)	1635(2)	21.8(10)
C38	4192(3)	5073(2)	2151(3)	25.4(11)
O2	1419(2)	4009(2)	1611.0(18)	35.2(9)
O4	1433.6(18)	5316.9(17)	2083.2(16)	22.7(7)
N2	1243(2)	3858(2)	2959(2)	23.5(9)
O3	2864.3(18)	5116.0(17)	1738.5(16)	23.1(7)
C45	2591(3)	5214(2)	3905(2)	26.3(11)
C56	740(3)	5341(2)	2296(3)	22.9(10)
C65	4865(3)	6636(3)	1023(3)	29.0(11)
C46	1310(3)	5386(2)	3447(2)	23.8(10)
C73	2428(3)	6791(2)	2874(2)	23.1(10)
C74	1138(3)	6958(3)	2460(3)	26.7(11)
O6	1069(2)	6635(2)	1090.6(18)	33.1(9)
N1	2738(2)	3718(2)	3368.5(19)	23.8(9)
C47	652(3)	5346(2)	2958(3)	24(1)
O5	2772(2)	6374(2)	677.6(17)	32.8(9)
C54	-637(3)	5412(3)	2012(3)	33.8(13)
C21	-1100(3)	3671(3)	2382(3)	33.0(12)
C37	4989(3)	5021(3)	2023(3)	31.3(12)
C77	-366(3)	7087(3)	2948(3)	35.9(13)
C18	556(3)	3689(2)	2704(3)	26.0(11)
C28	684(3)	3871(3)	1523(3)	28.6(11)
C41	3960(3)	5152(3)	4207(3)	37.8(14)
C19	238(3)	3768(2)	2040(3)	25.5(11)
C1	3800(3)	3558(2)	2347(3)	26.5(11)
C66	4058(3)	6585(3)	1137(3)	26.4(11)
C72	2339(3)	6901(3)	3532(3)	29.6(11)
C9	4793(3)	3380(3)	3271(3)	30.8(12)
C10	3998(3)	3483(2)	3019(3)	26.5(11)
C60	5061(3)	6618(3)	373(3)	37.5(13)
C17	1441(3)	3730(3)	3637(2)	25.7(10)
C20	-587(3)	3676(3)	1894(3)	26.9(11)
C44	2488(4)	5316(3)	4558(3)	35.5(13)
C76	-284(3)	7052(2)	2271(3)	28.6(11)
C30	3788(3)	4950(3)	994(3)	31.9(12)
C4	5357(3)	3325(3)	2832(3)	31.6(12)
C82	-915(3)	7047(3)	1155(3)	36.8(13)

C12	2230(3)	3652(2)	3857(2)	24.8(10)
C11	3422(3)	3453(3)	3466(3)	26.7(11)
C67	3877(3)	6698(2)	1786(3)	27.1(11)
C53	-763(3)	5398(3)	2679(3)	34.3(13)
C81	-968(3)	7104(3)	1833(3)	32.9(12)
C34	6514(3)	4889(3)	1733(4)	53.6(19)
C26	-438(3)	3678(3)	729(3)	42.7(15)
C16	913(3)	3719(3)	4096(3)	34.1(13)
C57	3490(3)	6475(3)	607(3)	31.0(12)
C69	3804(3)	6780(3)	3156(3)	31.3(12)
C48	-114(3)	5356(3)	3161(3)	31.8(12)
C36	5617(3)	5009(3)	2527(3)	42.1(15)
C31	4536(3)	4903(3)	867(3)	33.1(12)
C64	5475(3)	6678(3)	1531(3)	38.0(14)
C59	4467(4)	6540(4)	-146(3)	45.5(16)
C55	81(3)	5383(2)	1826(3)	28.0(11)
C78	-1063(4)	7199(3)	3170(4)	44.7(15)
C32	5148(3)	4944(3)	1372(3)	33.5(13)
C3	5123(3)	3342(3)	2154(3)	34.9(13)
C84	450(3)	6817(3)	1349(3)	29.8(12)
C13	2460(3)	3568(3)	4517(3)	35.5(13)
C42	3852(4)	5266(3)	4854(3)	45.9(16)
C58	3719(4)	6468(3)	-35(3)	39.7(14)
C83	-245(3)	6902(3)	922(3)	38.2(14)
C75	440(3)	6929(2)	2020(3)	27.3(11)
C15	1151(4)	3620(3)	4752(3)	43.6(15)
C2	4374(3)	3453(3)	1919(3)	30.8(12)
C25	-923(3)	3618(3)	1233(3)	33.1(12)
C24	-1726(3)	3527(3)	1093(3)	39.5(14)
C27	322(3)	3802(3)	867(3)	42.3(16)
C70	3711(3)	6908(3)	3804(3)	36.2(13)
C63	6223(4)	6718(4)	1407(4)	53.2(19)
C71	2974(3)	6964(3)	3988(3)	38.5(14)
C23	-2190(3)	3510(3)	1579(3)	40.8(14)
C5	6145(3)	3252(3)	3080(4)	43.5(16)
C8	5054(3)	3368(3)	3949(3)	39.1(14)
C14	1927(4)	3543(3)	4960(3)	46.0(16)
C7	5823(4)	3295(3)	4166(4)	50.9(18)
C43	3109(4)	5351(3)	5025(3)	46.0(16)
C35	6354(3)	4942(4)	2377(4)	55.6(19)
C33	5927(3)	4883(3)	1241(4)	47.5(17)
C62	6407(4)	6715(4)	762(4)	61(2)
C6	6377(3)	3242(3)	3734(4)	50.6(18)
C22	-1882(3)	3592(3)	2231(3)	40.1(14)
C61	5842(4)	6663(4)	263(4)	54.9(19)
O7	1538(3)	5174(2)	694(2)	46.6(11)
C80	-1680(3)	7225(3)	2079(4)	44.9(16)
C52	-1509(4)	5407(3)	2879(4)	52.9(19)
C79	-1729(4)	7280(3)	2735(4)	46.8(16)

C51	-1619(4)	5355(4)	3516(5)	64(2)
C49	-252(4)	5289(3)	3822(3)	41.7(15)
C50	-988(4)	5292(4)	3992(4)	57(2)
N4	1984(2)	5139(2)	3391(2)	23.4(9)
N6	1803(2)	6718(2)	2371(2)	23.1(9)
C39	4026(3)	5180(2)	2822(3)	27.0(11)
C85	1670(6)	4966(5)	55(5)	84(3)

Table SI32 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Tb2L3_final. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Tb1	15.23(11)	25.90(12)	21.42(12)	-0.63(9)	2.45(8)	-1.04(9)
Tb2	18.78(12)	27.82(13)	21.82(12)	2.67(9)	2.00(9)	0.54(9)
C40	12(2)	25(2)	13(2)	-4.0(17)	-5.8(16)	-1.1(17)
C68	22(2)	26(3)	22(2)	-3(2)	0.4(19)	0.5(19)
N3	19(2)	28(2)	20(2)	0.7(17)	0.2(16)	1.3(17)
N5	21(2)	22(2)	25(2)	1.2(16)	3.3(16)	0.8(16)
O1	21.3(17)	32(2)	26.0(18)	4.9(15)	1.3(14)	-4.6(15)
C29	15(2)	23(2)	28(3)	1.9(18)	6.1(19)	1.2(19)
C38	19(2)	21(2)	37(3)	-0.6(19)	7(2)	5(2)
O2	18.4(18)	59(3)	29(2)	-12.0(17)	5.2(15)	-16.8(18)
O4	17.6(16)	29.1(18)	22.1(17)	3.3(14)	5.1(13)	-1.1(14)
N2	22(2)	23(2)	26(2)	-2.7(17)	3.4(17)	-4.0(17)
O3	17.7(16)	30.5(19)	22.3(17)	2.2(14)	6.9(13)	3.5(14)
C45	32(3)	22(3)	24(3)	-4(2)	0(2)	1(2)
C56	15(2)	21(2)	32(3)	3.0(18)	1.5(19)	0(2)
C65	24(3)	24(3)	40(3)	-4(2)	8(2)	-2(2)
C46	23(2)	26(3)	24(2)	-3(2)	9.0(19)	-5(2)
C73	21(2)	18(2)	29(3)	1.2(18)	-1.4(19)	1.5(19)
C74	25(3)	27(3)	28(3)	4(2)	5(2)	-2(2)
O6	24.5(19)	48(2)	26.6(19)	14.8(17)	1.5(15)	3.4(17)
N1	28(2)	24(2)	19(2)	-5.4(17)	0.8(16)	2.9(16)
C47	19(2)	21(2)	33(3)	-0.8(19)	4(2)	-4(2)
O5	26.2(19)	48(2)	24.0(19)	0.7(17)	3.2(15)	6.3(17)
C54	18(2)	29(3)	53(4)	1(2)	-2(2)	-6(3)
C21	21(3)	39(3)	40(3)	-2(2)	4(2)	-2(2)
C37	14(2)	25(3)	54(4)	0(2)	2(2)	6(2)
C77	36(3)	32(3)	40(3)	3(2)	7(3)	0(2)
C18	22(2)	23(2)	33(3)	-4(2)	5(2)	-2(2)
C28	20(2)	32(3)	33(3)	-4(2)	2(2)	-9(2)
C41	32(3)	43(3)	36(3)	-7(3)	-8(2)	3(3)
C19	22(2)	19(2)	35(3)	-4.3(19)	3(2)	-4(2)
C1	27(3)	21(2)	33(3)	-2(2)	7(2)	-4(2)
C66	25(3)	28(3)	27(3)	-3(2)	5(2)	6(2)
C72	32(3)	32(3)	26(3)	4(2)	8(2)	-7(2)
C9	23(3)	26(3)	42(3)	0(2)	-2(2)	-1(2)
C10	29(3)	20(2)	31(3)	4(2)	5(2)	0(2)
C60	38(3)	37(3)	40(3)	-4(3)	15(3)	1(3)
C17	25(3)	28(3)	24(3)	-3(2)	5(2)	-2(2)

C20	20(2)	25(3)	35(3)	-2(2)	3(2)	-3(2)
C44	38(3)	41(3)	27(3)	-7(3)	4(2)	-2(2)
C76	24(3)	19(2)	42(3)	3(2)	4(2)	-2(2)
C30	28(3)	38(3)	31(3)	-1(2)	9(2)	-1(2)
C4	19(2)	27(3)	49(3)	2(2)	5(2)	1(2)
C82	27(3)	28(3)	54(4)	4(2)	-6(3)	3(3)
C12	31(3)	22(2)	23(2)	0(2)	7(2)	-0.7(19)
C11	24(3)	29(3)	26(3)	5(2)	-1(2)	1(2)
C67	26(3)	25(3)	30(3)	-4(2)	3(2)	-2(2)
C53	21(3)	24(3)	59(4)	0(2)	12(3)	-5(3)
C81	25(3)	25(3)	49(3)	4(2)	2(2)	3(2)
C34	18(3)	51(4)	95(6)	-1(3)	21(3)	-6(4)
C26	27(3)	65(4)	35(3)	-7(3)	0(2)	-22(3)
C16	28(3)	37(3)	39(3)	-9(2)	16(2)	-6(2)
C57	30(3)	38(3)	26(3)	1(2)	11(2)	5(2)
C69	24(3)	38(3)	31(3)	-1(2)	-1(2)	0(2)
C48	28(3)	24(3)	45(3)	-1(2)	15(2)	-4(2)
C36	15(3)	52(4)	59(4)	-1(2)	6(3)	10(3)
C31	30(3)	35(3)	37(3)	3(2)	16(2)	3(2)
C64	27(3)	46(4)	42(3)	-8(3)	9(2)	-8(3)
C59	46(4)	66(4)	28(3)	1(3)	18(3)	8(3)
C55	22(3)	25(3)	35(3)	0(2)	-3(2)	-3(2)
C78	38(3)	41(4)	58(4)	-1(3)	17(3)	-5(3)
C32	23(3)	25(3)	56(4)	1(2)	20(3)	-1(2)
C3	27(3)	34(3)	46(3)	8(2)	12(2)	2(3)
C84	25(3)	26(3)	38(3)	11(2)	0(2)	-2(2)
C13	33(3)	51(4)	24(3)	-1(3)	4(2)	1(2)
C42	46(4)	58(4)	28(3)	-7(3)	-20(3)	-1(3)
C58	37(3)	60(4)	22(3)	2(3)	5(2)	9(3)
C83	34(3)	44(3)	35(3)	11(3)	-2(2)	2(3)
C75	26(3)	20(2)	35(3)	6(2)	3(2)	2(2)
C15	46(4)	55(4)	33(3)	-9(3)	21(3)	-1(3)
C2	35(3)	27(3)	31(3)	5(2)	7(2)	1(2)
C25	22(3)	36(3)	41(3)	-2(2)	2(2)	-8(2)
C24	25(3)	46(4)	46(4)	-4(3)	-4(2)	-8(3)
C27	24(3)	70(5)	31(3)	-7(3)	1(2)	-20(3)
C70	24(3)	52(4)	30(3)	-3(3)	-7(2)	-4(3)
C63	24(3)	79(5)	57(4)	-17(3)	6(3)	-16(4)
C71	40(3)	48(4)	27(3)	5(3)	3(2)	-4(3)
C23	17(3)	49(4)	56(4)	-6(2)	-2(3)	-3(3)
C5	20(3)	35(3)	75(5)	2(2)	2(3)	5(3)
C8	34(3)	41(3)	41(3)	2(3)	-3(3)	4(3)
C14	51(4)	60(4)	28(3)	-3(3)	13(3)	7(3)
C7	34(3)	53(4)	61(4)	-3(3)	-17(3)	-3(3)
C43	63(4)	47(4)	27(3)	-10(3)	1(3)	-1(3)
C35	16(3)	65(5)	85(6)	-6(3)	2(3)	3(4)
C33	23(3)	47(4)	77(5)	5(3)	23(3)	-5(3)
C62	28(3)	94(6)	63(5)	-16(4)	23(3)	-10(4)
C6	19(3)	55(4)	72(5)	0(3)	-19(3)	1(4)

C22	28(3)	43(3)	51(4)	-1(3)	11(3)	2(3)
C61	40(4)	80(5)	49(4)	-7(4)	23(3)	-1(4)
O7	50(3)	57(3)	33(2)	-11(2)	2(2)	-14(2)
C80	26(3)	32(3)	76(5)	4(2)	7(3)	6(3)
C52	21(3)	51(4)	88(6)	0(3)	14(3)	-16(4)
C79	30(3)	46(4)	68(5)	3(3)	19(3)	-6(3)
C51	27(3)	63(5)	106(7)	-5(3)	32(4)	-15(5)
C49	37(3)	41(3)	51(4)	-2(3)	21(3)	-11(3)
C50	55(4)	54(4)	69(5)	-2(4)	40(4)	-12(4)
N4	27(2)	23(2)	21(2)	-4.5(17)	7.1(17)	-1.2(16)
N6	21(2)	24(2)	25(2)	2.9(16)	1.2(16)	-0.0(17)
C39	19(2)	24(3)	37(3)	-5(2)	-1(2)	4(2)

Table SI33 Bond Lengths for Tb2L3_final.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Tb1	N3	2.558(4)	C41	C42	1.388(9)
Tb1	O1	2.273(3)	C19	C20	1.454(7)
Tb1	O2	2.279(3)	C1	C10	1.396(7)
Tb1	O4	2.379(3)	C1	C2	1.426(7)
Tb1	N2	2.472(4)	C66	C67	1.429(7)
Tb1	O3	2.350(3)	C66	C57	1.410(7)
Tb1	N1	2.487(4)	C72	C71	1.379(8)
Tb1	N4	2.538(4)	C9	C10	1.443(7)
Tb2	N5	2.462(4)	C9	C4	1.416(8)
Tb2	O4	2.344(3)	C9	C8	1.421(8)
Tb2	O3	2.359(3)	C10	C11	1.442(7)
Tb2	O6	2.220(3)	C60	C59	1.413(9)
Tb2	O5	2.211(4)	C60	C61	1.413(8)
Tb2	O7	2.464(4)	C17	C12	1.413(7)
Tb2	N6	2.463(4)	C17	C16	1.395(7)
C40	N3	1.407(6)	C20	C25	1.426(8)
C40	C45	1.443(7)	C44	C43	1.371(8)
C40	C41	1.374(7)	C76	C81	1.420(7)
C68	N5	1.429(6)	C76	C75	1.443(7)
C68	C73	1.406(7)	C30	C31	1.368(7)
C68	C69	1.398(7)	C4	C3	1.412(8)
N3	C39	1.279(6)	C4	C5	1.423(7)
N5	C67	1.306(6)	C82	C81	1.416(9)
O1	C1	1.316(6)	C82	C83	1.349(8)
C29	C38	1.398(7)	C12	C13	1.385(7)
C29	O3	1.340(5)	C53	C48	1.424(8)
C29	C30	1.407(7)	C53	C52	1.412(8)
C38	C37	1.453(7)	C81	C80	1.419(8)
C38	C39	1.462(7)	C34	C35	1.391(11)
O2	C28	1.310(6)	C34	C33	1.360(10)
O4	C56	1.337(6)	C26	C25	1.419(8)
N2	C18	1.302(6)	C26	C27	1.352(8)
N2	C17	1.425(6)	C16	C15	1.384(8)
C45	C44	1.394(7)	C57	C58	1.425(7)

C45	N4	1.421(6)	C69	C70	1.388(8)
C56	C47	1.391(7)	C48	C49	1.418(8)
C56	C55	1.422(7)	C36	C35	1.367(8)
C65	C66	1.460(7)	C31	C32	1.409(8)
C65	C60	1.420(8)	C64	C63	1.364(8)
C65	C64	1.410(8)	C59	C58	1.361(8)
C46	C47	1.444(7)	C78	C79	1.398(9)
C46	N4	1.300(6)	C32	C33	1.425(7)
C73	C72	1.399(7)	C3	C2	1.363(8)
C73	N6	1.427(6)	C84	C83	1.430(7)
C74	C75	1.438(7)	C84	C75	1.403(8)
C74	N6	1.296(6)	C13	C14	1.378(8)
O6	C84	1.313(6)	C42	C43	1.395(10)
N1	C12	1.422(6)	C15	C14	1.384(9)
N1	C11	1.310(6)	C25	C24	1.414(7)
C47	C48	1.447(7)	C24	C23	1.360(9)
O5	C57	1.297(6)	C70	C71	1.389(8)
C54	C53	1.417(9)	C63	C62	1.403(10)
C54	C55	1.355(7)	C23	C22	1.399(9)
C21	C20	1.423(7)	C5	C6	1.363(10)
C21	C22	1.378(8)	C8	C7	1.377(8)
C37	C36	1.424(8)	C7	C6	1.392(10)
C37	C32	1.408(8)	C62	C61	1.347(10)
C77	C76	1.420(8)	O7	C85	1.427(10)
C77	C78	1.370(8)	C80	C79	1.368(10)
C18	C19	1.428(7)	C52	C51	1.352(11)
C28	C19	1.407(7)	C51	C50	1.397(11)
C28	C27	1.433(7)	C49	C50	1.373(8)

Table SI34 Bond Angles for Tb2L3_final.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O1	Tb1	N3	87.71(13)	C28	C19	C18	123.7(5)
O2	Tb1	N3	161.95(13)	C20	C19	C18	117.1(5)
O2	Tb1	O1	84.37(13)	C20	C19	C28	119.0(5)
O4	Tb1	N3	101.99(12)	C10	C1	O1	123.2(5)
O4	Tb1	O1	142.84(12)	C2	C1	O1	117.9(5)
O4	Tb1	O2	75.47(14)	C2	C1	C10	118.9(5)
N2	Tb1	N3	124.53(13)	C67	C66	C65	117.4(5)
N2	Tb1	O1	110.59(13)	C57	C66	C65	119.8(5)
N2	Tb1	O2	73.51(13)	C57	C66	C67	122.7(5)
N2	Tb1	O4	93.36(13)	C71	C72	C73	120.4(5)
O3	Tb1	N3	68.71(12)	C4	C9	C10	119.6(5)
O3	Tb1	O1	80.94(12)	C8	C9	C10	123.1(5)
O3	Tb1	O2	93.98(13)	C8	C9	C4	117.2(5)
O3	Tb1	O4	69.90(11)	C9	C10	C1	119.6(5)
O3	Tb1	N2	161.48(13)	C11	C10	C1	121.7(5)
N1	Tb1	N3	73.11(13)	C11	C10	C9	118.5(5)
N1	Tb1	O1	71.56(13)	C59	C60	C65	118.7(5)
N1	Tb1	O2	119.16(15)	C61	C60	C65	119.4(6)

N1	Tb1	O4	145.60(13)	C61	C60	C59	121.9(6)
N1	Tb1	N2	65.18(14)	C12	C17	N2	117.2(4)
N1	Tb1	O3	133.31(12)	C16	C17	N2	124.1(5)
N4	Tb1	N3	63.26(13)	C16	C17	C12	118.6(5)
N4	Tb1	O1	143.80(13)	C19	C20	C21	123.1(5)
N4	Tb1	O2	129.42(13)	C25	C20	C21	116.8(5)
N4	Tb1	O4	68.82(12)	C25	C20	C19	120.1(5)
N4	Tb1	N2	74.10(13)	C43	C44	C45	120.5(6)
N4	Tb1	O3	105.56(12)	C81	C76	C77	116.6(5)
N4	Tb1	N1	79.17(14)	C75	C76	C77	123.5(5)
O4	Tb2	N5	115.87(12)	C75	C76	C81	119.7(5)
O3	Tb2	N5	79.90(13)	C31	C30	C29	121.2(5)
O3	Tb2	O4	70.35(11)	C3	C4	C9	119.0(5)
O6	Tb2	N5	118.55(14)	C5	C4	C9	119.8(6)
O6	Tb2	O4	96.52(13)	C5	C4	C3	121.2(5)
O6	Tb2	O3	161.22(14)	C83	C82	C81	121.7(5)
O5	Tb2	N5	73.53(14)	C17	C12	N1	115.3(4)
O5	Tb2	O4	159.70(14)	C13	C12	N1	124.9(5)
O5	Tb2	O3	95.10(13)	C13	C12	C17	119.6(5)
O5	Tb2	O6	93.80(14)	C10	C11	N1	125.2(5)
O7	Tb2	N5	148.99(15)	C66	C67	N5	126.7(5)
O7	Tb2	O4	74.27(13)	C48	C53	C54	118.6(5)
O7	Tb2	O3	76.42(14)	C52	C53	C54	122.2(6)
O7	Tb2	O6	87.28(16)	C52	C53	C48	119.3(6)
O7	Tb2	O5	88.85(15)	C82	C81	C76	118.5(5)
N6	Tb2	N5	66.17(13)	C80	C81	C76	119.9(6)
N6	Tb2	O4	76.86(13)	C80	C81	C82	121.7(6)
N6	Tb2	O3	114.69(12)	C33	C34	C35	119.7(6)
N6	Tb2	O6	73.39(14)	C27	C26	C25	121.2(6)
N6	Tb2	O5	122.99(14)	C15	C16	C17	120.9(5)
N6	Tb2	O7	142.95(14)	C66	C57	O5	123.0(5)
C45	C40	N3	116.1(4)	C58	C57	O5	118.7(5)
C41	C40	N3	126.3(5)	C58	C57	C66	118.2(5)
C41	C40	C45	117.6(5)	C70	C69	C68	121.1(5)
C73	C68	N5	117.2(4)	C53	C48	C47	119.4(5)
C69	C68	N5	124.0(5)	C49	C48	C47	122.7(5)
C69	C68	C73	118.8(5)	C49	C48	C53	117.8(5)
C40	N3	Tb1	115.8(3)	C35	C36	C37	120.3(7)
C39	N3	Tb1	126.4(3)	C32	C31	C30	121.1(5)
C39	N3	C40	117.8(4)	C63	C64	C65	121.7(6)
C68	N5	Tb2	114.6(3)	C58	C59	C60	121.6(5)
C67	N5	Tb2	127.9(3)	C54	C55	C56	121.1(5)
C67	N5	C68	117.3(4)	C79	C78	C77	121.0(6)
C1	O1	Tb1	128.8(3)	C31	C32	C37	119.7(5)
O3	C29	C38	121.0(4)	C33	C32	C37	119.1(6)
C30	C29	C38	119.4(4)	C33	C32	C31	121.1(6)
C30	C29	O3	119.6(4)	C2	C3	C4	121.0(5)
C37	C38	C29	120.0(5)	C83	C84	O6	117.9(5)
C39	C38	C29	121.2(4)	C75	C84	O6	123.3(5)

C39	C38	C37	118.7(5)	C75	C84	C83	118.8(5)
C28	O2	Tb1	136.2(3)	C14	C13	C12	120.8(6)
Tb2	O4	Tb1	109.50(13)	C43	C42	C41	119.8(5)
C56	O4	Tb1	117.9(3)	C59	C58	C57	122.1(6)
C56	O4	Tb2	132.5(3)	C84	C83	C82	121.4(6)
C18	N2	Tb1	128.5(4)	C76	C75	C74	118.9(5)
C17	N2	Tb1	114.2(3)	C84	C75	C74	121.6(5)
C17	N2	C18	117.2(4)	C84	C75	C76	119.5(5)
Tb2	O3	Tb1	110.02(13)	C14	C15	C16	119.8(5)
C29	O3	Tb1	122.8(3)	C3	C2	C1	121.4(5)
C29	O3	Tb2	126.1(3)	C26	C25	C20	118.4(5)
C44	C45	C40	119.9(5)	C24	C25	C20	119.9(5)
N4	C45	C40	115.4(4)	C24	C25	C26	121.7(5)
N4	C45	C44	124.6(5)	C23	C24	C25	121.0(6)
C47	C56	O4	121.8(4)	C26	C27	C28	122.4(6)
C55	C56	O4	118.4(5)	C71	C70	C69	119.4(5)
C55	C56	C47	119.7(5)	C62	C63	C64	120.3(6)
C60	C65	C66	119.4(5)	C70	C71	C72	120.5(5)
C64	C65	C66	123.3(5)	C22	C23	C24	120.5(5)
C64	C65	C60	117.3(5)	C6	C5	C4	121.6(6)
N4	C46	C47	125.1(5)	C7	C8	C9	120.9(6)
C72	C73	C68	119.7(5)	C15	C14	C13	120.3(6)
N6	C73	C68	116.2(4)	C6	C7	C8	121.8(7)
N6	C73	C72	124.1(5)	C42	C43	C44	120.2(6)
N6	C74	C75	127.3(5)	C36	C35	C34	121.4(7)
C84	O6	Tb2	133.6(3)	C32	C33	C34	121.0(7)
C12	N1	Tb1	114.7(3)	C61	C62	C63	119.8(6)
C11	N1	Tb1	126.0(3)	C7	C6	C5	118.7(6)
C11	N1	C12	119.0(4)	C23	C22	C21	119.7(6)
C46	C47	C56	121.2(4)	C62	C61	C60	121.5(6)
C48	C47	C56	119.5(5)	C85	O7	Tb2	134.6(5)
C48	C47	C46	119.2(5)	C79	C80	C81	121.5(6)
C57	O5	Tb2	138.1(3)	C51	C52	C53	121.2(7)
C55	C54	C53	121.6(5)	C80	C79	C78	118.9(6)
C22	C21	C20	122.1(6)	C50	C51	C52	120.2(6)
C36	C37	C38	123.0(5)	C50	C49	C48	120.7(7)
C32	C37	C38	118.5(5)	C49	C50	C51	120.7(7)
C32	C37	C36	118.4(5)	C45	N4	Tb1	116.8(3)
C78	C77	C76	122.0(6)	C46	N4	Tb1	122.9(3)
C19	C18	N2	126.8(5)	C46	N4	C45	120.0(4)
C19	C28	O2	123.2(5)	C73	N6	Tb2	114.8(3)
C27	C28	O2	118.4(5)	C74	N6	Tb2	126.0(3)
C27	C28	C19	118.4(5)	C74	N6	C73	118.9(4)
C42	C41	C40	122.0(6)	C38	C39	N3	125.4(5)

Table SI35 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Tb2L3_final.

Atom	*x*	*y*	*z*	U(eq)
H46	1245(3)	5610(2)	3841(2)	28.6(12)
H74	1108(3)	7178(3)	2862(3)	32.0(13)

H54	-1067(3)	5443(3)	1687(3)	40.6(15)
H21	-898(3)	3724(3)	2826(3)	39.6(15)
H77	76(3)	7030(3)	3256(3)	43.0(15)
H18	234(3)	3493(2)	2990(3)	31.2(13)
H41	4468(3)	5086(3)	4098(3)	45.4(16)
H72	1837(3)	6933(3)	3664(3)	35.5(14)
H44	1983(4)	5362(3)	4680(3)	42.6(15)
H30	3386(3)	4920(3)	644(3)	38.2(14)
H82	-1364(3)	7112(3)	856(3)	44.1(16)
H11	3550(3)	3223(3)	3864(3)	32.0(13)
H67	4273(3)	6882(2)	2085(3)	32.5(13)
H34	7031(3)	4857(3)	1637(4)	64(2)
H26	-651(3)	3631(3)	287(3)	51.2(19)
H16	381(3)	3782(3)	3956(3)	40.9(15)
H69	4308(3)	6730(3)	3033(3)	37.5(14)
H36	5522(3)	5047(3)	2971(3)	50.5(18)
H31	4646(3)	4842(3)	430(3)	39.7(15)
H64	5361(3)	6678(3)	1971(3)	45.6(16)
H59	4592(4)	6539(4)	-582(3)	54.6(19)
H55	144(3)	5391(2)	1374(3)	33.5(13)
H78	-1094(4)	7222(3)	3626(4)	53.6(18)
H3	5493(3)	3275(3)	1857(3)	41.9(15)
H13	2992(3)	3526(3)	4667(3)	42.6(16)
H42	4281(4)	5285(3)	5180(3)	55.0(19)
H58	3338(4)	6412(3)	-397(3)	47.7(17)
H83	-236(3)	6856(3)	464(3)	45.8(16)
H15	785(4)	3604(3)	5058(3)	52.3(18)
H2	4232(3)	3461(3)	1461(3)	37.0(14)
H24	-1945(3)	3478(3)	652(3)	47.5(17)
H27	627(3)	3845(3)	516(3)	50.7(19)
H70	4148(3)	6956(3)	4119(3)	43.5(16)
H63	6621(4)	6747(4)	1759(4)	64(2)
H71	2908(3)	7047(3)	4432(3)	46.2(16)
H23	-2727(3)	3441(3)	1476(3)	49.0(17)
H5	6519(3)	3209(3)	2782(4)	52.2(19)
H8	4693(3)	3411(3)	4258(3)	46.9(16)
H14	2091(4)	3474(3)	5410(3)	55.2(19)
H7	5980(4)	3280(3)	4622(4)	61(2)
H43	3034(4)	5434(3)	5467(3)	55.2(19)
H35	6766(3)	4931(4)	2719(4)	67(2)
H33	6038(3)	4837(3)	802(4)	57(2)
H62	6928(4)	6749(4)	677(4)	73(3)
H6	6906(3)	3200(3)	3892(4)	61(2)
H22	-2211(3)	3593(3)	2568(3)	48.1(17)
H61	5972(4)	6657(4)	-172(4)	66(2)
H7a	1390(30)	4821(12)	891(10)	69.9(17)
H80	-2133(3)	7270(3)	1782(4)	53.9(19)
H52	-1943(4)	5450(3)	2560(4)	63(2)
H79	-2208(4)	7371(3)	2892(4)	56.2(19)

H51	-2125(4)	5362(4)	3640(5)	76(3)
H49	170(4)	5241(3)	4152(3)	50.1(18)
H50	-1070(4)	5252(4)	4438(4)	68(2)
H39	4411(3)	5391(2)	3111(3)	32.5(13)
H85a	1187(10)	4990(30)	-236(9)	125(4)
H85b	2050(30)	5250(20)	-112(14)	125(4)
H85c	1860(40)	4517(13)	75(7)	125(4)

Table SI36 Solvent masks information for Tb2L3_final.

Number	**X**	**Y**	**Z**	**Volume**	**Electron count**	**Content**
1	0.000	0.000	0.500	7.0	0.0	
2	0.152	0.204	0.032	346.2	109.5	2DCM/H2O
3	0.152	0.296	0.532	346.2	105.1	2DCM/H2O
4	0.000	0.500	0.000	7.0	0.0	
5	-0.152	0.704	0.468	346.2	112.3	2DCM/H2O
6	-0.152	0.796	0.968	346.2	107.9	2DCM/H2O

Refinement model description

Number of restraints - 3, number of constraints - 113.

Lu2L3_Final

Table SI37 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Lu2L3_Final. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Lu1	2271.0(3)	4440.2(3)	2482.5(2)	55.9(3)
Lu2	2082.3(3)	6010.9(3)	1524.0(2)	59.9(3)
O4	1448(5)	5289(5)	2130(4)	53.4(18)
O1	3093(5)	3751(5)	2093(4)	61(2)
O5	2723(5)	6371(6)	737(4)	72(3)
O3	2839(5)	5120(4)	1781(4)	58(2)
N3	3385(6)	5010(5)	3086(5)	54(2)
O2	1497(5)	4048(5)	1650(4)	67(2)
N1	2725(7)	3757(5)	3371(5)	56(2)
C40	3363(8)	5117(6)	3747(7)	62(3)
N4	1987(6)	5128(5)	3402(5)	57(2)
C39	4035(7)	5158(7)	2828(6)	58(3)
C38	4188(8)	5050(7)	2163(6)	61(3)
N5	3181(6)	6558(5)	2069(5)	55(2)
C45	2591(8)	5205(6)	3904(6)	57(3)
C68	3177(9)	6684(7)	2748(7)	66(3)
C32	5116(9)	4920(8)	1363(8)	71(4)
C29	3589(7)	5033(6)	1660(6)	57(3)
N2	1289(6)	3873(5)	2965(5)	55(2)
C47	635(6)	5350(6)	2996(7)	54(3)
C53	-763(8)	5373(7)	2714(7)	62(3)
C10	4010(7)	3487(7)	3013(6)	60(3)
C30	3750(8)	4943(7)	1024(6)	65(3)
C1	3784(7)	3574(7)	2347(7)	62(3)
O7	1549(6)	5207(5)	776(4)	66(2)
C11	3428(7)	3482(7)	3456(6)	60(3)
C4	5350(7)	3303(7)	2786(7)	64(3)
C54	-628(7)	5413(8)	2061(8)	70(4)
C60	5024(10)	6598(10)	401(8)	84(4)
C55	90(7)	5365(6)	1872(7)	58(3)
C34	6522(10)	4838(9)	1695(10)	93(6)
C73	2374(8)	6765(5)	2909(5)	53(3)
C65	4825(8)	6634(6)	1038(8)	68(3)
O6	1107(6)	6610(6)	1132(5)	79(3)
C41	3984(11)	5137(9)	4218(7)	82(5)
C19	291(8)	3787(7)	2058(7)	64(3)
C7	5842(9)	3305(8)	4105(8)	74(4)
C77	-406(10)	7067(7)	2947(9)	76(4)
C81	-977(9)	7085(8)	1834(7)	71(3)
C44	2503(10)	5309(7)	4580(7)	69(3)
C69	3796(9)	6738(7)	3192(7)	67(3)
C78	-1114(12)	7228(7)	3141(9)	84(5)
C37	4996(7)	5018(6)	2040(7)	59(3)
N6	1788(6)	6676(5)	2407(5)	56(2)

C74	1125(7)	6932(7)	2474(6)	61(3)
C57	3418(7)	6443(7)	653(6)	60(3)
C31	4518(9)	4907(9)	889(8)	77(4)
C25	-861(8)	3624(8)	1219(7)	67(3)
C36	5642(7)	4999(8)	2521(9)	74(4)
C46	1328(8)	5363(7)	3483(5)	59(3)
C76	-306(9)	7037(8)	2290(9)	78(4)
C17	1435(8)	3733(7)	3645(6)	63(3)
C70	3700(9)	6897(7)	3830(8)	72(4)
C21	-1072(10)	3669(7)	2351(7)	74(4)
C66	4030(10)	6568(8)	1181(7)	72(4)
C72	2313(10)	6880(6)	3574(8)	71(4)
C24	-1665(9)	3571(9)	1050(6)	77(4)
C67	3843(8)	6673(7)	1830(6)	63(3)
C56	776(7)	5346(6)	2364(7)	58(3)
C9	4792(9)	3367(8)	3256(7)	71(4)
C20	-540(9)	3666(7)	1875(8)	70(3)
C75	424(7)	6906(8)	2039(7)	64(3)
C13	2468(7)	3538(8)	4520(7)	72(4)
C48	-115(8)	5353(6)	3182(7)	64(3)
C82	-888(8)	7037(7)	1170(8)	67(3)
C3	5104(9)	3325(7)	2129(8)	73(4)
C83	-224(10)	6892(9)	948(8)	81(4)
C12	2236(9)	3667(7)	3849(7)	67(3)
C18	611(8)	3700(7)	2712(6)	62(3)
C5	6161(9)	3232(7)	3009(9)	77(4)
C26	-340(11)	3664(9)	756(9)	86(5)
C16	891(9)	3733(8)	4080(8)	71(4)
C43	3095(12)	5337(10)	5039(7)	87(5)
C35	6379(10)	4903(9)	2355(9)	86(5)
C2	4361(8)	3463(7)	1903(7)	67(3)
C84	477(8)	6805(7)	1398(7)	70(4)
C27	425(8)	3812(9)	875(7)	78(4)
C59	4380(11)	6535(11)	-128(9)	94(6)
C33	5901(9)	4876(9)	1233(8)	80(4)
C42	3868(10)	5231(9)	4882(7)	77(4)
C71	2910(11)	6924(9)	4018(7)	80(4)
C28	753(8)	3896(7)	1557(6)	61(3)
C58	3645(9)	6444(9)	7(8)	78(4)
C64	5438(9)	6667(9)	1533(8)	78(4)
C80	-1730(9)	7196(11)	2062(10)	95(6)
C6	6375(9)	3269(10)	3650(8)	89(5)
C15	1131(10)	3615(8)	4739(8)	78(4)
C61	5770(14)	6660(9)	271(9)	100(6)
C63	6190(10)	6645(12)	1364(10)	101(6)
C23	-2163(9)	3498(8)	1537(9)	79(4)
C22	-1846(9)	3568(8)	2177(8)	78(4)
C14	1916(11)	3536(10)	4942(8)	88(5)
C8	5074(10)	3355(9)	3919(7)	80(4)

C52	-1496(10)	5424(8)	2935(10)	82(4)
C49	-267(9)	5275(8)	3848(7)	71(4)
C50	-1019(10)	5303(9)	4036(9)	83(4)
C79	-1808(11)	7289(8)	2690(8)	82(5)
C51	-1655(9)	5352(10)	3561(11)	100(6)
C62	6357(12)	6689(12)	741(10)	106(7)
C85	1614(8)	5060(6)	105(6)	60

Table SI38 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Lu2L3_Final. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Lu1	48.1(4)	66.0(4)	54.5(4)	0.51(19)	9.3(2)	-1.78(19)
Lu2	53.7(4)	69.9(4)	56.9(4)	7.4(2)	9.8(2)	2.6(2)
O4	44(4)	74(5)	44(4)	6(4)	14(3)	1(3)
O1	50(4)	75(5)	61(5)	11(4)	18(4)	-18(4)
O5	55(5)	108(8)	56(5)	-8(5)	18(4)	17(5)
O3	59(5)	49(4)	72(5)	10(3)	34(4)	17(4)
N3	43(5)	71(6)	51(5)	-6(4)	17(4)	1(4)
O2	40(4)	101(7)	60(5)	-19(4)	1(4)	-29(5)
N1	63(6)	59(5)	46(4)	-4(5)	5(4)	0(4)
C40	59(7)	54(6)	74(8)	-3(5)	7(6)	10(5)
N4	55(6)	57(5)	60(5)	-14(4)	12(4)	-5(4)
C39	37(5)	71(7)	66(7)	1(5)	6(5)	12(6)
C38	58(7)	68(7)	59(6)	4(6)	20(5)	6(5)
N5	52(5)	52(5)	63(5)	1(4)	9(4)	-4(4)
C45	63(7)	64(7)	46(5)	-11(5)	11(5)	4(5)
C68	70(8)	59(7)	71(8)	1(6)	16(6)	-14(6)
C32	60(8)	79(9)	76(9)	15(7)	21(6)	4(7)
C29	39(5)	70(7)	65(7)	3(5)	21(5)	13(5)
N2	60(6)	49(5)	58(5)	-1(4)	20(4)	3(4)
C47	26(4)	58(6)	79(8)	-3(4)	10(4)	-7(5)
C53	56(7)	61(7)	69(7)	3(5)	8(6)	5(6)
C10	48(6)	66(7)	67(7)	0(5)	17(5)	-6(5)
C30	63(8)	86(9)	50(6)	1(6)	29(5)	-5(6)
C1	45(6)	75(8)	67(7)	5(5)	13(5)	2(6)
O7	77(6)	70(5)	49(4)	12(5)	4(4)	-5(4)
C11	48(6)	67(7)	63(7)	-11(5)	-3(5)	6(5)
C4	45(6)	79(8)	70(7)	-8(6)	17(5)	-8(6)
C54	30(5)	81(9)	98(10)	1(5)	-1(6)	-7(7)
C60	74(10)	109(13)	73(9)	3(9)	24(7)	12(8)
C55	45(6)	60(6)	67(7)	-2(5)	5(5)	-1(5)
C34	62(9)	94(11)	129(15)	20(8)	35(9)	38(11)
C73	83(8)	36(4)	39(4)	2(5)	5(5)	11(4)
C65	62(8)	51(6)	92(10)	7(5)	19(7)	-4(6)
O6	61(6)	106(8)	69(6)	43(6)	6(4)	21(5)
C41	86(11)	92(11)	64(8)	-40(9)	-5(7)	3(7)
C19	59(7)	64(7)	69(7)	0(6)	10(6)	-12(6)
C7	61(8)	74(8)	83(9)	12(6)	-7(7)	-21(7)
C77	73(9)	65(8)	94(11)	-6(7)	28(8)	-9(7)
C81	70(9)	76(9)	70(8)	8(7)	18(7)	8(6)

C44	82(10)	60(7)	64(7)	-1(7)	2(6)	-9(6)
C69	61(8)	57(7)	81(8)	3(6)	3(6)	8(6)
C78	110(13)	46(6)	99(11)	-10(7)	23(10)	-7(7)
C37	43(6)	56(6)	80(8)	10(5)	15(5)	14(5)
N6	50(5)	60(5)	60(5)	8(4)	15(4)	4(4)
C74	49(6)	70(7)	65(7)	4(5)	9(5)	-2(6)
C57	51(6)	76(8)	55(6)	8(5)	20(5)	2(5)
C31	54(8)	105(12)	78(9)	-6(7)	29(7)	10(8)
C25	51(7)	87(9)	62(7)	6(6)	3(5)	-17(6)
C36	40(6)	75(8)	107(12)	-9(6)	9(6)	4(7)
C46	61(7)	75(7)	42(5)	7(6)	5(5)	4(5)
C76	61(8)	68(8)	108(12)	14(6)	22(8)	8(8)
C17	59(7)	74(8)	55(6)	14(6)	12(5)	8(5)
C70	66(8)	65(7)	83(9)	-4(6)	1(7)	-22(7)
C21	88(10)	68(8)	72(8)	19(7)	28(7)	16(6)
C66	82(10)	73(8)	63(7)	6(7)	16(7)	17(6)
C72	87(10)	45(6)	87(9)	13(6)	37(8)	-4(6)
C24	71(9)	109(12)	48(6)	-12(8)	-1(6)	-4(7)
C67	59(7)	73(8)	58(6)	3(6)	12(5)	-15(6)
C56	47(6)	54(6)	72(7)	1(5)	6(5)	-16(5)
C9	66(8)	75(8)	70(8)	20(7)	-3(6)	6(6)
C20	59(8)	60(7)	93(10)	2(6)	16(7)	-9(6)
C75	41(6)	80(8)	74(8)	1(5)	15(5)	6(6)
C13	41(6)	110(11)	65(7)	26(7)	7(5)	-17(7)
C48	53(7)	58(6)	85(9)	2(5)	30(6)	2(6)
C82	50(6)	59(7)	88(9)	12(5)	-10(6)	-2(6)
C3	72(9)	55(7)	98(10)	14(6)	38(8)	4(6)
C83	69(9)	89(10)	82(10)	12(8)	1(7)	14(8)
C12	72(8)	65(7)	68(7)	-1(6)	26(6)	-12(6)
C18	66(8)	64(7)	57(6)	-3(6)	8(5)	0(5)
C5	60(8)	59(7)	110(12)	18(6)	0(7)	3(7)
C26	86(11)	94(11)	80(10)	8(9)	21(8)	-19(8)
C16	58(8)	75(8)	84(9)	-9(6)	24(7)	-11(7)
C43	96(12)	106(12)	55(7)	-2(10)	-12(7)	3(8)
C35	65(9)	92(11)	103(12)	-20(8)	10(8)	-6(9)
C2	62(8)	69(7)	70(7)	3(6)	15(6)	-9(6)
C84	63(8)	68(8)	80(9)	25(6)	22(7)	7(6)
C27	45(6)	128(13)	59(7)	-4(7)	-10(5)	-25(8)
C59	73(10)	128(16)	88(11)	-2(10)	33(9)	-8(11)
C33	55(8)	112(12)	81(9)	1(8)	36(7)	5(8)
C42	79(10)	89(10)	64(8)	-14(8)	7(7)	-19(7)
C71	85(11)	94(11)	60(7)	-1(9)	-2(7)	15(7)
C28	54(7)	74(8)	56(6)	11(6)	4(5)	-7(5)
C58	66(9)	97(11)	77(9)	4(8)	30(7)	21(8)
C64	56(8)	99(11)	83(9)	-22(7)	23(7)	-24(8)
C80	47(7)	120(15)	116(14)	-4(8)	4(8)	23(11)
C6	51(7)	134(15)	81(10)	-35(9)	1(7)	6(9)
C15	75(9)	85(10)	79(9)	7(8)	35(7)	15(7)
C61	140(18)	86(11)	81(11)	-30(12)	49(12)	-2(9)

C63	53(9)	139(17)	113(14)	6(10)	12(9)	13(13)
C23	62(8)	76(9)	98(11)	-6(7)	10(7)	8(8)
C22	66(9)	87(10)	82(9)	-3(7)	20(7)	-17(8)
C14	84(11)	118(14)	66(8)	-11(10)	23(8)	14(8)
C8	81(10)	95(11)	62(8)	15(9)	1(7)	-10(7)
C52	63(9)	78(9)	108(13)	0(7)	26(8)	1(8)
C49	73(9)	76(8)	69(8)	-4(7)	31(7)	2(6)
C50	78(10)	94(11)	85(10)	4(8)	41(8)	-4(8)
C79	100(12)	68(8)	85(10)	20(8)	48(9)	2(7)
C51	46(8)	112(14)	146(18)	-2(8)	31(9)	-33(12)
C62	93(13)	145(19)	90(12)	-22(13)	53(11)	-9(12)

Table SI39 Bond Lengths for Lu2L3_Final.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Lu1	O4	2.316(9)	C34	C35	1.42(2)
Lu1	O1	2.219(8)	C34	C33	1.36(2)
Lu1	O3	2.307(7)	C73	N6	1.387(15)
Lu1	N3	2.480(10)	C73	C72	1.410(17)
Lu1	O2	2.218(8)	C65	C66	1.45(2)
Lu1	N1	2.374(10)	C65	C64	1.40(2)
Lu1	N4	2.457(10)	O6	C84	1.338(15)
Lu1	N2	2.371(10)	C41	C42	1.42(2)
Lu2	O4	2.295(8)	C19	C20	1.48(2)
Lu2	O5	2.196(8)	C19	C18	1.417(19)
Lu2	O3	2.276(8)	C19	C28	1.397(19)
Lu2	N5	2.390(10)	C7	C6	1.39(2)
Lu2	O7	2.375(9)	C7	C8	1.35(2)
Lu2	O6	2.177(8)	C77	C78	1.38(2)
Lu2	N6	2.375(10)	C77	C76	1.39(2)
O4	C56	1.317(14)	C81	C76	1.42(2)
O1	C1	1.311(15)	C81	C82	1.40(2)
O5	C57	1.250(15)	C81	C80	1.46(2)
O3	C29	1.366(13)	C44	C43	1.33(2)
N3	C40	1.390(17)	C69	C70	1.39(2)
N3	C39	1.336(14)	C78	C79	1.45(3)
O2	C28	1.325(16)	C37	C36	1.42(2)
N1	C11	1.339(16)	N6	C74	1.288(15)
N1	C12	1.384(16)	C74	C75	1.436(18)
C40	C45	1.427(18)	C57	C66	1.46(2)
C40	C41	1.37(2)	C57	C58	1.433(17)
N4	C45	1.405(16)	C25	C24	1.410(19)
N4	C46	1.270(16)	C25	C20	1.41(2)
C39	C38	1.444(17)	C25	C26	1.39(2)
C38	C29	1.392(18)	C36	C35	1.38(2)
C38	C37	1.457(16)	C76	C75	1.447(18)
N5	C68	1.427(17)	C17	C12	1.42(2)
N5	C67	1.322(16)	C17	C16	1.375(18)
C45	C44	1.438(17)	C70	C71	1.47(2)
C68	C73	1.481(19)	C21	C20	1.42(2)

C68	C69	1.34(2)	C21	C22	1.37(2)
C32	C37	1.453(19)	C66	C67	1.430(18)
C32	C31	1.35(2)	C72	C71	1.31(2)
C32	C33	1.422(18)	C24	C23	1.41(2)
C29	C30	1.385(16)	C9	C8	1.406(19)
N2	C17	1.431(15)	C75	C84	1.36(2)
N2	C18	1.288(17)	C13	C12	1.43(2)
C47	C46	1.485(16)	C13	C14	1.37(2)
C47	C56	1.356(18)	C48	C49	1.438(18)
C47	C48	1.401(15)	C82	C83	1.32(2)
C53	C54	1.40(2)	C3	C2	1.36(2)
C53	C48	1.41(2)	C83	C84	1.46(2)
C53	C52	1.40(2)	C5	C6	1.34(2)
C10	C1	1.403(18)	C26	C27	1.36(2)
C10	C11	1.439(17)	C16	C15	1.40(2)
C10	C9	1.420(18)	C43	C42	1.43(3)
C30	C31	1.396(18)	C27	C28	1.473(17)
C1	C2	1.449(17)	C59	C58	1.35(2)
O7	C85	1.437(14)	C64	C63	1.39(2)
C4	C9	1.451(19)	C80	C79	1.33(2)
C4	C3	1.38(2)	C15	C14	1.39(2)
C4	C5	1.443(19)	C61	C62	1.33(3)
C54	C55	1.352(17)	C63	C62	1.35(3)
C60	C65	1.40(2)	C23	C22	1.38(2)
C60	C59	1.49(3)	C52	C51	1.36(3)
C60	C61	1.36(3)	C49	C50	1.406(19)
C55	C56	1.483(17)	C50	C51	1.40(3)

Table SI40 Bond Angles for Lu2L3_Final.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O1	Lu1	O4	139.6(3)	C59	C60	C65	117.0(15)
O3	Lu1	O4	69.1(3)	C61	C60	C65	121.2(18)
O3	Lu1	O1	79.5(3)	C61	C60	C59	121.6(16)
N3	Lu1	O4	103.3(3)	C56	C55	C54	120.3(13)
N3	Lu1	O1	89.0(3)	C33	C34	C35	117.3(15)
N3	Lu1	O3	70.7(3)	N6	C73	C68	116.9(10)
O2	Lu1	O4	73.9(4)	C72	C73	C68	114.2(12)
O2	Lu1	O1	81.4(3)	C72	C73	N6	128.8(13)
O2	Lu1	O3	89.7(4)	C66	C65	C60	121.6(15)
O2	Lu1	N3	159.5(3)	C64	C65	C60	116.5(14)
N1	Lu1	O4	145.7(3)	C64	C65	C66	121.6(14)
N1	Lu1	O1	74.6(4)	C84	O6	Lu2	130.8(9)
N1	Lu1	O3	135.4(4)	C42	C41	C40	120.4(17)
N1	Lu1	N3	73.1(4)	C18	C19	C20	119.9(13)
N1	Lu1	O2	120.8(4)	C28	C19	C20	117.5(13)
N4	Lu1	O4	69.3(3)	C28	C19	C18	122.0(13)
N4	Lu1	O1	146.6(4)	C8	C7	C6	121.4(15)
N4	Lu1	O3	106.2(3)	C76	C77	C78	120.4(18)
N4	Lu1	N3	63.5(3)	C82	C81	C76	118.4(14)

N4	Lu1	O2	130.6(4)	C80	C81	C76	119.9(15)
N4	Lu1	N1	79.3(4)	C80	C81	C82	121.7(15)
N2	Lu1	O4	92.8(3)	C43	C44	C45	123.2(16)
N2	Lu1	O1	111.3(4)	C70	C69	C68	120.1(14)
N2	Lu1	O3	159.4(4)	C79	C78	C77	122.9(17)
N2	Lu1	N3	125.3(3)	C32	C37	C38	114.6(12)
N2	Lu1	O2	75.2(4)	C36	C37	C38	125.9(13)
N2	Lu1	N1	65.3(4)	C36	C37	C32	119.1(12)
N2	Lu1	N4	74.9(3)	C73	N6	Lu2	116.7(7)
O5	Lu2	O4	158.9(4)	C74	N6	Lu2	125.8(9)
O3	Lu2	O4	70.0(3)	C74	N6	C73	117.4(11)
O3	Lu2	O5	96.6(3)	C75	C74	N6	128.8(13)
N5	Lu2	O4	116.8(3)	C66	C57	O5	123.7(11)
N5	Lu2	O5	75.5(4)	C58	C57	O5	119.7(13)
N5	Lu2	O3	81.4(3)	C58	C57	C66	116.4(12)
O7	Lu2	O4	74.6(3)	C30	C31	C32	122.3(14)
O7	Lu2	O5	86.7(4)	C20	C25	C24	121.5(13)
O7	Lu2	O3	77.0(3)	C26	C25	C24	122.4(14)
O7	Lu2	N5	150.1(3)	C26	C25	C20	116.0(14)
O6	Lu2	O4	99.4(4)	C35	C36	C37	121.2(16)
O6	Lu2	O5	88.4(4)	C47	C46	N4	125.6(11)
O6	Lu2	O3	160.9(4)	C81	C76	C77	117.7(14)
O6	Lu2	N5	117.7(4)	C75	C76	C77	124.4(16)
O6	Lu2	O7	85.0(4)	C75	C76	C81	117.7(15)
N6	Lu2	O4	78.0(3)	C12	C17	N2	112.1(11)
N6	Lu2	O5	123.1(4)	C16	C17	N2	125.5(13)
N6	Lu2	O3	116.5(3)	C16	C17	C12	122.0(13)
N6	Lu2	N5	66.3(4)	C71	C70	C69	118.1(14)
N6	Lu2	O7	142.6(4)	C22	C21	C20	120.7(15)
N6	Lu2	O6	75.0(4)	C57	C66	C65	119.8(12)
Lu2	O4	Lu1	109.6(3)	C67	C66	C65	119.7(14)
C56	O4	Lu1	119.6(8)	C67	C66	C57	120.4(13)
C56	O4	Lu2	129.9(8)	C71	C72	C73	123.9(15)
C1	O1	Lu1	129.0(8)	C23	C24	C25	120.1(13)
C57	O5	Lu2	135.9(9)	C66	C67	N5	128.3(13)
Lu2	O3	Lu1	110.6(3)	C47	C56	O4	127.9(11)
C29	O3	Lu1	121.3(7)	C55	C56	O4	115.5(11)
C29	O3	Lu2	127.0(7)	C55	C56	C47	116.5(11)
C40	N3	Lu1	117.8(7)	C4	C9	C10	117.6(13)
C39	N3	Lu1	123.7(8)	C8	C9	C10	124.7(15)
C39	N3	C40	118.2(11)	C8	C9	C4	117.6(14)
C28	O2	Lu1	134.4(8)	C25	C20	C19	122.2(13)
C11	N1	Lu1	124.8(8)	C21	C20	C19	120.9(15)
C12	N1	Lu1	116.9(9)	C21	C20	C25	116.5(14)
C12	N1	C11	118.2(11)	C76	C75	C74	119.2(14)
C45	C40	N3	111.6(11)	C84	C75	C74	118.5(12)
C41	C40	N3	126.8(14)	C84	C75	C76	122.2(14)
C41	C40	C45	121.5(14)	C14	C13	C12	118.5(13)
C45	N4	Lu1	116.0(8)	C53	C48	C47	120.9(13)

C46	N4	Lu1	125.3(9)	C49	C48	C47	122.3(14)
C46	N4	C45	118.3(11)	C49	C48	C53	116.6(12)
C38	C39	N3	126.6(12)	C83	C82	C81	123.3(14)
C29	C38	C39	121.1(11)	C2	C3	C4	122.0(13)
C37	C38	C39	116.9(13)	C84	C83	C82	120.5(15)
C37	C38	C29	121.8(11)	C17	C12	N1	115.7(13)
C68	N5	Lu2	117.4(8)	C13	C12	N1	126.0(14)
C67	N5	Lu2	126.2(8)	C13	C12	C17	118.2(12)
C67	N5	C68	115.6(11)	C19	C18	N2	127.0(13)
N4	C45	C40	117.8(11)	C6	C5	C4	118.0(15)
C44	C45	C40	116.1(13)	C27	C26	C25	125.9(16)
C44	C45	N4	125.8(12)	C15	C16	C17	118.8(14)
C73	C68	N5	110.3(12)	C42	C43	C44	120.4(16)
C69	C68	N5	126.8(13)	C36	C35	C34	121.2(17)
C69	C68	C73	122.9(13)	C3	C2	C1	120.9(14)
C31	C32	C37	121.5(13)	C75	C84	O6	126.3(14)
C33	C32	C37	115.6(14)	C83	C84	O6	116.0(14)
C33	C32	C31	122.9(14)	C83	C84	C75	117.6(13)
C38	C29	O3	120.8(11)	C28	C27	C26	118.0(15)
C30	C29	O3	119.1(12)	C58	C59	C60	121.0(16)
C30	C29	C38	120.1(11)	C34	C33	C32	125.1(15)
C17	N2	Lu1	116.8(8)	C43	C42	C41	118.2(15)
C18	N2	Lu1	129.3(9)	C72	C71	C70	120.3(15)
C18	N2	C17	113.8(11)	C19	C28	O2	124.1(12)
C56	C47	C46	115.9(10)	C27	C28	O2	116.0(12)
C48	C47	C46	121.8(12)	C27	C28	C19	119.8(13)
C48	C47	C56	122.4(12)	C59	C58	C57	123.7(17)
C48	C53	C54	117.5(12)	C63	C64	C65	118.6(16)
C52	C53	C54	124.3(14)	C79	C80	C81	121.8(17)
C52	C53	C48	117.8(14)	C5	C6	C7	122.4(15)
C11	C10	C1	119.0(12)	C14	C15	C16	119.5(13)
C9	C10	C1	121.7(12)	C62	C61	C60	122.2(17)
C9	C10	C11	119.2(12)	C62	C63	C64	122.7(19)
C31	C30	C29	119.5(14)	C22	C23	C24	117.4(15)
C10	C1	O1	125.2(11)	C23	C22	C21	123.1(15)
C2	C1	O1	117.3(12)	C15	C14	C13	122.7(15)
C2	C1	C10	117.6(12)	C9	C8	C7	120.6(16)
C85	O7	Lu2	135.0(8)	C51	C52	C53	126.0(17)
C10	C11	N1	127.5(12)	C50	C49	C48	122.2(16)
C3	C4	C9	119.7(13)	C51	C50	C49	119.8(15)
C5	C4	C9	119.8(14)	C80	C79	C78	116.7(15)
C5	C4	C3	120.5(13)	C50	C51	C52	116.6(15)
C55	C54	C53	122.1(13)	C63	C62	C61	117.8(18)

Table **SI41** Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Lu2L3_Final.

Atom	***x***	***y***	***z***	**U(eq)**
H39	4437(7)	5354(7)	3110(6)	70(3)
H30	3341(8)	4906(7)	683(6)	78(4)

H7	1370(70)	4840(30)	928(13)	98(3)
H11	3556(7)	3258(7)	3856(6)	72(3)
H54	-1054(7)	5476(8)	1739(8)	84(4)
H55	156(7)	5344(6)	1423(7)	69(3)
H34	7030(10)	4771(9)	1579(10)	112(7)
H41	4493(11)	5089(9)	4099(7)	98(6)
H7a	6021(9)	3295(8)	4555(8)	88(5)
H77	17(10)	6976(7)	3264(9)	91(5)
H44	1996(10)	5359(7)	4703(7)	83(4)
H69	4300(9)	6668(7)	3069(7)	80(4)
H78	-1149(12)	7303(7)	3590(9)	101(6)
H74	1095(7)	7171(7)	2865(6)	73(3)
H31	4624(9)	4872(9)	449(8)	93(5)
H36	5565(7)	5053(8)	2966(9)	89(5)
H46	1274(8)	5564(7)	3890(5)	71(3)
H70	4134(9)	6985(7)	4138(8)	86(4)
H21	-889(10)	3742(7)	2795(7)	89(5)
H72	1811(10)	6929(6)	3708(8)	85(4)
H24	-1871(9)	3586(9)	605(6)	92(5)
H67	4246(8)	6848(7)	2126(6)	76(4)
H13	2995(7)	3455(8)	4669(7)	86(5)
H82	-1327(8)	7112(7)	865(8)	80(4)
H3	5466(9)	3242(7)	1826(8)	87(5)
H83	-202(10)	6845(9)	494(8)	97(5)
H18	291(8)	3492(7)	2994(6)	75(3)
H5	6531(9)	3161(7)	2710(9)	92(5)
H26	-536(11)	3580(9)	317(9)	103(5)
H16	361(9)	3810(8)	3937(8)	85(4)
H43	3007(12)	5429(10)	5475(7)	105(6)
H35	6799(10)	4881(9)	2688(9)	104(6)
H2	4217(8)	3487(7)	1447(7)	80(4)
H27	737(8)	3860(9)	528(7)	94(5)
H59	4486(11)	6559(11)	-569(9)	113(7)
H33	6001(9)	4874(9)	790(8)	97(5)
H42	4292(10)	5223(9)	5213(7)	93(5)
H71	2830(11)	6975(9)	4463(7)	96(5)
H58	3256(9)	6376(9)	-345(8)	94(5)
H64	5343(9)	6704(9)	1975(8)	94(5)
H80	-2178(9)	7202(11)	1755(10)	114(7)
H6	6911(9)	3270(10)	3799(8)	107(6)
H15	762(10)	3590(8)	5045(8)	94(5)
H61	5877(14)	6684(9)	-169(9)	120(8)
H63	6604(10)	6597(12)	1700(10)	122(7)
H23	-2697(9)	3404(8)	1432(9)	94(5)
H22	-2180(9)	3545(8)	2510(8)	93(5)
H14	2073(11)	3479(10)	5393(8)	106(6)
H8	4723(10)	3381(9)	4239(7)	96(5)
H52	-1919(10)	5516(8)	2618(10)	98(5)
H49	155(9)	5202(8)	4171(7)	85(4)

H50	-1097(10)	5289(9)	4484(9)	100(5)
H79	-2294(11)	7389(8)	2835(8)	98(5)
H51	-2172(9)	5337(10)	3670(11)	120(7)
H62	6874(12)	6739(12)	643(10)	128(8)
H85a	1293(8)	4679(6)	-27(6)	90
H85b	1439(8)	5437(6)	-164(6)	90
H85c	2155(8)	4964(6)	49(6)	90

Table SI42 Solvent masks information for Lu2L3_Final.

Number	X	Y	Z	Volume	Electron count	Content
1	0.155	0.209	0.033	327.6	127.0	3DCM
2	0.155	0.291	0.533	327.6	121.2	3DCM
3	-0.155	0.709	0.467	327.6	131.6	3DCM
4	-0.155	0.791	0.967	327.6	125.9	3DCM

Refinement model description

Number of restraints - 3, number of constraints - 113.

Details:

```
1. Others
 Fixed Uiso: C85(0.06) H85a(0.09) H85b(0.09) H85c(0.09)
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References

1. E. J. Bowen and R. J. Cook, *J. Chem. Soc*., **1953**, 3059-3061. DOI:10.1039/JR9530003059