Supporting Information

Self-Assembly of a Unique 3d/4f Heterometallic Square Prismatic Box-Like Coordination Cage

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Cotents

Materials

All chemicals and solvents used were of commercial grade and used without further purification.

Experimental Section

$[DyH_3L(NO_3)](NO_3)_2$: This was prepared as reported previously.[1] It was obtained as pale yellow crystals in 65% yield following recrystallization of the initial product from ethanol.

1: An excess of triethylamine (1 mL) was added to a solution of $[DyH_3\mathbf{L}(NO_3)](NO_3)_2$ (100 mg, 0.14 mmol) in methanol (10 mL). The mixture was heated at 60°C with stirring for 2 hrs leading to a clear yellow solution. $Cu(NO_3)_2.3H_2O$ (24 mg, 0.1 mmol) in methanol (10 mL) was slowly added to the stirred solution. This mixture was then heated at 80 °C for a further 2 hrs leading to a purple suspension. The precipitate was filtered off. Slow diffusion of diethyl ether into the methanol filtrate resulted in the formation of purple crystals which were air dried. Yield: 69%. FT-IR (ATR, ν_{max}/cm^{-1}): 1616, 1462, 1336, 1254, 1113, 1019, 907, 869, 805, 651, 494, 433; UV/Vis (solid state): λ_{max} 560 nm; Elemental analysis (%) (calcd., found for $C_{144}H_{232}Cu_6Dy_8N_{92}O_{68}$): C (28.72, 28.64), H (3.88, 3.73), N(21.40, 21.31); ESI-HRMS (positive-ion detection, Milli-Q water, *m/z*): cald. for $\{[Cu_6Dy_8L_8](NO_3)_7\}^{5+}$, 1026.8961; found, 1026.8967; found for $\{[Cu_6Dy_8L_8](NO_3)_{11}\}^{1+}$ 5382.4414; found for $\{[Cu_6Dy_8L_8](NO_3)_{10}\}^{2+}$ 2660.2480; found for $\{[Cu_6Dy_8L_8](NO_3)_9\}^{3+}$ 1752.8469; found for $\{[Cu_6Dy_8L_8](NO_3)_8\}^{4+}$ 1299.1299; found for $\{[Cu_6Dy_8L_8](NO_3)_6\}^{6+}$ 845.4147; found for $\{[Cu_6Dy_8L_8](NO_3)_5\}^{7+}$ 715.7747; found for $\{[Cu_6Dy_8L_8](NO_3)_4\}^{8+}$ 618.6202; Single crystals were taken from the same sample and used directly for the X-ray study.

General physical measurements

The UV-vis-NIR spectra (Figure 4) of cage **1** were measured using a Cary 5000 spectrophotometer equipped with a Labsphere Biconical Accessory. The spectrum was referenced to that of a Labsphere certified standard (Spectralon), and transformed into Kubelka-Munk units[2], $F(R) = (1-R)^2/2R$. High resolution ESI-MS data were acquired using a Waters Xevo QToF mass spectrometer, operating in positive ion mode. FT-IR spectra were recorded on a Bruker Tensor 27 Fourier transform infrared

spectrometer using a diamond single bounce ATR sampling device. The Raman spectrum (Figure S9) was recorded on a Renishaw inVia spectrometer equipped with a 514 nm excitation Ar laser. The spectrum was collected in the range 2,000-100 cm^{-1} with a spectral resolution of ~1.7 cm^{-1} and calibrated using the 520.5 cm^{-1} line of a silicon wafer. A Zeiss Ultra Plus SEM (Carl Zeiss NTS GmbH, Oberkochen, Germany) operating under an accelerating voltage of 20 kV and equipped with an electron disperse spectroscopy (EDS) unit was used to confirm the presence of key elements (Figure S7).

Magnetic measurements

Susceptibility data were collected using a PPMS9 magnetometer (Quantum Design) calibrated against a standard palladium sample. Zero-field cooled DC susceptibility was measured under the field of 1000 Oe in the range 2.5-300 K. AC susceptibility was measured using the field with the amplitude 3 Oe in the frequency range 0.1-5 kHz without DC field. The data were corrected for diamagnetism using the Pascal's constants.

Single crystal X-ray diffraction measurements

The single crystal data for cage **1** were collected on the MX1 beamline at the Australian Synchrotron. Diffraction data were collected using Si<111> monochromated synchrotron X-ray radiation (λ = 0.71074) at 100(2) K with BlueIce software[3] and were corrected for Lorentz and polarization effects using the XDS software[4]. An empirical absorption correction was then applied using SADABS[5]. The structure was solved by direct methods and the full-matrix least-squares refinements were carried out using SHELX suite of programme[6] via Olex^2 interface[7]. All non-hydrogen atoms with occupancies over 0.5 were located from the electron density map and refined anisotropically. Some disordered solvent molecules were refined isotropically. Hydrogen atoms bound to carbon atoms were added in the ideal positions and refined using a riding model.

Formula $C_{161}H_{236}Cu_6Dy_8N_{80}O_{27}$, M 5405.52, monoclinic, space group $C2/c$ (#15), a 24.673(12), b 42.718(9), c 24.298(5) Å, V 25610(15) A^3, D_c 1.402 g cm^{-3}, Z 4, crystal size 0.101 by 0.08 by 0.05 mm, colour purple, habit plate, temperature 100(2) K, λ(Synchrotron) 0.71074 Å, μ(Synchrotron) 2.854 mm^{-1},

$2\theta_{max}$ 49.508, *hkl* range -29 28, -50 50, -28 28, *N* 155733, N_{ind} 21649(R_{merge} 0.0461), N_{obs} 16971(I > 2σ(I)), N_{var} 1286, residuals* $R_1(F)$ 0.0589, $wR_2(F^2)$ 0.1652, GoF(all) 1.035, $\Delta\rho_{min,max}$ -0.78, 2.51 e^- Å^{-3}.

Table S1 | Crystal data and structure refinement for Cage 1

Empirical formula	$C_{161}H_{236}N_{80}O_{27}Cu_6Dy_8$
Formula weight	5405.52
Temperature/K	100(2)
Crystal system	monoclinic
Space group	*C*2/*c*
a/Å	24.673(12)
b/Å	42.718(9)
c/Å	24.298(5)
α/°	90
β/°	90.01(4)
γ/°	90
Volume/Å^3	25610(15)
Z	4
ρ_{calc}g/cm^3	1.402
μ/mm^{-1}	2.854 (Synchrotron)
F(000)	10720.0
Radiation	Synchrotron (λ = 0.71074)
2Θ range for data collection/°	1.906 to 49.508
Index ranges	-29 ≤ h ≤ 28, -50 ≤ k ≤ 50, -28 ≤ l ≤ 28
Reflections collected	155733
Independent reflections	21649 [R_{int} = 0.0461, R_{sigma} = 0.0231]
Data/restraints/parameters	21649/0/1286
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0589, wR_2 = 0.1652
Final R indexes [all data]	R_1 = 0.0741, wR_2 = 0.1779
Largest diff. peak/hole / e Å^{-3}	2.51/-0.78

* $R_1 = \Sigma||F_O| - |F_C||/\Sigma|F_O|$ for $F_O > 2\sigma(F_O)$; $wR_2 = (\Sigma w(F_O^2 - F_C^2)^2/\Sigma(wF_C^2)^2)^{1/2}$ all reflections
$w=1/[\sigma^2(F_O^2)+(0.2000P)^2+100.0000P]$ where $P=(F_O^2+2F_C^2)/3$

Specific details. The crystals employed in this study decayed rapidly out of solvent. Rapid handling (< 1 min) at dry-ice temperature, quenching in the nitrogen cryostream and much shorter time for data collection at the Australian Synchrotron significantly improved the data quality. In addition, the unit cell contains substantial solvent accessible voids (1913.84 Å^3, ~7.5 % of the unit cell) with a large amount of disordered nitrate anions and solvent molecules (methanol, water and diethyl ether) shown in figure S12.

The voids are mainly between the cages in the crystal lattice, which is common for such type of cage compound. As the contribution from these disordered anions and solvent molecules is quite small with the largest electron residue peak at around 2, they were not removed for the final structure refinement.

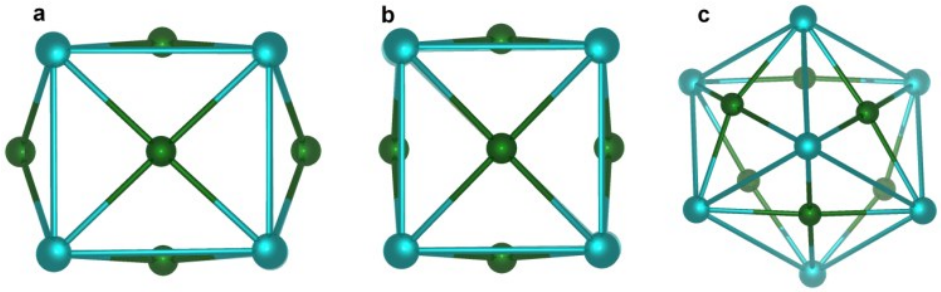
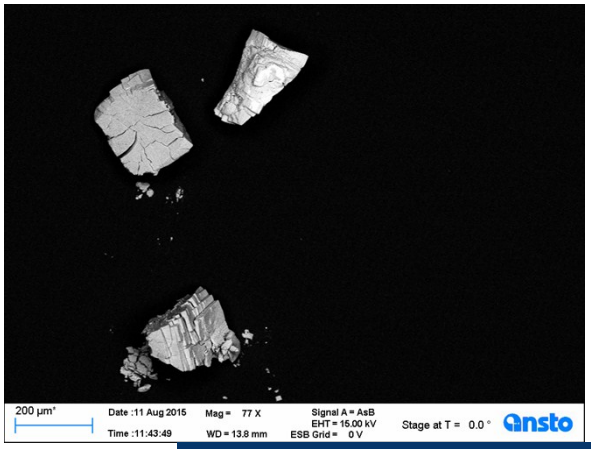


Figure S1. Three schematics of the nanocage **1** topology. Color codes: Cu-green, Dy-cyan. (a) Perspective view along a C2 symmetry axis highlighting one of the face-centred Cu(II) ions (coordinated by one of two disorder waters); (b) Perspective view along a C4 symmetry axis highlighting a second face-centred Cu(II) site (coordinated with one of four waters); (c) view through one of the Dy(III) corners.



Element	Weight%
C K	16.54
N K	5.59
O K	61.98
Dy L	9.25
Cu K	6.64
Totals	100.00
Dy: Cu= 4.0 : 2.9	

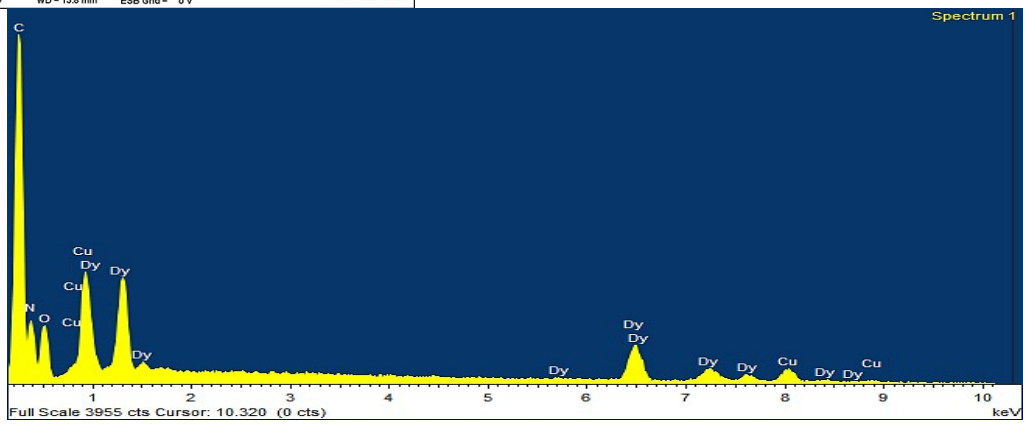


Figure S2 A backscattered SEM image and an EDS spectrum of cage **1** confirming the atomic ratio of Dy:Cu =4:3.

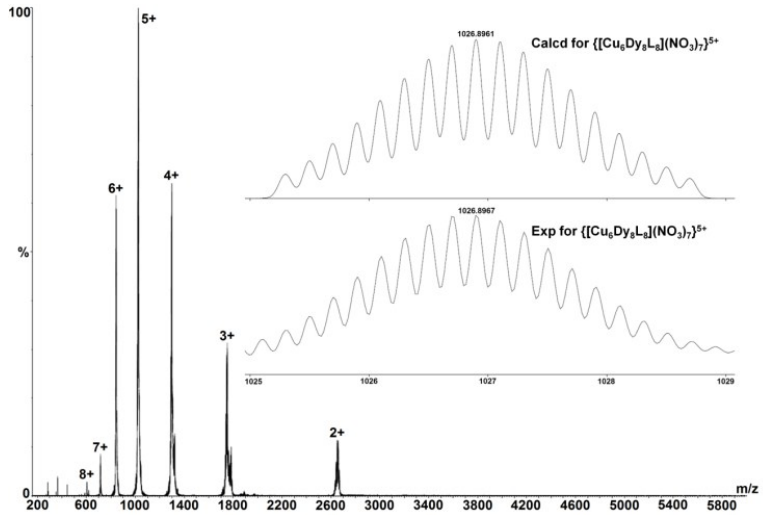


Figure S3. ESI-HRMS spectrum of coordination cage **1**. The inset shows the isotope pattern for $\{[Cu_6Dy_8L_8](NO_3)_7\}^{5+}$.

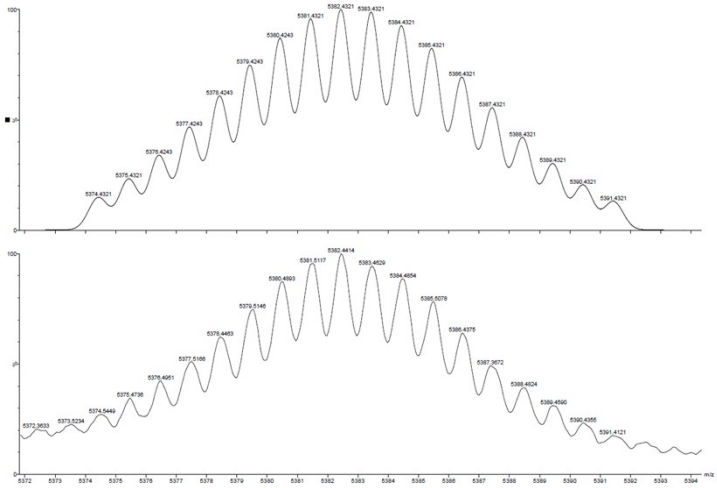


Figure S4 The isotope pattern (bottom) with the simulated distribution (top) for $\{[Cu_6Dy_8L_8](NO_3)_{11}\}^{1+}$.

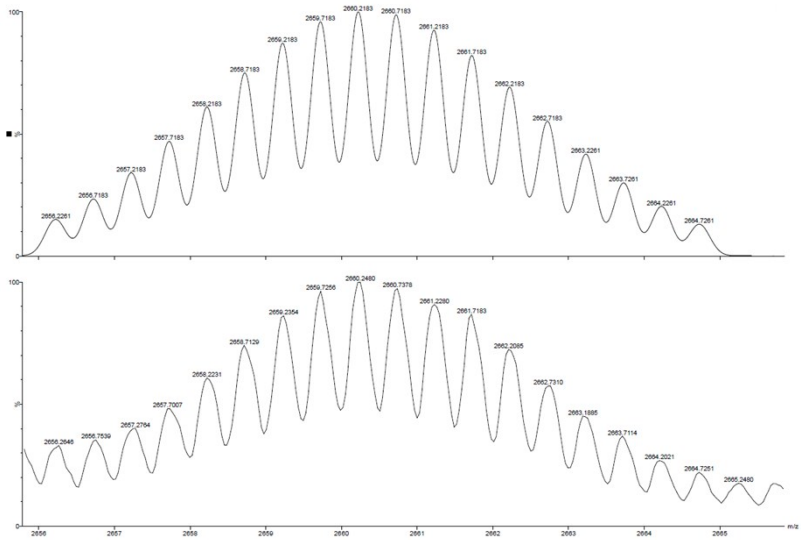


Figure S5 The isotope pattern (bottom) with the simulated distribution (top) for $\{[Cu_6Dy_8L_8](NO_3)_{10}\}^{2+}$.

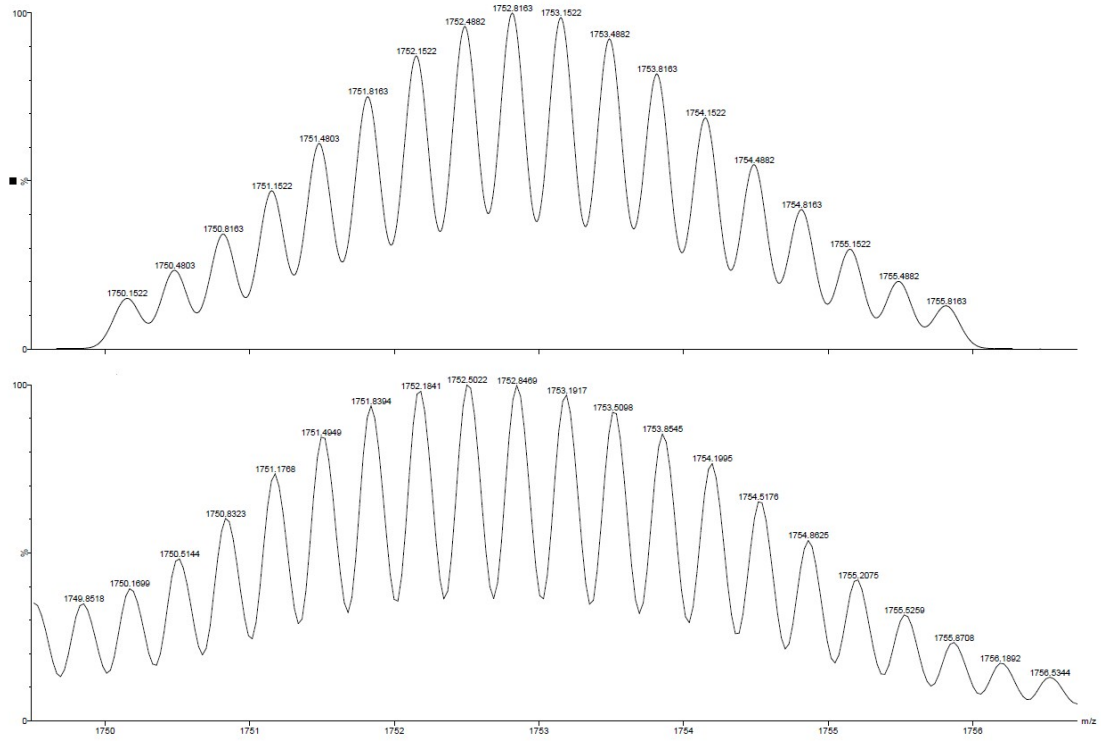


Figure S6 The isotope pattern (bottom) with the simulated distribution (top) for $\{[Cu_6Dy_8L_8](NO_3)_9\}^{3+}$.

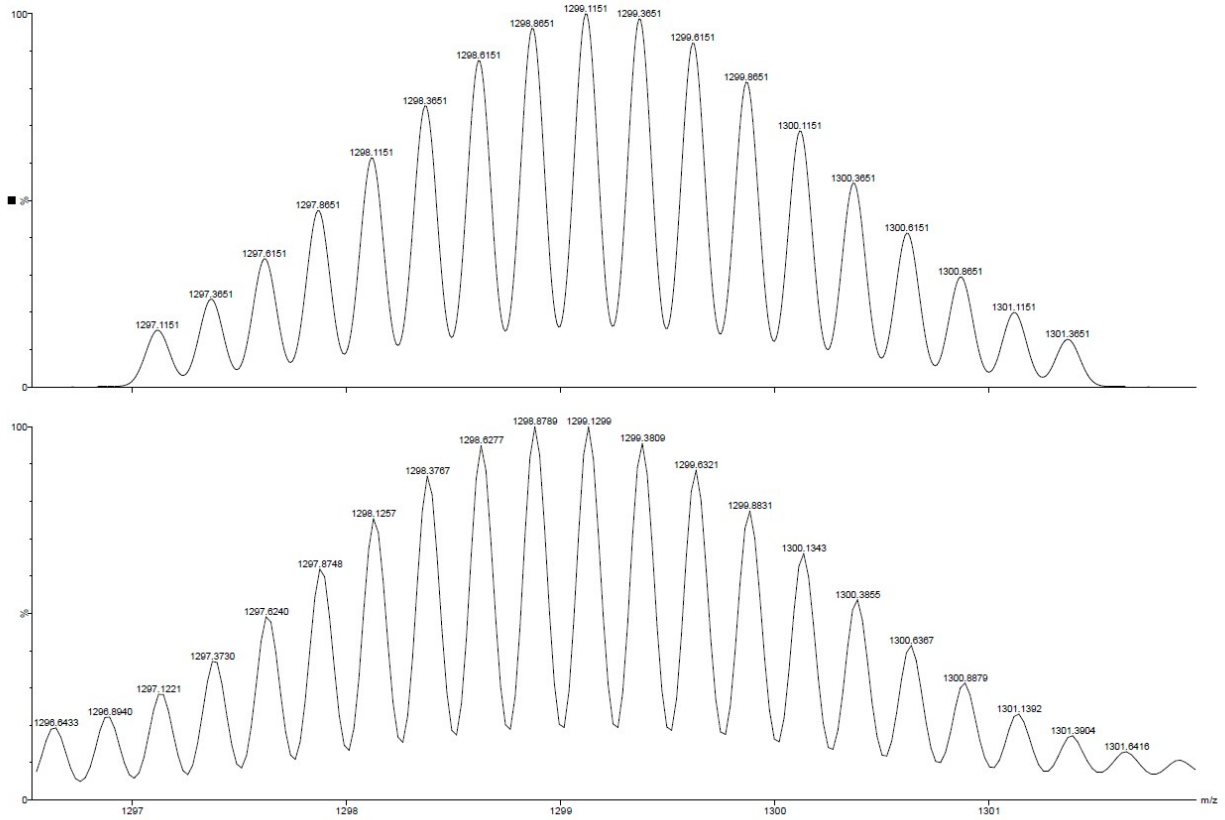


Figure S7 The isotope pattern (bottom) with the simulated distribution (top) for $\{[Cu_6Dy_8L_8](NO_3)_8\}^{4+}$.

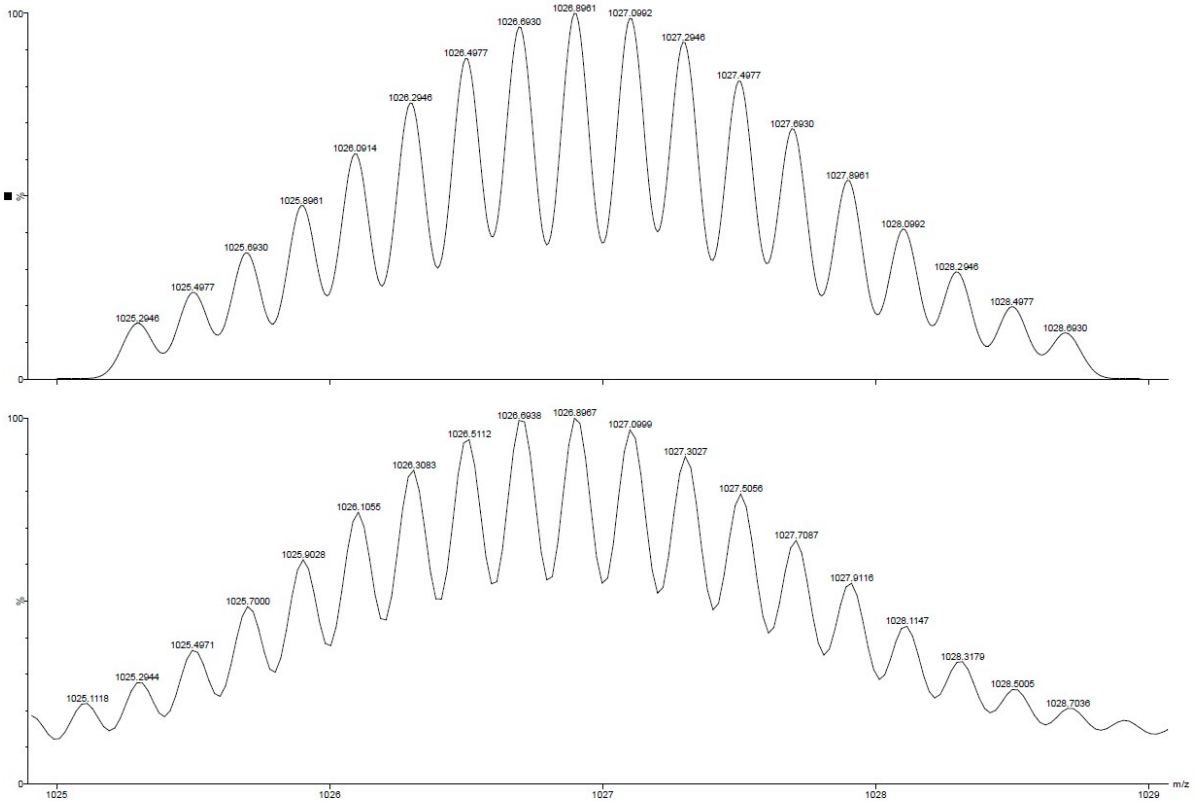


Figure S8 The isotope pattern (bottom) with the simulated distribution (top) for $\{[Cu_6Dy_8L_8](NO_3)_7\}^{5+}$.

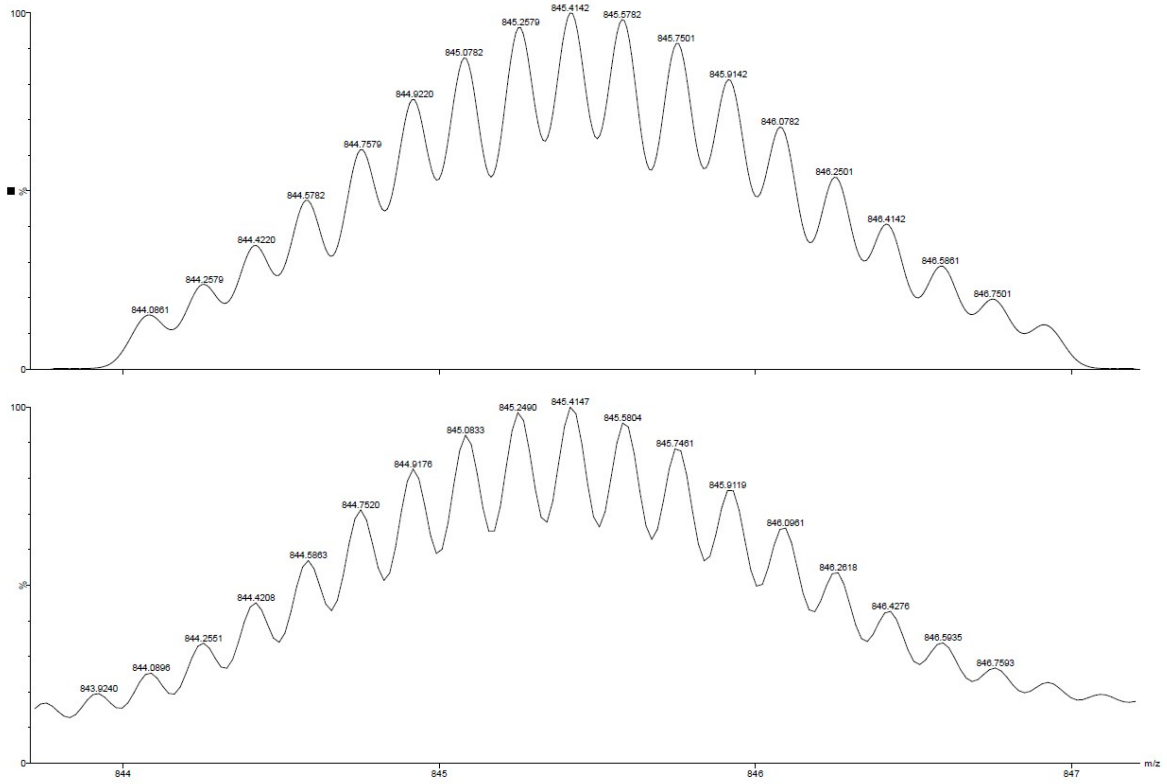


Figure S9 The isotope pattern (bottom) with the simulated distribution (top) for $\{[Cu_6Dy_8L_8](NO_3)_6\}^{6+}$.

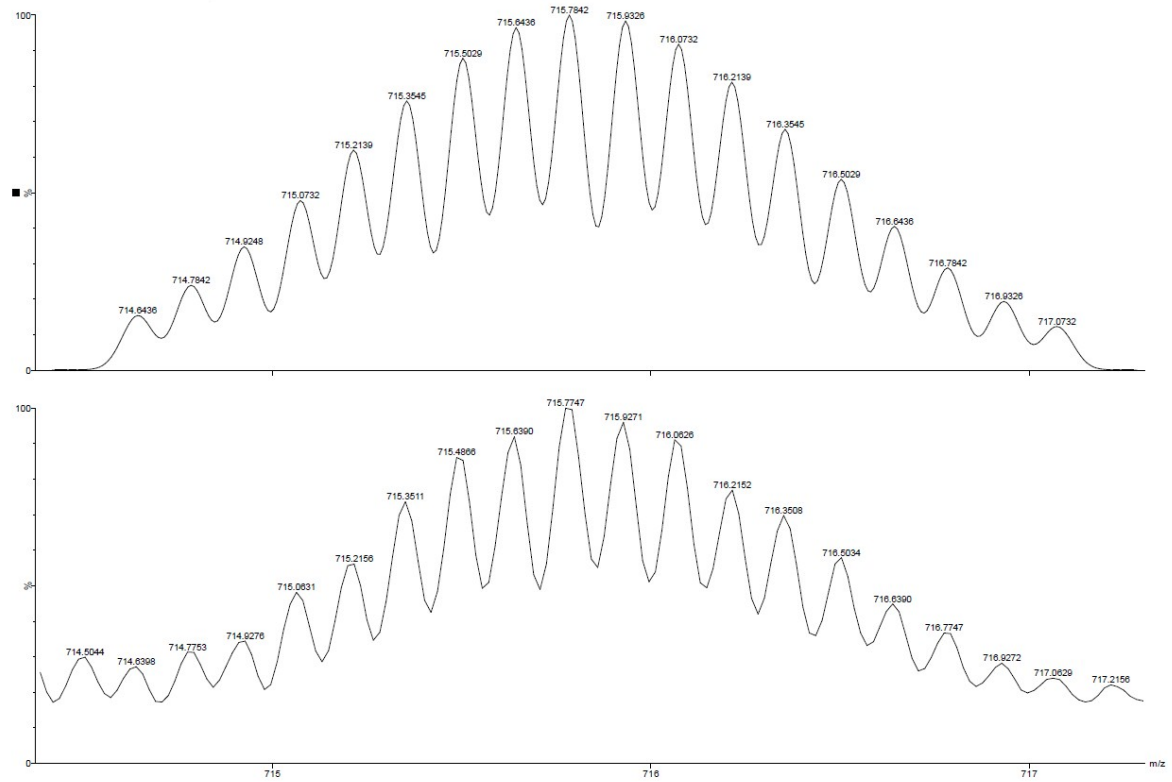


Figure S10 The isotope pattern (bottom) with the simulated distribution (top) for $\{[Cu_6Dy_8L_8](NO_3)_5\}^{7+}$.

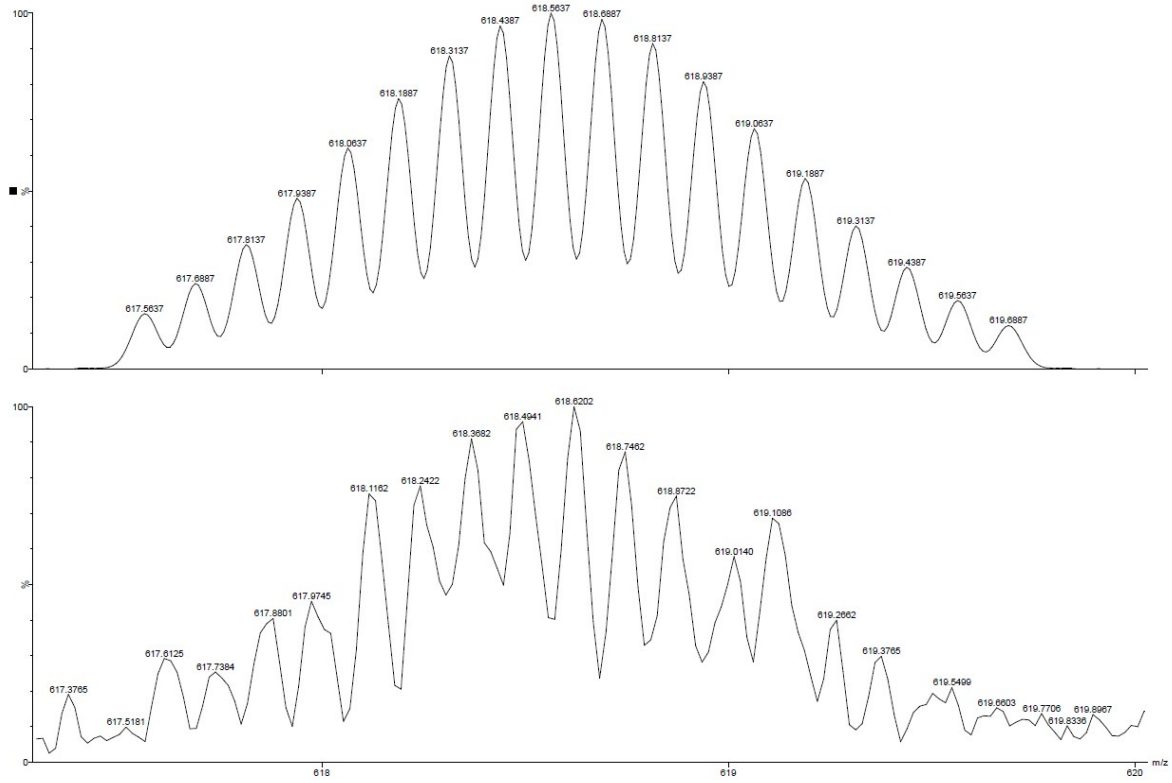


Figure S11 The isotope pattern (bottom) with the simulated distribution (top) for $\{[Cu_6Dy_8L_8](NO_3)_4\}^{8+}$.

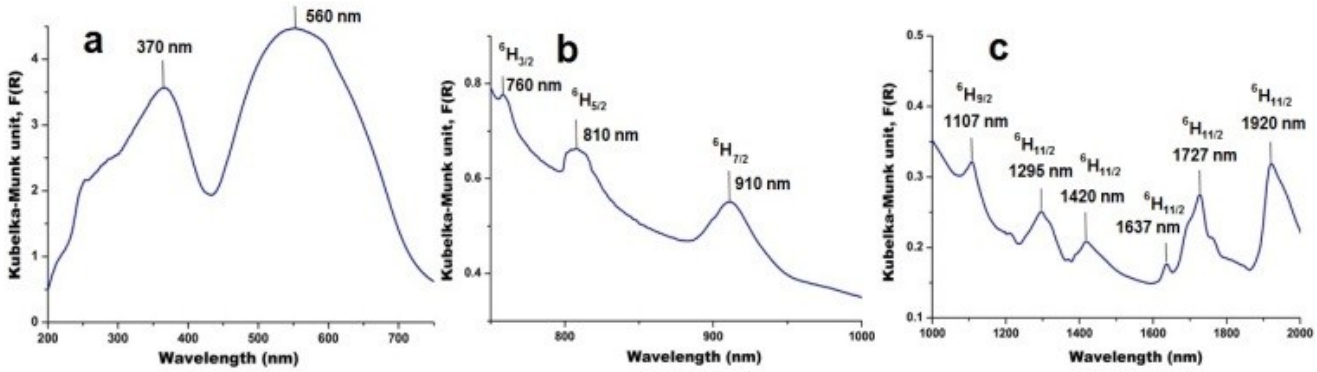


Figure S12. The absorption spectrum of cage **1** in 2,000–200 nm region.

Table S2 Upper states of Dy(III) ions.

Cage 1	**Dy(III)**		
nm		**nm**	**cm^{-1}**
1920	$^6H_{11/2}$		
1637, 1727	$^6H_{11/2}$	1674	5973
1295, 1420	$^6H_{11/2}$	1262	7924
1107	$^6H_{9/2}$	1097	9116
910	$^6H_{7/2}$	890	11236
810	$^6H_{5/2}$	792	12626
760	$^6H_{3/2}$	753	13280

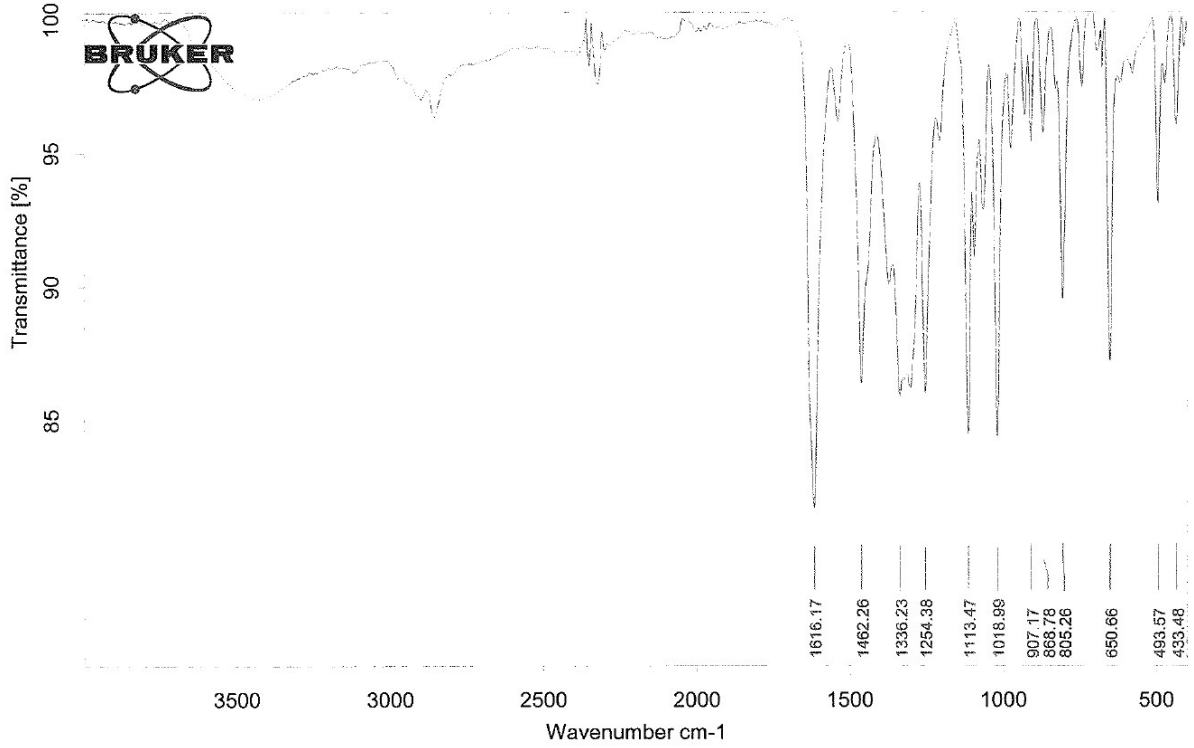


Figure S13 FT-IR spectrum of Cage **1.**

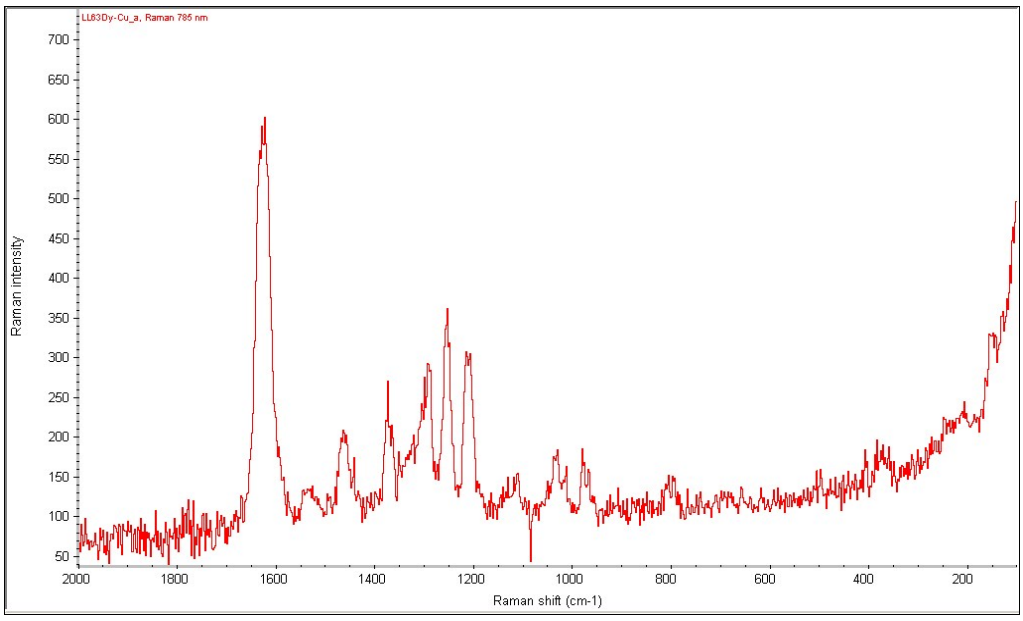


Figure S14 A Raman spectrum of cage **1** in 2,000–200 cm^{-1} region.

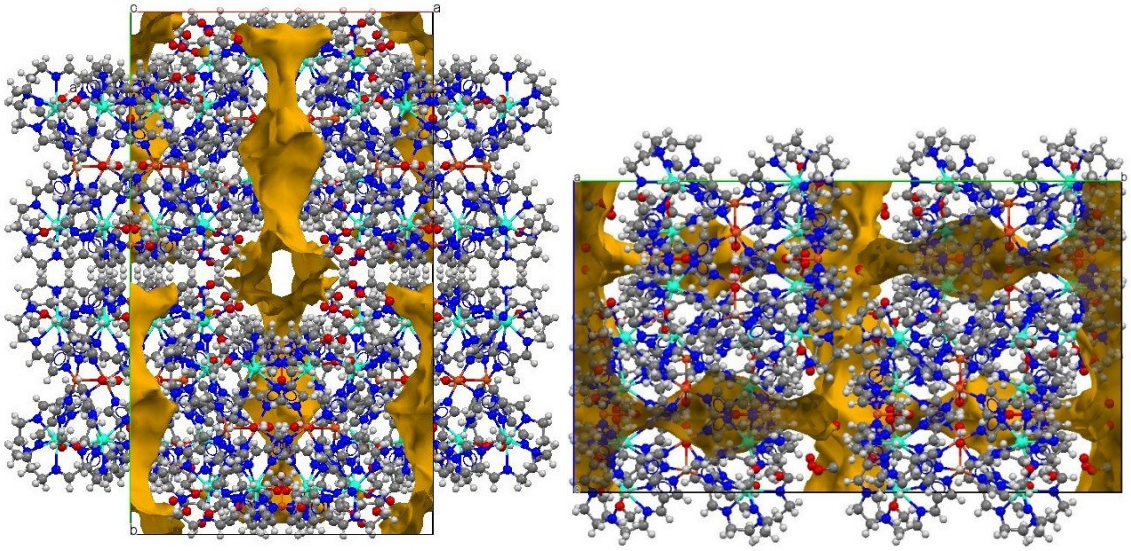


Figure S15 The representation of the crystal packing of **1** containing substantial solvent accessible voids.

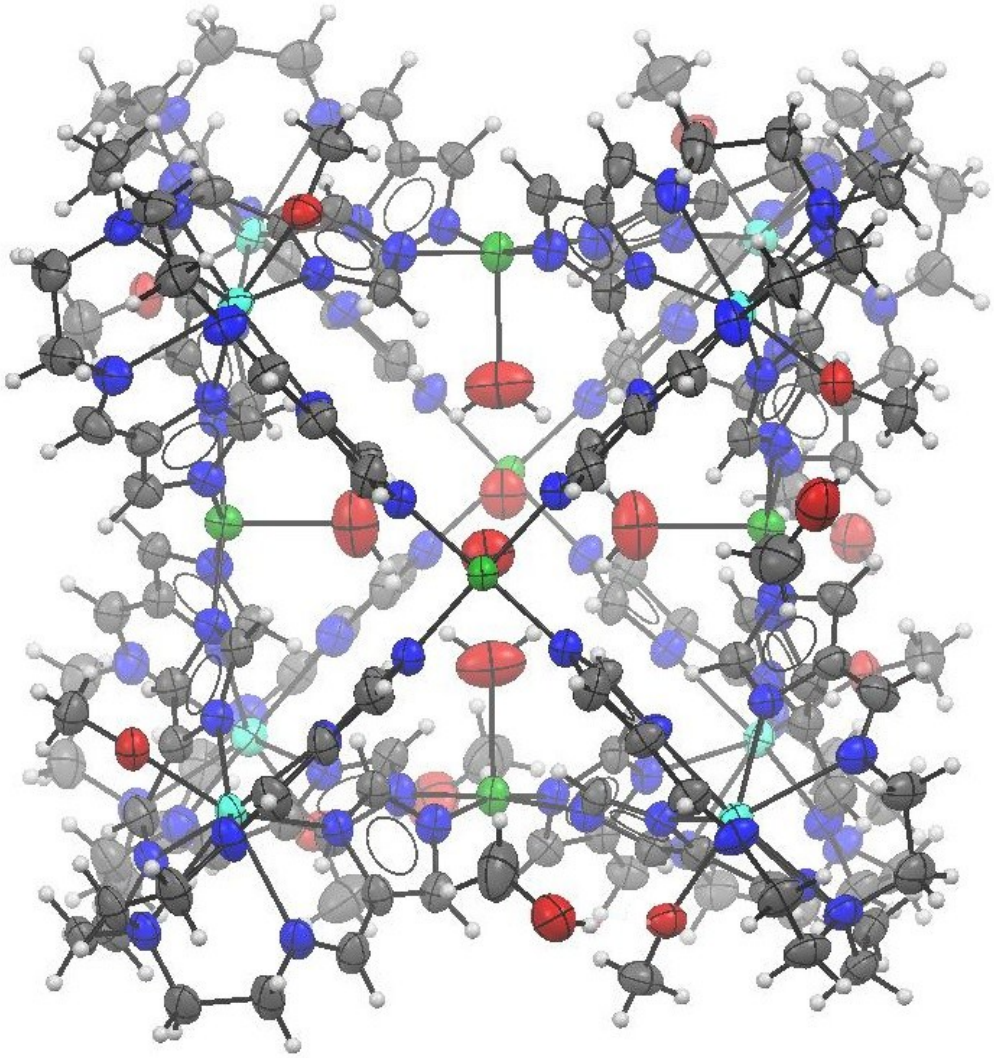


Figure S16 The ORTEP representation of **1** in 50% ellipsoid.

Table S3 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **1**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Dy1	866.0(2)	4072.5(2)	4951.7(2)	37.24(12)
Dy2	-2421.7(2)	1818.9(2)	3394.3(2)	38.93(12)
Dy3	917.9(2)	1818.1(2)	4938.3(2)	38.98(12)
Dy4	2417.9(2)	4082.8(2)	1595.8(2)	42.49(13)
Cu1	0	1472.4(3)	2500	35.0(3)
Cu2	0	4457.6(3)	2500	39.8(3)
Cu3	-816.7(4)	2943.5(2)	4287.5(4)	40.0(2)
Cu4	1784.5(4)	2959.6(2)	3331.4(4)	39.7(2)
O1	136(2)	4159.9(13)	5446(2)	49.7(14)
O2	-2272(2)	1678.8(13)	4244(2)	50.2(14)
O3	1761(2)	1687.9(13)	4795(2)	48.7(13)
O4	2855(3)	4222.7(14)	2346(3)	58.0(16)
O5	-422(4)	2945.1(16)	3420(4)	94(3)

O6	927(4)	2953.2(16)	2906(4)	95(3)
N1	1355(3)	4299.4(16)	5843(3)	48.8(17)
N2	839(3)	4651.9(15)	5014(3)	44.4(16)
N3	616(3)	4318.4(14)	4088(3)	38.6(14)
N4	288(3)	4482.0(14)	3262(3)	42.6(15)
N5	1844(3)	4204.7(15)	4827(3)	42.6(15)
N6	1360(2)	3720.8(13)	4309(2)	34.7(13)
N7	1699(3)	3354.6(14)	3742(3)	38.9(14)
N8	1106(3)	3660.1(15)	5614(3)	46.2(16)
N9	327(3)	3593.2(13)	4803(2)	37.0(14)
N10	-216(3)	3183.1(14)	4629(3)	43.6(15)
N11	-3401(3)	1576.7(16)	3607(3)	46.2(16)
N12	-2458(3)	1240.2(15)	3347(3)	49.5(17)
N13	-1598(3)	1596.9(14)	3010(3)	40.7(15)
N14	-768(3)	1450.3(14)	2731(3)	38.4(14)
N15	-3068(3)	2213.5(15)	3751(3)	42.4(15)
N16	-1957(3)	2287.8(14)	3755(3)	37.8(14)
N17	-1468(2)	2698.7(13)	4052(3)	38.0(14)
N18	-3021(3)	1729.4(17)	2569(3)	50.7(18)
N19	-2286(2)	2198.0(14)	2627(3)	38.1(14)
N20	-2054(3)	2561.8(14)	1992(3)	41.9(15)
N21	1137(3)	1568.8(17)	5926(3)	49.0(17)
N22	101(3)	1715.6(17)	5531(3)	51.7(18)
N23	144(2)	2193.0(14)	4791(3)	38.4(14)
N24	-488(3)	2542.5(14)	4556(3)	39.7(14)
N25	887(3)	1234.3(16)	4972(3)	51.5(18)
N26	537(3)	1595.4(14)	4115(3)	40.0(14)
N27	231(3)	1448.2(14)	3276(3)	38.3(14)
N28	1242(3)	2209.5(16)	5606(3)	44.4(15)
N29	1257(2)	2294.3(13)	4477(2)	36.3(13)
N30	1542(3)	2713.3(13)	3986(3)	40.0(14)
N31	3293(3)	4323.9(18)	1100(3)	55.2(18)
N32	2320(3)	4178.4(16)	597(3)	49.9(17)
N33	1814(3)	3701.1(14)	1120(3)	41.5(15)
N34	1227(3)	3340.5(14)	802(3)	39.8(14)
N35	2429(3)	4666.4(16)	1546(3)	52.5(18)
N36	1550(3)	4312.4(14)	1854(3)	44.4(15)
N37	745(3)	4467.8(14)	2194(3)	40.7(14)
N38	3117(3)	3690.9(17)	1407(3)	52.8(18)
N39	2296(3)	3612.0(14)	2176(3)	39.6(14)
N40	2119(3)	3198.4(14)	2720(3)	43.5(15)
C1	1009(4)	4572.6(19)	6005(4)	55(2)
C2	970(4)	4813.5(19)	5533(3)	53(2)
C3	622(3)	4802.4(18)	4620(3)	45.3(19)
C4	511(3)	4634.5(17)	4116(3)	40.8(17)
C5	324(3)	4733.7(18)	3599(3)	45.3(19)
C6	469(3)	4239.8(18)	3574(3)	42.3(18)

C7	1929(4)	4395(2)	5757(4)	54(2)
C8	2080(4)	4460(2)	5160(4)	54(2)
C9	2137(3)	4045.2(17)	4502(4)	44.3(19)
C10	1905(3)	3789.3(16)	4204(3)	36.7(16)
C11	2110(3)	3571.1(17)	3862(3)	42.3(18)
C12	1265(3)	3462.7(17)	4021(3)	37.5(16)
C13	1308(4)	4060.6(19)	6278(3)	54(2)
C14	1479(4)	3735(2)	6055(4)	55(2)
C15	843(4)	3404.8(19)	5603(4)	51(2)
C16	443(3)	3355.8(17)	5177(3)	39.9(17)
C17	108(3)	3107.5(19)	5065(3)	45.5(19)
C18	-65(3)	3478.1(18)	4493(3)	42.0(18)
C19	-202(4)	3974(3)	5783(4)	69(3)
C20	-3278(4)	1276(2)	3899(4)	53(2)
C21	-2925(4)	1061(2)	3559(4)	60(2)
C22	-2023(4)	1092.8(19)	3204(4)	52(2)
C23	-1567(3)	1271.6(17)	3022(3)	41.3(17)
C24	-1058(3)	1183.4(19)	2848(4)	47.9(19)
C25	-1109(3)	1689.6(17)	2838(3)	38.2(16)
C26	-3751(4)	1524(2)	3128(4)	56(2)
C27	-3433(4)	1485(2)	2591(4)	62(3)
C28	-2984(4)	1911(2)	2153(3)	51(2)
C29	-2590(3)	2157.6(18)	2157(3)	41.8(18)
C30	-2444(3)	2378.3(19)	1766(3)	45.4(19)
C31	-1981(3)	2448.4(16)	2503(3)	38.8(17)
C32	-3675(3)	1794(2)	3993(4)	51(2)
C33	-3638(3)	2133(2)	3794(4)	52(2)
C34	-2877(3)	2462.4(19)	3943(3)	46.0(19)
C35	-2310(3)	2523.9(18)	3933(3)	41.8(17)
C36	-2005(3)	2770.8(17)	4115(3)	40.6(17)
C37	-1462(3)	2409.9(17)	3838(3)	39.1(17)
C38	-2260(4)	1832(2)	4750(4)	57(2)
C39	648(4)	1507(2)	6270(4)	59(2)
C40	133(4)	1465(2)	5938(4)	61(3)
C41	-322(3)	1889(2)	5490(4)	54(2)
C42	-321(3)	2142(2)	5104(3)	46.5(19)
C43	-707(3)	2353.0(18)	4945(3)	45.7(19)
C44	21(3)	2433.4(16)	4486(3)	38.6(17)
C45	1428(4)	1277(2)	5796(4)	57(2)
C46	1109(4)	1057(2)	5445(4)	59(2)
C47	739(4)	1090.0(19)	4539(4)	48(2)
C48	544(3)	1269.0(17)	4071(3)	43.0(18)
C49	353(4)	1179.3(19)	3562(3)	47.8(19)
C50	340(3)	1686.3(17)	3623(3)	37.8(16)
C51	1503(4)	1797(2)	6214(4)	53(2)
C52	1286(4)	2127(2)	6182(3)	51(2)
C53	1419(3)	2468.7(19)	5419(4)	46.6(19)

C54	1425(3)	2532.0(17)	4839(3)	38.3(16)
C55	1590(3)	2784.4(18)	4535(3)	41.0(17)
C56	1341(3)	2417.9(18)	3980(3)	40.9(17)
C57	2256(3)	1849(2)	4813(4)	58(2)
C58	3227(4)	4383(2)	494(4)	62(3)
C59	2630(4)	4427(2)	326(4)	59(2)
C60	2003(4)	4006.5(19)	304(4)	49(2)
C61	1715(3)	3756.3(17)	563(3)	39.0(17)
C62	1360(3)	3539.6(17)	371(3)	41.1(17)
C63	1515(3)	3451.2(17)	1230(3)	38.5(17)
C64	3404(4)	4615(2)	1406(4)	61(2)
C65	2926(4)	4835(2)	1403(4)	64(3)
C66	2024(4)	4809.8(19)	1744(3)	49(2)
C67	1546(4)	4637.4(17)	1890(3)	44.2(19)
C68	1054(4)	4729.6(19)	2098(3)	47.3(19)
C69	1063(3)	4228.6(18)	2038(3)	43.9(18)
C70	3738(4)	4099(2)	1183(5)	66(3)
C71	3566(4)	3768(2)	1056(4)	63(3)
C72	3095(4)	3429(2)	1676(4)	54(2)
C73	2679(3)	3377.0(18)	2069(3)	42.6(18)
C74	2563(4)	3126.8(18)	2407(3)	47.4(19)
C75	1980(3)	3496.6(17)	2558(3)	42.0(18)
C76	3170(6)	4048(3)	2729(5)	89(4)
O16	0	3878.8(18)	2500	61(2)
O14	3135(7)	4555(4)	3925(8)	100(5)
O9	1989(3)	1275.5(18)	4026(3)	77(2)
C77	1894(6)	1451(3)	3525(5)	95(4)
O18	-1413(6)	645(4)	4154(7)	80(4)
O10	2400(4)	4604(2)	3028(4)	106(3)
C78	1924(6)	4476(3)	3256(5)	88(4)
O15	2643(8)	5219(5)	2856(8)	105(6)
O11	-636(3)	4482.5(16)	4963(3)	71.1(19)
C79	-764(5)	4359(2)	4427(5)	71(3)
O17	0	2045.3(19)	2500	70(3)
O12	-1529(4)	1249.9(19)	4478(3)	84(2)
C80	-1004(6)	1416(3)	4389(6)	98(4)
O19	1712(5)	683(3)	3905(6)	65(3)
O13	-1435(5)	4465(3)	5709(5)	52(3)
C81	-1712(7)	4736(4)	5797(7)	48(4)

Table S4 Anisotropic Displacement Parameters ($Å^2 \times 10^3$). 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_{23}**	**U_{13}**	**U_{12}**
Dy1	48.4(2)	30.5(2)	32.8(2)	-4.04(13)	1.17(15)	-1.53(14)
Dy2	42.6(2)	33.5(2)	40.7(2)	-2.55(14)	11.57(16)	-6.24(14)
Dy3	42.8(2)	35.7(2)	38.4(2)	6.34(14)	-5.73(15)	-1.67(15)

Dy4	48.0(2)	34.3(2)	45.1(2)	4.42(15)	1.19(17)	-7.40(15)
Cu1	38.8(7)	32.3(6)	33.8(7)	0	4.0(5)	0
Cu2	53.1(8)	34.0(7)	32.4(7)	0	-0.1(6)	0
Cu3	44.0(5)	28.4(5)	47.5(5)	0.2(4)	-1.1(4)	1.0(4)
Cu4	52.8(6)	27.2(5)	39.1(5)	-1.1(4)	5.7(4)	2.0(4)
O1	61(4)	40(3)	48(3)	-3(3)	15(3)	-1(3)
O2	59(4)	48(3)	44(3)	-1(3)	11(3)	-4(3)
O3	45(3)	49(3)	52(3)	9(3)	-6(3)	-1(3)
O4	67(4)	50(4)	57(4)	2(3)	-13(3)	-12(3)
O5	136(8)	52(4)	92(6)	-1(4)	38(6)	-11(5)
O6	96(6)	54(4)	135(8)	9(5)	-39(6)	-2(4)
N1	61(4)	44(4)	42(4)	-6(3)	-11(3)	-1(3)
N2	61(4)	41(4)	32(3)	-7(3)	0(3)	-3(3)
N3	51(4)	28(3)	37(3)	-2(3)	-3(3)	-2(3)
N4	60(4)	34(3)	34(3)	1(3)	-3(3)	1(3)
N5	49(4)	37(3)	42(4)	-8(3)	-1(3)	-4(3)
N6	46(4)	22(3)	36(3)	-5(2)	4(3)	0(2)
N7	48(4)	32(3)	36(3)	1(3)	3(3)	-1(3)
N8	55(4)	41(4)	43(4)	-1(3)	-7(3)	2(3)
N9	45(4)	29(3)	36(3)	-4(3)	-1(3)	0(3)
N10	44(4)	33(3)	54(4)	7(3)	-3(3)	1(3)
N11	48(4)	43(4)	47(4)	2(3)	10(3)	-11(3)
N12	57(4)	34(3)	58(4)	-2(3)	19(3)	-15(3)
N13	44(4)	35(3)	43(4)	-5(3)	10(3)	-4(3)
N14	45(4)	31(3)	39(3)	1(3)	4(3)	-3(3)
N15	41(4)	37(4)	50(4)	-1(3)	11(3)	0(3)
N16	43(4)	31(3)	39(3)	-3(3)	3(3)	5(3)
N17	40(3)	26(3)	48(4)	-3(3)	0(3)	3(3)
N18	57(4)	49(4)	46(4)	-8(3)	10(3)	-23(3)
N19	42(3)	33(3)	39(3)	-3(3)	7(3)	-3(3)
N20	57(4)	27(3)	42(4)	-3(3)	4(3)	-5(3)
N21	50(4)	52(4)	45(4)	12(3)	-8(3)	3(3)
N22	53(4)	48(4)	54(4)	22(3)	-4(3)	-8(3)
N23	39(3)	36(3)	41(4)	4(3)	-1(3)	-3(3)
N24	42(4)	27(3)	49(4)	2(3)	0(3)	-2(3)
N25	65(5)	36(4)	53(4)	14(3)	-15(4)	-1(3)
N26	44(4)	34(3)	41(4)	2(3)	-8(3)	-1(3)
N27	47(4)	31(3)	37(3)	0(3)	3(3)	2(3)
N28	48(4)	49(4)	36(4)	3(3)	-6(3)	-2(3)
N29	41(3)	31(3)	37(3)	-2(3)	0(3)	1(3)
N30	54(4)	26(3)	40(4)	-1(3)	4(3)	-1(3)
N31	56(4)	55(4)	55(4)	11(4)	7(3)	-15(4)
N32	55(4)	46(4)	49(4)	8(3)	8(3)	-15(3)
N33	47(4)	32(3)	46(4)	5(3)	4(3)	-5(3)
N34	45(4)	27(3)	47(4)	6(3)	2(3)	1(3)
N35	61(5)	38(4)	58(5)	5(3)	-1(4)	-16(3)
N36	56(4)	31(3)	47(4)	3(3)	2(3)	-5(3)

N37	55(4)	31(3)	36(3)	2(3)	1(3)	-1(3)
N38	52(4)	51(4)	55(4)	8(3)	8(3)	1(3)
N39	49(4)	30(3)	40(3)	0(3)	0(3)	-2(3)
N40	60(4)	28(3)	42(4)	-1(3)	8(3)	4(3)
C1	83(6)	40(5)	43(5)	-22(4)	-7(4)	-1(4)
C2	81(6)	39(4)	39(4)	-16(4)	1(4)	-1(4)
C3	58(5)	33(4)	44(5)	-6(3)	3(4)	4(4)
C4	57(5)	30(4)	35(4)	-1(3)	-4(3)	-1(3)
C5	63(5)	32(4)	42(4)	0(3)	-2(4)	0(4)
C6	59(5)	32(4)	36(4)	-5(3)	6(3)	-2(3)
C7	68(6)	44(5)	50(5)	-12(4)	-12(4)	-5(4)
C8	60(5)	41(5)	60(6)	-15(4)	-9(4)	-5(4)
C9	38(4)	35(4)	60(5)	0(4)	-3(4)	-5(3)
C10	44(4)	24(3)	42(4)	0(3)	2(3)	-3(3)
C11	42(4)	35(4)	50(5)	2(3)	3(3)	-2(3)
C12	44(4)	37(4)	31(4)	-5(3)	6(3)	-4(3)
C13	85(7)	48(5)	30(4)	-3(3)	-16(4)	-4(4)
C14	77(6)	43(5)	45(5)	4(4)	-17(4)	0(4)
C15	62(5)	35(4)	55(5)	5(4)	-5(4)	1(4)
C16	47(4)	34(4)	39(4)	2(3)	2(3)	3(3)
C17	49(5)	39(4)	49(5)	5(4)	1(4)	-2(4)
C18	44(4)	34(4)	48(5)	-2(3)	3(4)	7(3)
C19	74(7)	71(7)	61(6)	-2(5)	18(5)	-4(5)
C20	51(5)	50(5)	59(5)	5(4)	21(4)	-15(4)
C21	62(6)	49(5)	69(6)	-1(4)	25(5)	-15(4)
C22	58(5)	33(4)	64(6)	-5(4)	13(4)	-11(4)
C23	47(4)	33(4)	44(4)	-2(3)	11(3)	-5(3)
C24	52(5)	36(4)	55(5)	-3(4)	3(4)	-7(4)
C25	39(4)	34(4)	41(4)	1(3)	8(3)	-4(3)
C26	56(5)	62(6)	51(5)	-7(4)	9(4)	-29(4)
C27	69(6)	66(6)	50(5)	-8(4)	18(4)	-38(5)
C28	65(6)	51(5)	38(4)	-7(4)	6(4)	-19(4)
C29	50(5)	33(4)	42(4)	-3(3)	13(4)	-8(3)
C30	54(5)	44(4)	38(4)	-2(3)	3(4)	0(4)
C31	47(4)	28(4)	41(4)	-1(3)	4(3)	-8(3)
C32	43(5)	63(6)	47(5)	-3(4)	14(4)	-9(4)
C33	42(5)	56(5)	60(5)	-4(4)	12(4)	4(4)
C34	48(5)	38(4)	53(5)	-5(4)	10(4)	8(4)
C35	45(4)	37(4)	43(4)	-3(3)	4(3)	-1(3)
C36	49(5)	27(4)	45(4)	-3(3)	7(3)	-1(3)
C37	46(4)	31(4)	41(4)	2(3)	7(3)	-1(3)
C38	69(6)	61(6)	41(5)	-6(4)	6(4)	-2(5)
C39	63(6)	62(6)	52(5)	28(4)	-4(4)	-7(4)
C40	53(5)	65(6)	65(6)	35(5)	-9(4)	-13(4)
C41	40(5)	55(5)	66(6)	23(4)	3(4)	-2(4)
C42	44(5)	49(5)	46(5)	9(4)	-5(4)	0(4)
C43	42(4)	41(4)	54(5)	3(4)	1(4)	2(3)

C44	44(4)	27(4)	44(4)	4(3)	-1(3)	-1(3)
C45	55(5)	56(5)	60(6)	21(4)	-18(4)	-1(4)
C46	72(6)	51(5)	56(5)	18(4)	-14(5)	7(4)
C47	60(5)	32(4)	52(5)	8(4)	-8(4)	3(4)
C48	53(5)	32(4)	45(4)	4(3)	-8(4)	3(3)
C49	67(5)	33(4)	43(5)	2(3)	3(4)	-1(4)
C50	41(4)	33(4)	39(4)	5(3)	-5(3)	2(3)
C51	52(5)	68(6)	39(5)	12(4)	-11(4)	1(4)
C52	62(5)	60(5)	33(4)	2(4)	-4(4)	-4(4)
C53	48(5)	39(4)	53(5)	-8(4)	-11(4)	-1(4)
C54	46(4)	34(4)	36(4)	1(3)	-2(3)	4(3)
C55	46(4)	35(4)	42(4)	-1(3)	-1(3)	-5(3)
C56	51(5)	37(4)	35(4)	-2(3)	3(3)	5(3)
C57	39(5)	63(6)	72(6)	14(5)	-5(4)	-2(4)
C58	68(6)	58(6)	61(6)	11(5)	16(5)	-18(5)
C59	75(6)	48(5)	53(5)	14(4)	3(5)	-24(4)
C60	58(5)	43(4)	45(5)	7(4)	4(4)	-2(4)
C61	46(4)	34(4)	37(4)	0(3)	4(3)	0(3)
C62	47(4)	39(4)	37(4)	2(3)	1(3)	0(3)
C63	44(4)	34(4)	37(4)	5(3)	3(3)	-5(3)
C64	54(5)	56(5)	73(7)	8(5)	3(5)	-22(4)
C65	75(7)	42(5)	74(7)	3(4)	7(5)	-27(5)
C66	71(6)	31(4)	46(5)	5(3)	-3(4)	-4(4)
C67	62(5)	29(4)	42(4)	9(3)	-1(4)	-4(3)
C68	66(5)	34(4)	41(4)	1(3)	-2(4)	3(4)
C69	59(5)	35(4)	37(4)	6(3)	6(4)	-7(4)
C70	41(5)	72(7)	86(7)	14(5)	12(5)	-8(4)
C71	53(5)	63(6)	73(7)	9(5)	19(5)	5(4)
C72	58(5)	43(5)	62(6)	0(4)	11(4)	7(4)
C73	52(5)	36(4)	40(4)	-1(3)	3(3)	1(3)
C74	61(5)	33(4)	48(5)	3(3)	7(4)	2(4)
C75	55(5)	30(4)	41(4)	-2(3)	-1(4)	1(3)
C76	104(9)	91(9)	72(8)	11(6)	-29(7)	-18(7)
O16	82(6)	27(4)	73(6)	0	6(5)	0
O9	72(5)	82(5)	75(5)	-7(4)	7(4)	10(4)
C77	114(10)	104(10)	66(7)	9(7)	22(7)	-30(8)
O10	117(7)	112(7)	89(7)	-38(5)	-2(5)	-20(6)
C78	101(9)	90(9)	72(8)	21(6)	-7(7)	1(7)
O11	83(5)	58(4)	72(5)	-2(3)	8(4)	10(4)
C79	79(7)	56(6)	78(7)	-3(5)	7(6)	4(5)
O17	86(7)	33(5)	90(7)	0	-5(6)	0
O12	107(6)	80(5)	66(5)	5(4)	7(4)	26(5)
C80	94(9)	102(10)	97(10)	-25(8)	-12(8)	4(8)

Table S5 Bond Lengths.

Atom	Atom	Length/Å	Atom	Atom	Length/Å

Dy1	O1	2.197(6)	N18	C28	1.275(11)
Dy1	N1	2.662(7)	N19	C29	1.376(10)
Dy1	N2	2.481(7)	N19	C31	1.341(9)
Dy1	N3	2.427(6)	N20	Cu4[1]	1.986(6)
Dy1	N5	2.496(7)	N20	C30	1.357(10)
Dy1	N6	2.487(6)	N20	C31	1.345(10)
Dy1	N8	2.457(7)	N21	C39	1.492(11)
Dy1	N9	2.468(6)	N21	C45	1.472(12)
Dy2	O2	2.181(6)	N21	C51	1.500(11)
Dy2	N11	2.679(6)	N22	C40	1.461(10)
Dy2	N12	2.476(7)	N22	C41	1.282(11)
Dy2	N13	2.430(6)	N23	C42	1.391(10)
Dy2	N15	2.477(6)	N23	C44	1.303(9)
Dy2	N16	2.469(6)	N24	C43	1.356(10)
Dy2	N18	2.522(7)	N24	C44	1.352(10)
Dy2	N19	2.493(6)	N25	C46	1.481(10)
Dy3	O3	2.182(6)	N25	C47	1.274(11)
Dy3	N21	2.680(7)	N26	C48	1.398(10)
Dy3	N22	2.517(7)	N26	C50	1.346(9)
Dy3	N23	2.518(6)	N27	C49	1.376(10)
Dy3	N25	2.497(7)	N27	C50	1.349(10)
Dy3	N26	2.407(6)	N28	C52	1.447(10)
Dy3	N28	2.463(7)	N28	C53	1.274(10)
Dy3	N29	2.468(6)	N29	C54	1.407(9)
Dy4	O4	2.201(6)	N29	C56	1.334(10)
Dy4	N31	2.679(7)	N30	C55	1.375(10)
Dy4	N32	2.473(7)	N30	C56	1.356(10)
Dy4	N33	2.493(6)	N31	C58	1.503(12)
Dy4	N35	2.496(7)	N31	C64	1.475(12)
Dy4	N36	2.438(7)	N31	C70	1.472(12)
Dy4	N38	2.446(7)	N32	C59	1.466(10)
Dy4	N39	2.474(6)	N32	C60	1.287(11)
Cu1	N14[1]	1.978(6)	N33	C61	1.395(10)
Cu1	N14	1.978(6)	N33	C63	1.325(9)
Cu1	N27[1]	1.972(6)	N34	Cu3[1]	1.987(6)
Cu1	N27	1.972(6)	N34	C62	1.388(10)
Cu2	N4[1]	1.987(6)	N34	C63	1.346(10)
Cu2	N4	1.987(6)	N35	C65	1.466(11)
Cu2	N37	1.983(7)	N35	C66	1.265(11)
Cu2	N37[1]	1.983(7)	N36	C67	1.391(10)
Cu3	O5	2.322(8)	N36	C69	1.329(10)
Cu3	N10	1.984(7)	N37	C68	1.373(10)
Cu3	N17	2.000(6)	N37	C69	1.344(10)
Cu3	N24	2.004(6)	N38	C71	1.439(11)
Cu3	N34[1]	1.987(6)	N38	C72	1.296(11)
Cu4	O6	2.355(9)	N39	C73	1.403(10)
Cu4	N7	1.972(6)	N39	C75	1.309(10)

Cu4	N20[1]	1.987(6)	N40	C74	1.368(10)
Cu4	N30	1.998(6)	N40	C75	1.376(10)
Cu4	N40	1.983(7)	C1	C2	1.544(12)
O1	C19	1.411(11)	C3	C4	1.445(11)
O2	C38	1.393(10)	C4	C5	1.403(11)
O3	C57	1.403(10)	C7	C8	1.524(13)
O4	C76	1.423(13)	C9	C10	1.430(10)
N1	C1	1.499(11)	C10	C11	1.346(11)
N1	C7	1.489(11)	C13	C14	1.551(12)
N1	C13	1.474(11)	C15	C16	1.446(12)
N2	C2	1.472(10)	C16	C17	1.373(11)
N2	C3	1.272(10)	C20	C21	1.513(12)
N3	C4	1.377(9)	C22	C23	1.430(11)
N3	C6	1.342(10)	C23	C24	1.377(11)
N4	C5	1.353(10)	C26	C27	1.532(12)
N4	C6	1.358(10)	C28	C29	1.436(11)
N5	C8	1.477(10)	C29	C30	1.386(11)
N5	C9	1.270(10)	C32	C33	1.530(12)
N6	C10	1.399(9)	C34	C35	1.423(11)
N6	C12	1.327(9)	C35	C36	1.369(11)
N7	C11	1.402(10)	C39	C40	1.517(12)
N7	C12	1.349(9)	C41	C42	1.432(12)
N8	C14	1.451(11)	C42	C43	1.368(11)
N8	C15	1.268(10)	C45	C46	1.495(13)
N9	C16	1.392(9)	C47	C48	1.450(11)
N9	C18	1.321(10)	C48	C49	1.380(11)
N10	C17	1.366(10)	C51	C52	1.511(13)
N10	C18	1.355(10)	C53	C54	1.435(11)
N11	C20	1.497(11)	C54	C55	1.369(11)
N11	C26	1.467(11)	C58	C59	1.539(14)
N11	C32	1.481(11)	C60	C61	1.429(11)
N12	C21	1.477(10)	C61	C62	1.358(11)
N12	C22	1.293(11)	C64	C65	1.507(14)
N13	C23	1.392(10)	C66	C67	1.437(12)
N13	C25	1.337(9)	C67	C68	1.373(12)
N14	C24	1.376(10)	C70	C71	1.506(14)
N14	C25	1.349(9)	C72	C73	1.420(12)
N15	C33	1.451(10)	C73	C74	1.377(11)
N15	C34	1.253(10)	O9	C77	1.451(14)
N16	C35	1.401(10)	O10	C78	1.408(15)
N16	C37	1.343(10)	O11	C79	1.439(13)
N17	C36	1.369(10)	O12	C80	1.491(15)
N17	C37	1.339(9)	O13	C81	1.361(19)
N18	C27	1.457(10)			

Table S6 Bond Angles.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°

O1	Dy1	N1	82.2(2)	C22	N12	Dy2	117.9(5)
O1	Dy1	N2	77.0(2)	C22	N12	C21	119.3(7)
O1	Dy1	N3	101.0(2)	C23	N13	Dy2	115.3(5)
O1	Dy1	N5	145.1(2)	C25	N13	Dy2	139.4(5)
O1	Dy1	N6	148.0(2)	C25	N13	C23	104.6(6)
O1	Dy1	N8	87.8(2)	C24	N14	Cu1	126.7(5)
O1	Dy1	N9	77.3(2)	C25	N14	Cu1	128.0(5)
N2	Dy1	N1	66.4(2)	C25	N14	C24	105.2(6)
N2	Dy1	N5	78.9(2)	C33	N15	Dy2	119.2(5)
N2	Dy1	N6	130.9(2)	C34	N15	Dy2	117.7(5)
N3	Dy1	N1	131.4(2)	C34	N15	C33	122.7(7)
N3	Dy1	N2	67.3(2)	C35	N16	Dy2	113.9(5)
N3	Dy1	N5	92.4(2)	C37	N16	Dy2	142.3(5)
N3	Dy1	N6	81.0(2)	C37	N16	C35	103.8(6)
N3	Dy1	N8	159.6(2)	C36	N17	Cu3	128.9(5)
N3	Dy1	N9	95.5(2)	C37	N17	Cu3	125.8(5)
N5	Dy1	N1	65.1(2)	C37	N17	C36	105.1(6)
N6	Dy1	N1	120.6(2)	C27	N18	Dy2	119.2(6)
N6	Dy1	N5	65.6(2)	C28	N18	Dy2	119.7(6)
N8	Dy1	N1	67.6(2)	C28	N18	C27	120.9(8)
N8	Dy1	N2	133.0(2)	C29	N19	Dy2	117.7(5)
N8	Dy1	N5	90.5(2)	C31	N19	Dy2	139.6(5)
N8	Dy1	N6	82.0(2)	C31	N19	C29	102.7(6)
N8	Dy1	N9	68.4(2)	C30	N20	Cu4[1]	124.9(5)
N9	Dy1	N1	131.7(2)	C31	N20	Cu4[1]	128.9(5)
N9	Dy1	N2	145.3(2)	C31	N20	C30	105.0(6)
N9	Dy1	N5	133.7(2)	C39	N21	Dy3	114.2(5)
N9	Dy1	N6	70.8(2)	C39	N21	C51	109.8(7)
O2	Dy2	N11	82.2(2)	C45	N21	Dy3	104.1(5)
O2	Dy2	N12	77.1(2)	C45	N21	C39	111.3(7)
O2	Dy2	N13	96.6(2)	C45	N21	C51	110.9(7)
O2	Dy2	N15	87.9(2)	C51	N21	Dy3	106.3(5)
O2	Dy2	N16	78.9(2)	C40	N22	Dy3	118.2(6)
O2	Dy2	N18	144.2(2)	C41	N22	Dy3	120.4(6)
O2	Dy2	N19	149.7(2)	C41	N22	C40	121.4(8)
N12	Dy2	N11	65.8(2)	C42	N23	Dy3	116.6(5)
N12	Dy2	N15	132.3(2)	C44	N23	Dy3	139.3(5)
N12	Dy2	N18	77.9(2)	C44	N23	C42	104.1(6)
N12	Dy2	N19	128.2(2)	C43	N24	Cu3	125.2(5)
N13	Dy2	N11	132.7(2)	C44	N24	Cu3	129.0(5)
N13	Dy2	N12	67.8(2)	C44	N24	C43	104.6(6)
N13	Dy2	N15	159.8(2)	C46	N25	Dy3	121.8(6)
N13	Dy2	N16	93.7(2)	C47	N25	Dy3	117.7(5)
N13	Dy2	N18	97.2(2)	C47	N25	C46	119.9(7)
N13	Dy2	N19	81.6(2)	C48	N26	Dy3	116.8(5)
N15	Dy2	N11	67.3(2)	C50	N26	Dy3	139.8(5)
N15	Dy2	N18	90.3(2)	C50	N26	C48	103.0(6)

N15	Dy2	N19	84.6(2)	C49	N27	Cu1	126.1(5)
N16	Dy2	N11	131.6(2)	C50	N27	Cu1	128.0(5)
N16	Dy2	N12	147.5(2)	C50	N27	C49	105.7(6)
N16	Dy2	N15	67.8(2)	C52	N28	Dy3	119.8(5)
N16	Dy2	N18	132.7(2)	C53	N28	Dy3	117.8(5)
N16	Dy2	N19	71.1(2)	C53	N28	C52	122.0(7)
N18	Dy2	N11	64.3(2)	C54	N29	Dy3	114.2(4)
N19	Dy2	N11	121.1(2)	C56	N29	Dy3	142.2(5)
N19	Dy2	N18	65.3(2)	C56	N29	C54	103.6(6)
O3	Dy3	N21	81.3(2)	C55	N30	Cu4	129.1(5)
O3	Dy3	N22	144.2(2)	C56	N30	Cu4	126.3(5)
O3	Dy3	N23	149.7(2)	C56	N30	C55	104.3(6)
O3	Dy3	N25	77.3(2)	C58	N31	Dy4	114.7(5)
O3	Dy3	N26	98.0(2)	C64	N31	Dy4	104.3(5)
O3	Dy3	N28	88.2(2)	C64	N31	C58	111.9(7)
O3	Dy3	N29	79.3(2)	C70	N31	Dy4	106.7(5)
N22	Dy3	N21	65.2(2)	C70	N31	C58	109.0(8)
N22	Dy3	N23	65.4(2)	C70	N31	C64	110.1(8)
N23	Dy3	N21	122.2(2)	C59	N32	Dy4	120.6(6)
N25	Dy3	N21	65.1(2)	C60	N32	Dy4	120.5(5)
N25	Dy3	N22	77.5(2)	C60	N32	C59	118.9(7)
N25	Dy3	N23	128.1(2)	C61	N33	Dy4	116.3(5)
N26	Dy3	N21	131.7(2)	C63	N33	Dy4	140.0(5)
N26	Dy3	N22	95.4(2)	C63	N33	C61	103.6(6)
N26	Dy3	N23	80.6(2)	C62	N34	Cu3[1]	124.1(5)
N26	Dy3	N25	67.7(2)	C63	N34	Cu3[1]	130.8(5)
N26	Dy3	N28	160.5(2)	C63	N34	C62	104.1(6)
N26	Dy3	N29	94.6(2)	C65	N35	Dy4	120.7(6)
N28	Dy3	N21	67.3(2)	C66	N35	Dy4	117.2(5)
N28	Dy3	N22	90.1(2)	C66	N35	C65	120.9(8)
N28	Dy3	N23	84.7(2)	C67	N36	Dy4	115.1(5)
N28	Dy3	N25	131.8(2)	C69	N36	Dy4	140.5(5)
N28	Dy3	N29	68.3(2)	C69	N36	C67	103.9(7)
N29	Dy3	N21	131.7(2)	C68	N37	Cu2	126.6(5)
N29	Dy3	N22	132.4(2)	C69	N37	Cu2	129.2(5)
N29	Dy3	N23	70.7(2)	C69	N37	C68	104.3(7)
N29	Dy3	N25	148.0(2)	C71	N38	Dy4	119.8(6)
O4	Dy4	N31	82.7(2)	C72	N38	Dy4	117.8(6)
O4	Dy4	N32	144.7(2)	C72	N38	C71	122.0(8)
O4	Dy4	N33	148.7(2)	C73	N39	Dy4	113.2(5)
O4	Dy4	N35	76.3(2)	C75	N39	Dy4	141.5(5)
O4	Dy4	N36	96.2(2)	C75	N39	C73	105.2(6)
O4	Dy4	N38	89.7(3)	C74	N40	Cu4	129.4(5)
O4	Dy4	N39	79.0(2)	C74	N40	C75	104.3(6)
N32	Dy4	N31	64.8(2)	C75	N40	Cu4	125.9(5)
N32	Dy4	N33	66.1(2)	N1	C1	C2	111.1(7)
N32	Dy4	N35	77.8(2)	N2	C2	C1	109.7(6)

N32	Dy4	N39	132.9(2)	N2	C3	C4	117.9(7)
N33	Dy4	N31	121.7(2)	N3	C4	C3	119.5(7)
N33	Dy4	N35	129.6(2)	N3	C4	C5	108.3(6)
N35	Dy4	N31	65.5(2)	C5	C4	C3	132.1(7)
N36	Dy4	N31	132.0(2)	N4	C5	C4	108.8(7)
N36	Dy4	N32	95.8(2)	N3	C6	N4	114.7(6)
N36	Dy4	N33	81.8(2)	N1	C7	C8	114.6(7)
N36	Dy4	N35	67.7(2)	N5	C8	C7	107.0(7)
N36	Dy4	N38	160.5(2)	N5	C9	C10	119.8(7)
N36	Dy4	N39	94.2(2)	N6	C10	C9	116.9(6)
N38	Dy4	N31	67.1(2)	C11	C10	N6	109.1(6)
N38	Dy4	N32	89.9(2)	C11	C10	C9	133.7(7)
N38	Dy4	N33	83.5(2)	C10	C11	N7	108.3(7)
N38	Dy4	N35	131.8(2)	N6	C12	N7	114.1(7)
N38	Dy4	N39	68.7(2)	N1	C13	C14	110.4(7)
N39	Dy4	N31	131.8(2)	N8	C14	C13	106.4(7)
N39	Dy4	N33	70.1(2)	N8	C15	C16	119.1(8)
N39	Dy4	N35	147.2(2)	N9	C16	C15	120.2(7)
N14[1]	Cu1	N14	174.5(3)	C17	C16	N9	108.0(7)
N27	Cu1	N14	90.2(3)	C17	C16	C15	131.7(7)
N27[1]	Cu1	N14	89.6(3)	N10	C17	C16	108.8(7)
N27	Cu1	N14[1]	89.6(3)	N9	C18	N10	114.1(7)
N27[1]	Cu1	N14[1]	90.2(3)	N11	C20	C21	112.3(7)
N27	Cu1	N27[1]	174.0(3)	N12	C21	C20	108.9(7)
N4[1]	Cu2	N4	174.0(4)	N12	C22	C23	118.5(7)
N37	Cu2	N4[1]	88.9(3)	N13	C23	C22	119.7(7)
N37	Cu2	N4	91.0(3)	C24	C23	N13	108.5(7)
N37[1]	Cu2	N4[1]	91.0(3)	C24	C23	C22	131.8(7)
N37[1]	Cu2	N4	88.9(3)	N14	C24	C23	108.2(7)
N37[1]	Cu2	N37	177.5(4)	N13	C25	N14	113.5(6)
N10	Cu3	O5	93.7(3)	N11	C26	C27	113.0(7)
N10	Cu3	N17	171.7(3)	N18	C27	C26	108.1(7)
N10	Cu3	N24	90.2(2)	N18	C28	C29	119.3(8)
N10	Cu3	N34[1]	89.2(3)	N19	C29	C28	117.9(7)
N17	Cu3	O5	94.6(3)	N19	C29	C30	110.0(7)
N17	Cu3	N24	88.3(2)	C30	C29	C28	132.2(8)
N24	Cu3	O5	97.4(3)	N20	C30	C29	107.5(7)
N34[1]	Cu3	O5	96.5(3)	N19	C31	N20	114.8(7)
N34[1]	Cu3	N17	90.3(2)	N11	C32	C33	111.5(7)
N34[1]	Cu3	N24	166.2(3)	N15	C33	C32	107.7(7)
N7	Cu4	O6	97.8(3)	N15	C34	C35	121.4(7)
N7	Cu4	N20[1]	165.4(3)	N16	C35	C34	118.9(7)
N7	Cu4	N30	90.9(2)	C36	C35	N16	108.2(7)
N7	Cu4	N40	89.1(2)	C36	C35	C34	132.6(7)
N20[1]	Cu4	O6	96.7(3)	N17	C36	C35	108.8(6)
N20[1]	Cu4	N30	87.9(2)	N17	C37	N16	114.0(7)
N30	Cu4	O6	94.3(3)	N21	C39	C40	113.6(7)

N40	Cu4	O6	92.9(3)	N22	C40	C39	108.6(7)
N40	Cu4	N20[1]	90.2(3)	N22	C41	C42	119.0(8)
N40	Cu4	N30	172.7(3)	N23	C42	C41	118.5(7)
C19	O1	Dy1	134.8(6)	C43	C42	N23	108.5(7)
C38	O2	Dy2	135.3(5)	C43	C42	C41	132.9(8)
C57	O3	Dy3	134.5(6)	N24	C43	C42	108.2(7)
C76	O4	Dy4	131.9(6)	N23	C44	N24	114.5(7)
C1	N1	Dy1	103.8(5)	N21	C45	C46	113.5(7)
C7	N1	Dy1	114.6(5)	N25	C46	C45	108.3(7)
C7	N1	C1	111.4(7)	N25	C47	C48	119.1(7)
C13	N1	Dy1	107.2(5)	N26	C48	C47	118.1(7)
C13	N1	C1	107.8(7)	C49	C48	N26	109.9(7)
C13	N1	C7	111.5(7)	C49	C48	C47	132.0(7)
C2	N2	Dy1	120.9(5)	N27	C49	C48	107.2(7)
C3	N2	Dy1	118.0(5)	N26	C50	N27	114.2(6)
C3	N2	C2	120.0(7)	N21	C51	C52	111.7(7)
C4	N3	Dy1	115.5(5)	N28	C52	C51	107.6(7)
C6	N3	Dy1	139.9(5)	N28	C53	C54	121.1(7)
C6	N3	C4	103.9(6)	N29	C54	C53	118.4(7)
C5	N4	Cu2	128.9(5)	C55	C54	N29	108.5(6)
C5	N4	C6	104.3(6)	C55	C54	C53	133.0(7)
C6	N4	Cu2	126.7(5)	C54	C55	N30	109.0(7)
C8	N5	Dy1	118.8(5)	N29	C56	N30	114.6(7)
C9	N5	Dy1	120.3(5)	N31	C58	C59	112.6(7)
C9	N5	C8	120.7(7)	N32	C59	C58	107.0(7)
C10	N6	Dy1	117.4(4)	N32	C60	C61	119.1(8)
C12	N6	Dy1	138.3(5)	N33	C61	C60	117.8(7)
C12	N6	C10	104.4(6)	C62	C61	N33	109.4(7)
C11	N7	Cu4	126.4(5)	C62	C61	C60	132.8(8)
C12	N7	Cu4	129.2(5)	C61	C62	N34	108.1(7)
C12	N7	C11	104.1(6)	N33	C63	N34	114.9(7)
C14	N8	Dy1	118.6(5)	N31	C64	C65	112.2(8)
C15	N8	Dy1	118.7(6)	N35	C65	C64	110.4(7)
C15	N8	C14	121.9(7)	N35	C66	C67	119.6(8)
C16	N9	Dy1	113.4(5)	N36	C67	C66	119.3(8)
C18	N9	Dy1	141.9(5)	C68	C67	N36	108.4(7)
C18	N9	C16	104.6(6)	C68	C67	C66	132.1(7)
C17	N10	Cu3	129.8(5)	C67	C68	N37	108.6(7)
C18	N10	Cu3	125.6(5)	N36	C69	N37	114.7(7)
C18	N10	C17	104.4(7)	N31	C70	C71	112.0(8)
C20	N11	Dy2	103.9(5)	N38	C71	C70	108.0(8)
C26	N11	Dy2	115.9(5)	N38	C72	C73	120.3(8)
C26	N11	C20	111.3(7)	N39	C73	C72	119.9(7)
C26	N11	C32	109.3(7)	C74	C73	N39	107.8(7)
C32	N11	Dy2	106.9(5)	C74	C73	C72	132.2(8)
C32	N11	C20	109.2(6)	N40	C74	C73	108.9(7)
C21	N12	Dy2	122.0(5)	N39	C75	N40	113.8(7)

Table S7 Torsion Angles.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Dy1	N1	C1	C2	-58.3(8)	N31	C58	C59	N32	-45.7(10)
Dy1	N1	C7	C8	20.9(9)	N31	C64	C65	N35	47.9(11)
Dy1	N1	C13	C14	48.8(8)	N31	C70	C71	N38	-58.6(11)
Dy1	N2	C2	C1	-10.3(10)	N32	C60	C61	N33	-3.1(12)
Dy1	N2	C3	C4	-12.8(10)	N32	C60	C61	C62	180.0(9)
Dy1	N3	C4	C3	8.1(9)	N33	C61	C62	N34	-0.3(9)
Dy1	N3	C4	C5	-174.5(5)	N35	C66	C67	N36	5.1(12)
Dy1	N3	C6	N4	170.1(6)	N35	C66	C67	C68	-178.6(9)
Dy1	N5	C8	C7	50.4(8)	N36	C67	C68	N37	-0.2(9)
Dy1	N5	C9	C10	0.3(10)	N38	C72	C73	N39	-1.4(13)
Dy1	N6	C10	C9	3.5(8)	N38	C72	C73	C74	-179.7(9)
Dy1	N6	C10	C11	178.3(5)	N39	C73	C74	N40	0.2(9)
Dy1	N6	C12	N7	-177.2(5)	C1	N1	C7	C8	-96.6(8)
Dy1	N8	C14	C13	43.1(9)	C1	N1	C13	C14	160.0(7)
Dy1	N8	C15	C16	4.8(11)	C2	N2	C3	C4	178.9(8)
Dy1	N9	C16	C15	0.6(9)	C3	N2	C2	C1	157.7(8)
Dy1	N9	C16	C17	177.9(5)	C3	C4	C5	N4	179.9(9)
Dy1	N9	C18	N10	-177.1(6)	C4	N3	C6	N4	1.4(9)
Dy2	N11	C20	C21	-57.7(8)	C5	N4	C6	N3	0.4(9)
Dy2	N11	C26	C27	24.0(10)	C6	N3	C4	C3	-180.0(7)
Dy2	N11	C32	C33	48.8(8)	C6	N3	C4	C5	-2.6(9)
Dy2	N12	C21	C20	-12.3(11)	C6	N4	C5	C4	-2.0(9)
Dy2	N12	C22	C23	-7.1(11)	C7	N1	C1	C2	65.6(9)
Dy2	N13	C23	C22	5.6(10)	C7	N1	C13	C14	-77.5(9)
Dy2	N13	C23	C24	-173.5(5)	C8	N5	C9	C10	176.8(7)
Dy2	N13	C25	N14	170.7(6)	C9	N5	C8	C7	-126.2(8)
Dy2	N15	C33	C32	39.3(9)	C9	C10	C11	N7	173.1(8)
Dy2	N15	C34	C35	2.9(11)	C10	N6	C12	N7	0.7(8)
Dy2	N16	C35	C34	6.2(9)	C11	N7	C12	N6	-0.9(8)
Dy2	N16	C35	C36	-179.2(5)	C12	N6	C10	C9	-174.9(7)
Dy2	N16	C37	N17	178.4(6)	C12	N6	C10	C11	-0.1(8)
Dy2	N18	C27	C26	48.8(10)	C12	N7	C11	C10	0.8(8)
Dy2	N18	C28	C29	1.8(11)	C13	N1	C1	C2	-171.8(7)
Dy2	N19	C29	C28	3.2(9)	C13	N1	C7	C8	143.0(7)
Dy2	N19	C29	C30	-177.1(5)	C14	N8	C15	C16	174.8(8)
Dy2	N19	C31	N20	176.4(5)	C15	N8	C14	C13	-126.9(9)
Dy3	N21	C39	C40	24.3(10)	C15	C16	C17	N10	177.0(8)
Dy3	N21	C45	C46	-58.5(8)	C16	N9	C18	N10	-0.4(9)
Dy3	N21	C51	C52	48.4(8)	C17	N10	C18	N9	0.4(9)
Dy3	N22	C40	C39	49.9(10)	C18	N9	C16	C15	-177.2(7)
Dy3	N22	C41	C42	-0.1(12)	C18	N9	C16	C17	0.2(8)
Dy3	N23	C42	C41	1.5(10)	C18	N10	C17	C16	-0.3(9)
Dy3	N23	C42	C43	-176.1(5)	C20	N11	C26	C27	-94.4(9)
Dy3	N23	C44	N24	176.3(5)	C20	N11	C32	C33	160.6(7)

Dy3 N25 C46 C45	-11.2(11)	C21 N12 C22 C23	-177.4(8)
Dy3 N25 C47 C48	-6.2(11)	C22 N12 C21 C20	157.6(9)
Dy3 N26 C48 C47	4.8(10)	C22 C23 C24 N14	-178.6(9)
Dy3 N26 C48 C49	-175.2(5)	C23 N13 C25 N14	0.9(9)
Dy3 N26 C50 N27	172.4(5)	C24 N14 C25 N13	-0.6(9)
Dy3 N28 C52 C51	39.7(9)	C25 N13 C23 C22	178.4(8)
Dy3 N28 C53 C54	0.6(10)	C25 N13 C23 C24	-0.8(9)
Dy3 N29 C54 C53	4.1(8)	C25 N14 C24 C23	0.0(9)
Dy3 N29 C54 C55	-178.5(5)	C26 N11 C20 C21	67.7(9)
Dy3 N29 C56 N30	178.7(5)	C26 N11 C32 C33	-77.4(8)
Dy4 N31 C58 C59	24.2(9)	C27 N18 C28 C29	177.1(8)
Dy4 N31 C64 C65	-57.5(8)	C28 N18 C27 C26	-126.6(9)
Dy4 N31 C70 C71	47.3(9)	C28 C29 C30 N20	178.6(9)
Dy4 N32 C59 C58	50.6(9)	C29 N19 C31 N20	-2.2(9)
Dy4 N32 C60 C61	-1.0(11)	C30 N20 C31 N19	1.6(9)
Dy4 N33 C61 C60	5.5(9)	C31 N19 C29 C28	-177.8(7)
Dy4 N33 C61 C62	-176.9(5)	C31 N19 C29 C30	1.9(8)
Dy4 N33 C63 N34	175.8(5)	C31 N20 C30 C29	-0.3(9)
Dy4 N35 C65 C64	-10.5(11)	C32 N11 C20 C21	-171.5(7)
Dy4 N35 C66 C67	-11.3(10)	C32 N11 C26 C27	144.9(8)
Dy4 N36 C67 C66	3.9(9)	C33 N15 C34 C35	175.1(8)
Dy4 N36 C67 C68	-173.2(5)	C34 N15 C33 C32	-132.7(8)
Dy4 N36 C69 N37	170.4(6)	C34 C35 C36 N17	174.2(8)
Dy4 N38 C71 C70	39.5(10)	C35 N16 C37 N17	0.2(9)
Dy4 N38 C72 C73	-0.5(12)	C36 N17 C37 N16	0.2(9)
Dy4 N39 C73 C72	2.4(9)	C37 N16 C35 C34	-175.1(7)
Dy4 N39 C73 C74	-178.9(5)	C37 N16 C35 C36	-0.5(8)
Dy4 N39 C75 N40	178.1(6)	C37 N17 C36 C35	-0.5(9)
Cu1 N14 C24 C23	176.7(5)	C39 N21 C45 C46	65.0(10)
Cu1 N14 C25 N13	-177.1(5)	C39 N21 C51 C52	-75.6(8)
Cu1 N27 C49 C48	174.4(5)	C40 N22 C41 C42	176.8(9)
Cu1 N27 C50 N26	-174.2(5)	C41 N22 C40 C39	-127.1(10)
Cu2 N4 C5 C4	174.9(6)	C41 C42 C43 N24	-179.5(10)
Cu2 N4 C6 N3	-176.7(5)	C42 N23 C44 N24	-1.6(9)
Cu2 N37 C68 C67	179.4(5)	C43 N24 C44 N23	0.2(9)
Cu2 N37 C69 N36	-179.1(5)	C44 N23 C42 C41	180.0(8)
Cu3 N10 C17 C16	-175.9(6)	C44 N23 C42 C43	2.3(9)
Cu3 N10 C18 N9	176.3(5)	C44 N24 C43 C42	1.3(9)
Cu3 N17 C36 C35	-175.1(5)	C45 N21 C39 C40	-93.3(9)
Cu3 N17 C37 N16	175.0(5)	C45 N21 C51 C52	161.0(7)
Cu3 N24 C43 C42	-167.2(6)	C46 N25 C47 C48	-177.4(8)
Cu3 N24 C44 N23	168.1(5)	C47 N25 C46 C45	159.7(9)
Cu3[1] N34 C62 C61	-169.7(5)	C47 C48 C49 N27	-179.1(9)
Cu3[1] N34 C63 N33	169.1(5)	C48 N26 C50 N27	-0.8(9)
Cu4 N7 C11 C10	-172.7(5)	C49 N27 C50 N26	1.4(9)
Cu4 N7 C12 N6	172.3(5)	C50 N26 C48 C47	179.9(7)
Cu4[1] N20 C30 C29	-169.0(5)	C50 N26 C48 C49	-0.1(9)

Cu4[1]	N20	C31	N19	169.7(5)	C50	N27	C49	C48	-1.3(9)
Cu4	N30	C55	C54	-172.9(5)	C51	N21	C39	C40	143.5(8)
Cu4	N30	C56	N29	173.9(5)	C51	N21	C45	C46	-172.4(7)
Cu4	N40	C74	C73	-173.8(6)	C52	N28	C53	C54	173.2(8)
Cu4	N40	C75	N39	174.1(5)	C53	N28	C52	C51	-132.7(8)
N1	C1	C2	N2	48.2(10)	C53	C54	C55	N30	175.7(8)
N1	C7	C8	N5	-44.2(10)	C54	N29	C56	N30	-0.7(9)
N1	C13	C14	N8	-61.7(10)	C55	N30	C56	N29	0.0(9)
N2	C3	C4	N3	3.2(12)	C56	N29	C54	C53	-176.3(7)
N2	C3	C4	C5	-173.5(9)	C56	N29	C54	C55	1.2(8)
N3	C4	C5	N4	3.0(10)	C56	N30	C55	C54	0.8(8)
N5	C9	C10	N6	-2.6(11)	C58	N31	C64	C65	67.0(10)
N5	C9	C10	C11	-175.7(8)	C58	N31	C70	C71	-77.1(10)
N6	C10	C11	N7	-0.4(9)	C59	N32	C60	C61	177.7(8)
N8	C15	C16	N9	-3.7(12)	C60	N32	C59	C58	-128.1(9)
N8	C15	C16	C17	179.7(9)	C60	C61	C62	N34	176.8(8)
N9	C16	C17	N10	0.1(9)	C61	N33	C63	N34	-0.7(9)
N11	C20	C21	N12	49.0(11)	C62	N34	C63	N33	0.5(9)
N11	C26	C27	N18	-45.5(11)	C63	N33	C61	C60	-177.0(7)
N11	C32	C33	N15	-59.5(9)	C63	N33	C61	C62	0.6(8)
N12	C22	C23	N13	0.9(13)	C63	N34	C62	C61	-0.1(8)
N12	C22	C23	C24	179.9(9)	C64	N31	C58	C59	-94.3(9)
N13	C23	C24	N14	0.5(9)	C64	N31	C70	C71	159.9(8)
N15	C34	C35	N16	-6.4(12)	C65	N35	C66	C67	-178.8(8)
N15	C34	C35	C36	-179.4(9)	C66	N35	C65	C64	156.5(9)
N16	C35	C36	N17	0.6(9)	C66	C67	C68	N37	-176.7(8)
N18	C28	C29	N19	-3.4(13)	C67	N36	C69	N37	-0.5(9)
N18	C28	C29	C30	177.1(9)	C68	N37	C69	N36	0.5(9)
N19	C29	C30	N20	-1.0(9)	C69	N36	C67	C66	177.5(7)
N21	C39	C40	N22	-46.9(11)	C69	N36	C67	C68	0.4(9)
N21	C45	C46	N25	48.7(11)	C69	N37	C68	C67	-0.2(9)
N21	C51	C52	N28	-59.4(9)	C70	N31	C58	C59	143.7(8)
N22	C41	C42	N23	-1.0(14)	C70	N31	C64	C65	-171.6(8)
N22	C41	C42	C43	176.0(10)	C71	N38	C72	C73	172.5(9)
N23	C42	C43	N24	-2.3(10)	C72	N38	C71	C70	-133.3(10)
N25	C47	C48	N26	1.0(12)	C72	C73	C74	N40	178.7(9)
N25	C47	C48	C49	-178.9(9)	C73	N39	C75	N40	-0.2(9)
N26	C48	C49	N27	0.9(10)	C74	N40	C75	N39	0.3(9)
N28	C53	C54	N29	-3.3(11)	C75	N39	C73	C72	-178.7(8)
N28	C53	C54	C55	-180.0(9)	C75	N39	C73	C74	0.0(9)
N29	C54	C55	N30	-1.3(9)	C75	N40	C74	C73	-0.3(9)

Table S8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3).

Atom	*x*	*y*	*z*	U(eq)
H5A	-52	2995	3341	140
H5B	-598	2896	3081	140
H6A	593	2950	3090	142

H6B	861	2955	2526	142
H1A	1162	4672	6328	66
H1B	648	4499	6098	66
H2A	690	4966	5616	63
H2B	1312	4923	5496	63
H3	538	5014	4654	54
H5	239	4939	3503	54
H6	490	4036	3443	51
H7A	2163	4231	5897	65
H7B	1998	4583	5971	65
H8A	1936	4660	5044	65
H8B	2471	4463	5118	65
H9	2502	4095	4457	53
H11	2463	3565	3729	51
H12	928	3365	4012	45
H13A	936	4052	6408	65
H13B	1537	4117	6587	65
H14A	1848	3742	5919	66
H14B	1458	3579	6344	66
H15	907	3251	5867	61
H17	102	2919	5255	55
H18	-224	3590	4207	50
H19A	-386	3822	5560	103
H19B	-463	4105	5963	103
H19C	15	3869	6054	103
H20A	-3615	1170	3985	64
H20B	-3096	1323	4243	64
H21A	-2799	888	3784	72
H21B	-3133	976	3255	72
H22	-2006	875	3220	62
H24	-933	979	2815	58
H25	-1013	1899	2796	46
H26A	-3998	1699	3090	68
H26B	-3967	1337	3190	68
H27A	-3263	1281	2579	74
H27B	-3675	1504	2278	74
H28	-3210	1883	1851	61
H30	-2588	2397	1414	54
H31	-1739	2537	2751	47
H32A	-3508	1777	4353	61
H32B	-4053	1735	4028	61
H33A	-3812	2155	3438	63
H33B	-3817	2271	4053	63
H34	-3110	2610	4095	55
H36	-2140	2957	4259	49
H37	-1144	2303	3755	47
H38A	-1982	1989	4746	85

H38B	-2185	1683	5037	85
H38C	-2605	1929	4817	85
H39A	599	1680	6524	71
H39B	710	1320	6487	71
H40A	136	1263	5755	73
H40B	-180	1472	6180	73
H41	-624	1851	5709	65
H43	-1059	2365	5081	55
H44	265	2523	4239	46
H45A	1521	1172	6138	69
H45B	1763	1328	5609	69
H46A	1341	889	5314	71
H46B	816	965	5657	71
H47	755	873	4522	58
H49	314	975	3435	57
H50	284	1895	3531	45
H51A	1860	1789	6047	63
H51B	1539	1736	6597	63
H52A	934	2139	6358	62
H52B	1530	2270	6369	62
H53	1547	2619	5663	56
H55	1714	2973	4677	49
H56	1269	2310	3656	49
H57A	2282	1986	4501	87
H57B	2550	1701	4804	87
H57C	2276	1970	5145	87
H58A	3377	4208	291	75
H58B	3430	4569	393	75
H59A	2501	4631	443	70
H59B	2592	4412	-70	70
H60	1962	4045	-70	58
H62	1229	3527	13	49
H63	1505	3359	1577	46
H64A	3714	4720	1243	73
H64B	3496	4563	1783	73
H65A	2987	5002	1666	76
H65B	2888	4928	1041	76
H66	2037	5026	1794	59
H68	947	4935	2164	57
H69	952	4021	2056	53
H70A	3860	4110	1562	80
H70B	4040	4155	948	80
H71A	3459	3751	673	76
H71B	3865	3625	1121	76
H72	3353	3275	1612	65
H74	2756	2940	2420	57
H75	1689	3606	2707	50

H76A	3447	3935	2536	133
H76B	2941	3904	2922	133
H76C	3336	4189	2988	133
H9A	1954	1391	4293	115
H77A	2169	1401	3260	142
H77B	1905	1671	3605	142
H77C	1545	1398	3378	142
H10	2538	4476	2819	159
H78A	1623	4520	3019	132
H78B	1860	4566	3611	132
H78C	1965	4253	3293	132
H11A	-540	4339	5165	107
H79A	-577	4478	4151	106
H79B	-1148	4373	4366	106
H79C	-653	4144	4407	106
H12A	-1765	1378	4554	127
H80A	-904	1401	4008	147
H80B	-728	1321	4612	147
H80C	-1043	1632	4488	147
H13	-1272	4476	5416	79
H81A	-1729	4854	5461	73
H81B	-1529	4857	6073	73
H81C	-2072	4688	5919	73

Table S9 Atomic Occupancy.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
O14	0.5	O18	0.5	O15	0.5
O19	0.5	O13	0.5	H13	0.5
C81	0.5	H81A	0.5	H81B	0.5
H81C	0.5				

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