Supplemental Information

Analysis of Solid State π–π Stacking and Higher Order Dimensional Crystal Packing, Reactivity, and Electrochemical Behaviour of Recently Characterized Salphenazine Actinide and Transition Metal Complexes

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Additional Electronic Spectroscopy

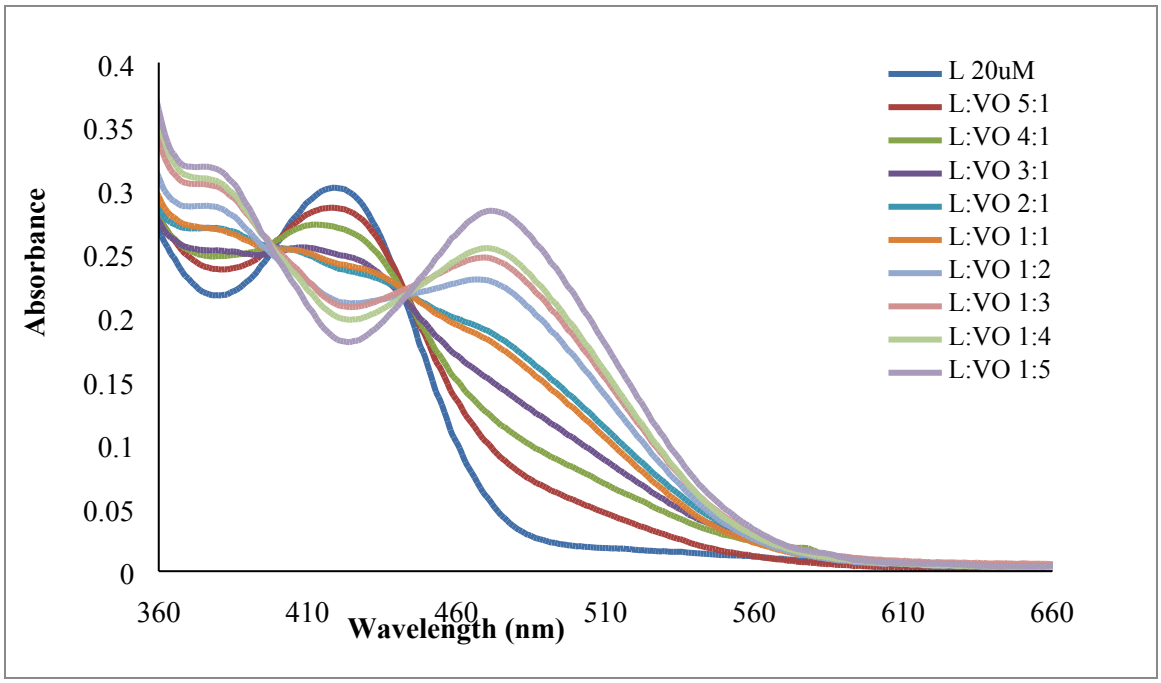

Figure SI1. UV Vis spectrum of 20 μM salphenazine **[H_2L^I]** solution with varying $VO(acac)_2$ concentrations in pyridine after 72 hours stir time.

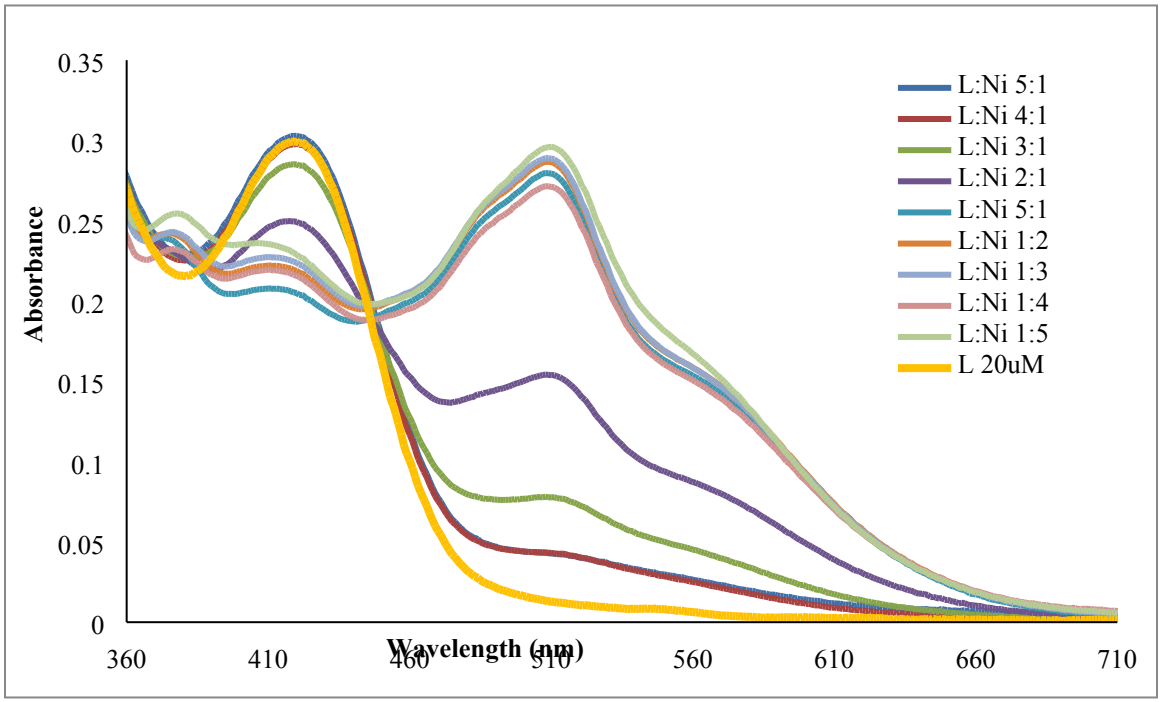

Figure SI2. UV Vis spectrum of 20 μM salphenazine **[H_2L^I]** solution with varying $Ni(acetate)_2$ concentrations in pyridine after 15 minute stir time.

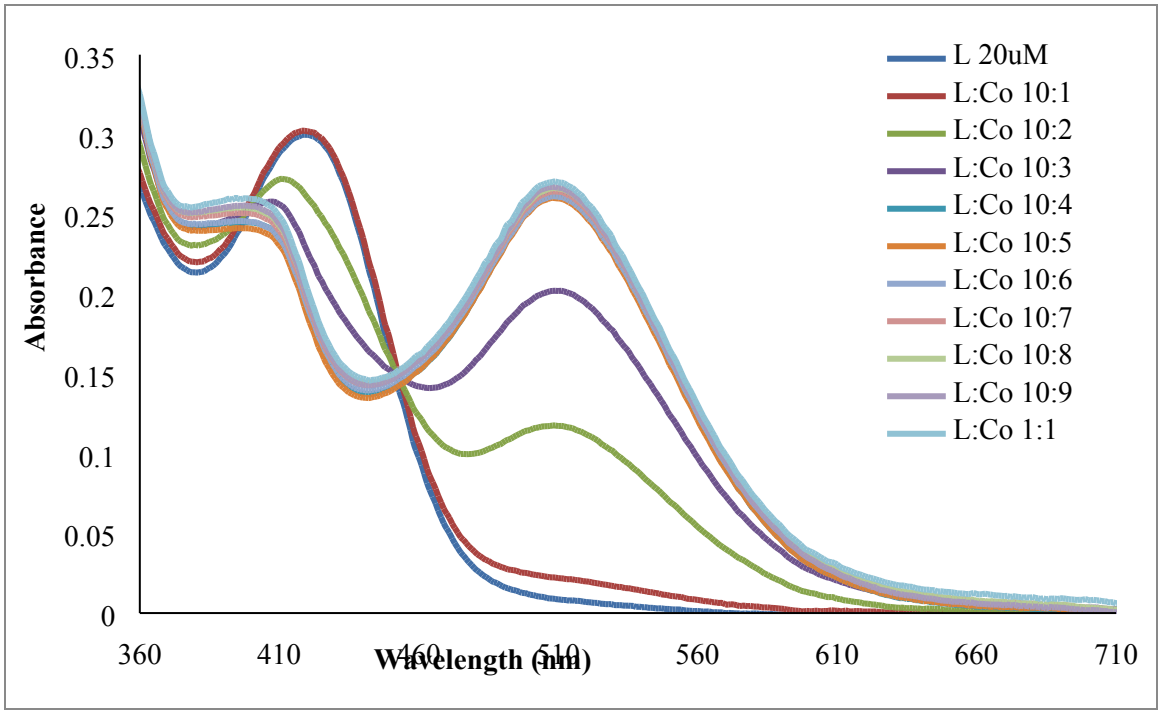

Figure SI3. UV Vis spectrum of 20 μM salphenazine **[H_2L^I]** solution with varying Co(acetate)$_2$ concentrations in pyridine after 15 minute stir time.

Cyclic Voltammatry

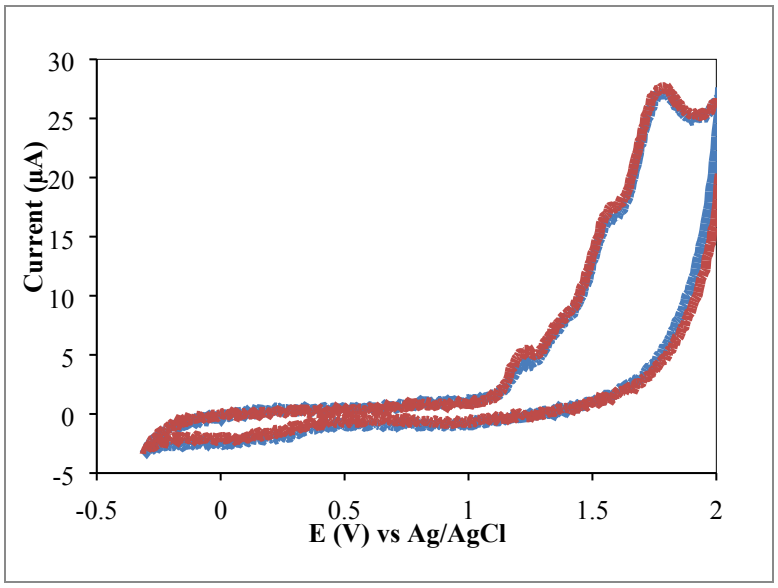

Figure SI4. Cyclic Voltammagram of Salphenazine **[H_2L^I]** Conditions: 0.5 mM ligand in dichloromethane, room temperature, tetra-n-butylammonium perchlorate (0.1 M) as electrolyte. Scan rate 0.100 V/s.

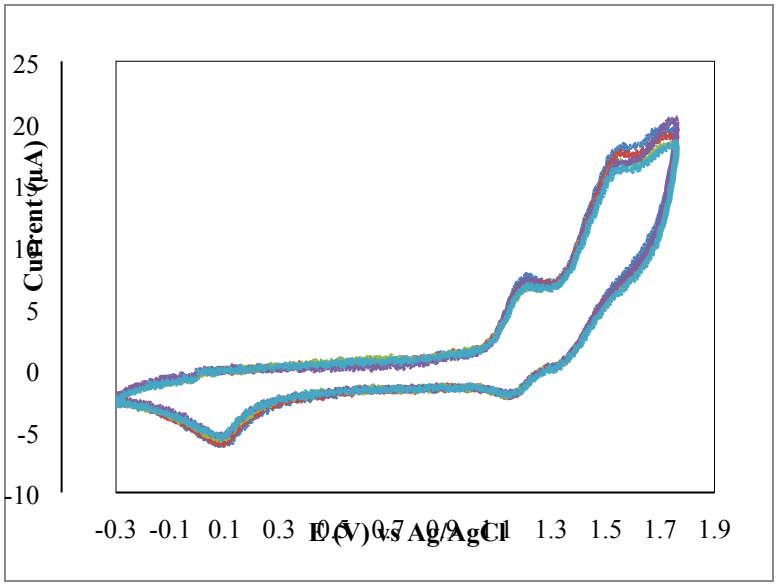

Figure SI5. Cyclic Voltammagram of $UO_2[L^I]$ Conditions: 0.5 mM complex in dichloromethane, room temperature, tetra-n-butylammonium perchlorate (0.1 M) as electrolyte. Scan rate 0.100 V/s.

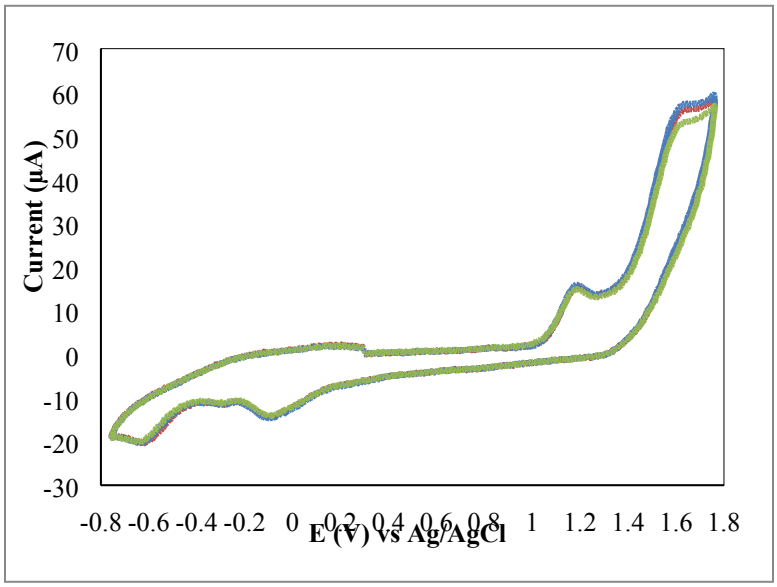

Figure SI6. Cyclic Voltammagram of Salqu $[H_2L^{II}]$ Conditions: 1.0 mM ligand in dichloromethane, room temperature, tetra-n-butylammonium perchlorate (0.1 M) as electrolyte. Scan rate 0.100 V/s.

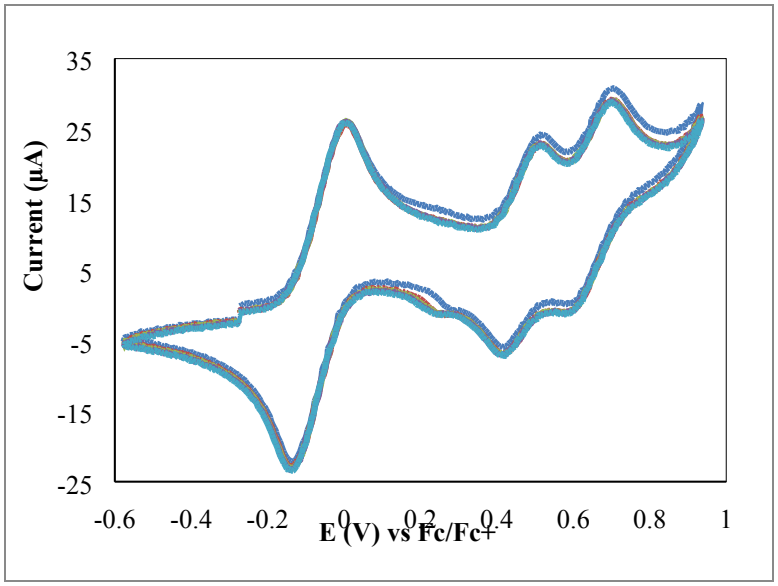

Figure SI7. Cyclic Voltammagram of **Cu[L^{II}]** Conditions: 1.0 mM ligand in dichloromethane, room temperature, tetra-n-butylammonium perchlorate (0.1 M) as electrolyte. Scan rate 0.100 V/s.

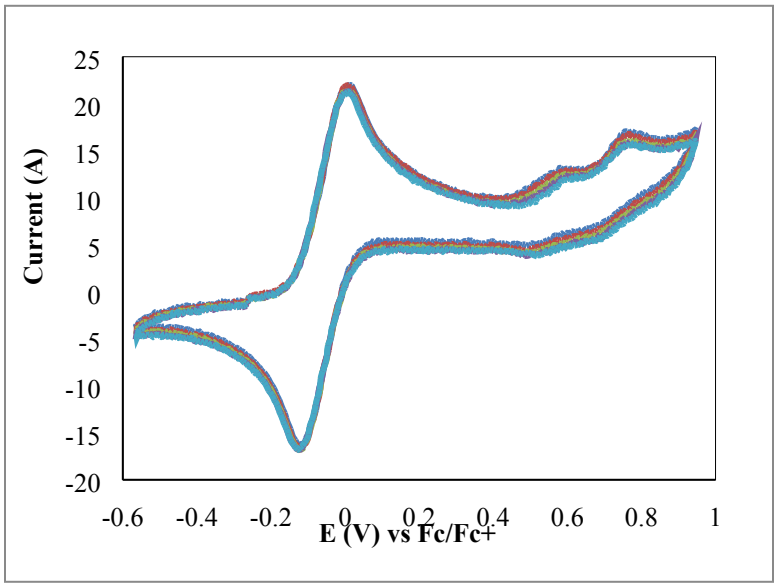

Figure SI8. Cyclic Voltammagram of **UO_2[L^{II}]** Conditions: 1.0 mM ligand in dichloromethane, room temperature, tetra-n-butylammonium perchlorate (0.1 M) as electrolyte. Scan rate 0.100 V/s.

Crystal Structures

[H_2L^I] Hardy012815

Table SI1 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Hardy012815_0mFINALCIF. Ueq is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
C1	6188(3)	6822.0(8)	1866.4(7)	23.1(4)
N1	2784(2)	6263.1(7)	2334.9(6)	25.3(4)
O1	5574(2)	7089.4(6)	2272.1(5)	33.1(4)
C2	7814(3)	7079.0(8)	1609.3(7)	21.9(4)
N2	2317(2)	6652.3(7)	3252.1(6)	27.2(4)
O2	3940(2)	7705.4(6)	3283.5(5)	35.8(4)
C3	8827(3)	7669.2(8)	1772.6(7)	25.6(5)
N3	-3479(2)	5020.1(7)	2404.7(6)	27.5(4)
C4	7084(3)	8145.7(9)	1766.6(8)	36.4(5)
N4	-3907(2)	5432.9(7)	3376.4(6)	29.6(4)
C5	9969(3)	7613.8(9)	2288.8(7)	32.2(5)
C6	10500(4)	7869.7(9)	1431.3(8)	42.0(6)
C7	8441(3)	6774.7(8)	1206.0(7)	24.1(4)
C8	7558(3)	6239.3(8)	1035.4(7)	25.3(4)
C13	5951(3)	6007.6(8)	1295.0(7)	25.5(5)
C14	5231(3)	6289.2(8)	1705.5(7)	22.9(4)
C15	3537(3)	6022.5(8)	1959.5(7)	25.0(5)
C16	1055(3)	6021.2(8)	2568.9(7)	23.1(4)
C17	-403(3)	5631.7(8)	2359.5(7)	25.0(5)
C18	-2102(3)	5412.5(8)	2623.6(7)	23.3(4)
C19	-5060(3)	4830.7(8)	2673.2(7)	27.0(5)
C20	-6584(3)	4417.6(9)	2463.2(8)	33.3(5)
C21	-8210(3)	4227.4(9)	2724.7(8)	37.6(6)
C22	-8423(3)	4432.7(9)	3204.4(9)	38.5(6)
C23	-7009(3)	4827.0(9)	3417.7(8)	35.4(5)
C24	-5280(3)	5037.5(8)	3158.3(8)	28.0(5)
C25	-2323(3)	5619.4(8)	3110.0(7)	25.4(5)
C26	-810(3)	6035.1(8)	3316.8(7)	27.9(5)
C27	831(3)	6226.7(8)	3060.3(7)	24.7(4)
C28	3351(3)	6562.8(9)	3669.6(7)	27.7(5)
C29	4845(3)	6985.9(8)	3902.0(7)	26.5(5)
C30	6045(3)	6825.1(9)	4336.5(7)	30.2(5)
C31	7510(3)	7200.5(9)	4574.0(7)	29.4(5)
C32	8876(3)	7043.9(10)	5046.6(7)	36.4(5)

C33	8122(4)	6479.4(11)	5272.2(8)	51.0(7)
C34	8729(4)	7532.8(11)	5427.5(8)	46.9(6)
C35	11229(4)	6975.6(13)	4929.5(9)	56.7(7)
C36	7747(3)	7749.8(9)	4355.2(7)	30.3(5)
C37	6604(3)	7940.9(9)	3929.8(7)	27.5(5)
C38	6956(3)	8546.0(9)	3708.8(7)	31.1(5)
C39	4847(3)	8899.1(10)	3678.8(9)	42.6(6)
C40	8668(4)	8899.3(10)	4015.9(8)	43.7(6)
C41	7750(4)	8477.9(10)	3197.9(8)	40.0(6)
C42	5107(3)	7541.4(9)	3699.2(7)	26.3(5)
C43S	7042(8)	4618(2)	4496.1(15)	118.9(15)
C44S	8738(14)	4920(3)	4454(2)	84(2)
C45S	8267(13)	4726(3)	5012(3)	74.4(18)
O46S	7458(8)	4552.6(19)	5368.2(17)	90.6(14)
O3S	10000	5000	5000	85.3(10)
C9	8373(3)	5926.9(9)	590.5(7)	30.4(5)
C1A	9667(12)	5354(3)	796(2)	50(2)
C1b	10628(9)	5739(3)	705.6(19)	55(2)
C2A	9950(16)	6267(3)	326(3)	67(3)
C2b	8347(11)	6381(2)	145.3(16)	45.4(17)
C3A	6512(16)	5700(5)	263(4)	62(3)
C3b	6953(15)	5432(4)	400(4)	63(3)

Table SI2 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Hardy012815_0mFINALCIF. 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}**
C1	22.6(10)	25.4(11)	21.2(10)	4.3(8)	0.8(8)	-4.6(8)
N1	20.8(8)	29.1(9)	26.0(9)	-1.5(7)	1.9(7)	1.2(7)
O1	31.5(8)	35.5(8)	33.9(8)	-6.6(6)	12.7(6)	-10.6(7)
C2	21.8(10)	21.4(10)	22.4(11)	0.4(8)	1.0(8)	-0.2(8)
N2	25.6(9)	30.3(9)	25.5(9)	-5.4(7)	1.6(8)	-3.6(7)
O2	41.5(9)	35.4(8)	28.1(8)	-10.0(7)	-11.1(7)	1.6(7)
C3	28.3(11)	22(1)	26.8(11)	-2.0(8)	4.6(9)	-4.1(8)
N3	23.3(9)	24.0(9)	34.9(10)	-0.8(7)	0.8(8)	-2.6(7)
C4	41.4(13)	24.1(11)	42.4(13)	3.9(9)	-5.1(11)	-3.9(10)
N4	27.4(9)	29.0(9)	33.1(10)	-4.5(7)	6.2(8)	-1.4(8)
C5	30.8(11)	28.4(12)	36.7(12)	1.5(9)	-2.6(10)	-7.2(9)
C6	50.8(14)	32.0(13)	45.0(14)	-16.5(11)	15.1(12)	-10.1(10)
C7	25.4(10)	26.2(11)	20.9(10)	-1.4(8)	3.6(8)	1.0(9)
C8	26.9(10)	24.9(11)	23.7(11)	-0.4(9)	0.5(9)	-1.4(9)
C13	27.4(10)	23.1(11)	25.8(11)	-3.7(8)	0.9(9)	-3.0(9)
C14	21.9(10)	24.7(11)	22.1(11)	0.5(8)	1.2(8)	1.2(8)

C15	23.5(10)	24.7(11)	26.2(11)	-1.3(8)	-2.0(9)	-0.0(9)
C16	19.3(10)	23.6(10)	26.4(11)	0.1(8)	1.4(8)	1.2(9)
C17	23.7(10)	28.9(11)	22.3(11)	1.1(9)	1.8(9)	-2.1(8)
C18	21(1)	21.3(10)	27.1(11)	2.2(8)	-1.1(9)	-0.4(8)
C19	22.7(10)	21.8(10)	36.2(12)	2.7(8)	1.1(9)	2.5(9)
C20	27.8(11)	26.7(11)	44.7(14)	-2.8(9)	-1.2(10)	-5.3(10)
C21	28.4(11)	27.3(12)	56.3(16)	-5.7(9)	-1.0(11)	0.4(11)
C22	30.6(12)	32.7(12)	52.9(15)	-6(1)	8.2(11)	6.9(11)
C23	33.3(12)	34.4(12)	39.4(13)	-4.8(10)	8.9(10)	2.3(10)
C24	25.0(11)	22.6(11)	36.6(12)	-1.0(9)	2.6(9)	2.8(9)
C25	23.2(10)	25.2(11)	27.9(11)	1.5(8)	2.7(9)	1.2(9)
C26	28.8(11)	30.7(11)	24.4(11)	-4.0(9)	3.4(9)	-3.7(9)
C27	23.3(10)	22.6(10)	27.6(11)	-2.0(8)	-1.1(9)	-0.1(8)
C28	28.3(11)	27.9(11)	27.6(12)	-3.1(9)	7.1(9)	0.1(9)
C29	25.1(10)	30.2(11)	24.2(11)	-3.0(9)	2.0(9)	-3.2(9)
C30	30.5(11)	33.5(12)	26.6(11)	0.3(9)	2.8(9)	0.9(9)
C31	26.4(11)	37.0(12)	24.9(11)	2.1(9)	2.2(9)	-2.8(9)
C32	32.9(12)	47.4(14)	27.9(12)	4.9(10)	-3.3(10)	-0.1(10)
C33	58.5(16)	52.4(15)	39.5(14)	6.0(13)	-11.1(12)	9.2(12)
C34	53.1(15)	58.6(16)	27.7(13)	-2.0(12)	-4.6(11)	1.3(11)
C35	37.2(13)	82(2)	49.2(16)	14.6(13)	-5.6(12)	2.0(14)
C36	26.5(11)	38.7(13)	25.4(11)	-4.0(9)	0.3(9)	-8.1(9)
C37	26.6(10)	33.3(12)	22.8(11)	-1.8(9)	3.3(9)	-5.5(9)
C38	35.5(12)	30.0(11)	27.8(12)	-4.7(9)	1.8(9)	-3.3(9)
C39	44.8(13)	35.9(13)	46.6(15)	0.9(11)	0.5(11)	-2.6(11)
C40	48.0(14)	36.9(13)	45.2(14)	-12.8(11)	-2.4(11)	-6.4(11)
C41	46.4(14)	39.0(13)	35.4(13)	-9.9(11)	7.3(11)	0.3(10)
C42	25.3(10)	34.0(12)	19.5(11)	-1.9(9)	0.2(9)	-1.8(9)
C43S	129(4)	134(4)	89(3)	33(3)	-15(3)	26(3)
C44S	125(6)	79(5)	46(4)	-8(4)	-10(4)	14(3)
C45S	97(5)	53(4)	76(5)	25(4)	23(5)	11(4)
O46S	125(4)	78(3)	72(3)	7(3)	30(3)	11(2)
O3S	113(3)	65(2)	82(2)	13(2)	31(2)	12.5(17)
C9	33.7(11)	31.2(12)	27.2(12)	-4.1(9)	7.4(9)	-9.0(9)
C1A	61(4)	46(4)	44(3)	24(4)	12(3)	-6(3)
C1b	55(3)	68(5)	42(3)	26(3)	4(3)	-13(3)
C2A	109(8)	49(4)	51(5)	-18(4)	48(5)	-21(3)
C2b	60(4)	52(3)	24(3)	4(3)	6(2)	-7(2)
C3A	54(4)	90(8)	39(5)	19(5)	-9(3)	-42(5)
C3b	64(5)	60(5)	68(6)	-22(4)	31(4)	-41(4)

Table SI3 Bond Lengths for Hardy012815_0mFINALCIF.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
C1	O1	1.351(2)	C23	C24	1.424(3)
C1	C2	1.410(3)	C25	C26	1.425(3)
C1	C14	1.413(3)	C26	C27	1.361(3)

N1	C15	1.289(2)	C28	C29	1.454(3)
N1	C16	1.413(2)	C29	C30	1.402(3)
C2	C3	1.543(3)	C29	C42	1.403(3)
C2	C7	1.389(3)	C30	C31	1.378(3)
N2	C27	1.417(2)	C31	C32	1.533(3)
N2	C28	1.282(2)	C31	C36	1.406(3)
O2	C42	1.353(2)	C32	C33	1.524(3)
C3	C4	1.540(3)	C32	C34	1.538(3)
C3	C5	1.535(3)	C32	C35	1.537(3)
C3	C6	1.528(3)	C36	C37	1.386(3)
N3	C18	1.349(2)	C37	C38	1.535(3)
N3	C19	1.350(2)	C37	C42	1.419(3)
N4	C24	1.352(2)	C38	C39	1.541(3)
N4	C25	1.346(2)	C38	C40	1.535(3)
C7	C8	1.408(3)	C38	C41	1.530(3)
C8	C13	1.382(3)	C43S	C44S	1.277(8)
C8	C9	1.535(3)	C43S	C45S	1.570(8)
C13	C14	1.402(3)	C44S	C45S	1.641(10)
C14	C15	1.448(3)	C44S	O3S1	1.642(6)
C16	C17	1.367(3)	C45S	O46S	1.202(7)
C16	C27	1.443(3)	C45S	O3S1	1.253(9)
C17	C18	1.423(3)	C9	C1A	1.617(6)
C18	C25	1.431(3)	C9	C1b	1.481(5)
C19	C20	1.428(3)	C9	C2A	1.489(6)
C19	C24	1.428(3)	C9	C2b	1.601(5)
C20	C21	1.361(3)	C9	C3A	1.501(10)
C21	C22	1.412(3)	C9	C3b	1.505(8)
C22	C23	1.360(3)			

[1]2-X,1-Y,1-Z

Table SI4 Bond Angles for Hardy012815_0mFINALCIF.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C2	C1	O1	119.05(16)	C29	C28	N2	122.78(18)
C14	C1	O1	120.42(17)	C30	C29	C28	118.37(18)
C14	C1	C2	120.53(17)	C42	C29	C28	121.47(17)
C16	N1	C15	122.43(16)	C42	C29	C30	120.16(17)
C3	C2	C1	121.04(16)	C31	C30	C29	121.60(19)
C7	C2	C1	116.66(16)	C32	C31	C30	123.63(19)
C7	C2	C3	122.31(16)	C36	C31	C30	116.47(18)
C28	N2	C27	119.16(16)	C36	C31	C32	119.88(17)
C4	C3	C2	110.19(15)	C33	C32	C31	111.82(17)
C5	C3	C2	110.05(15)	C34	C32	C31	110.01(17)

C5	C3	C4	110.04(16)	C34	C32	C33	107.76(18)
C6	C3	C2	111.74(16)	C35	C32	C31	108.84(17)
C6	C3	C4	107.37(16)	C35	C32	C33	109.3(2)
C6	C3	C5	107.38(16)	C35	C32	C34	109.08(19)
C19	N3	C18	116.06(16)	C37	C36	C31	125.15(18)
C25	N4	C24	116.14(17)	C38	C37	C36	122.42(17)
C8	C7	C2	124.93(18)	C42	C37	C36	116.44(18)
C13	C8	C7	116.39(17)	C42	C37	C38	121.12(17)
C9	C8	C7	121.53(17)	C39	C38	C37	110.22(16)
C9	C8	C13	122.07(17)	C40	C38	C37	112.04(16)
C14	C13	C8	122.00(17)	C40	C38	C39	107.82(17)
C13	C14	C1	119.47(17)	C41	C38	C37	109.63(16)
C15	C14	C1	121.42(17)	C41	C38	C39	110.13(17)
C15	C14	C13	119.10(17)	C41	C38	C40	106.93(17)
C14	C15	N1	122.11(17)	C29	C42	O2	120.83(16)
C17	C16	N1	124.98(17)	C37	C42	O2	119.01(17)
C27	C16	N1	115.55(16)	C37	C42	C29	120.16(17)
C27	C16	C17	119.44(17)	C45S	C43S	C44S	69.5(5)
C18	C17	C16	121.04(18)	C45S	C44S	C43S	63.7(5)
C17	C18	N3	118.88(17)	O3S1	C44S	C43S	108.5(5)
C25	C18	N3	121.84(17)	O3S1	C44S	C45S	44.9(3)
C25	C18	C17	119.27(17)	C44S	C45S	C43S	46.8(3)
C20	C19	N3	119.08(18)	O46S	C45S	C43S	118.2(7)
C24	C19	N3	122.05(17)	O46S	C45S	C44S	164.6(8)
C24	C19	C20	118.87(18)	O3S1	C45S	C43S	114.4(6)
C21	C20	C19	120.1(2)	O3S1	C45S	C44S	67.6(5)
C22	C21	C20	120.94(19)	O3S1	C45S	O46S	127.5(7)
C23	C22	C21	120.9(2)	C44S	O3S	C44S1	180
C24	C23	C22	120.1(2)	C45S	O3S	C44S	67.5(4)
C19	C24	N4	121.85(17)	C45S	O3S	C44S1	112.5(4)
C23	C24	N4	119.04(19)	C45S1	O3S	C44S	112.5(4)
C23	C24	C19	119.11(18)	C45S1	O3S	C44S1	67.5(4)
C18	C25	N4	122.05(17)	C45S1	O3S	C45S	180
C26	C25	N4	119.28(17)	C2A	C9	C1A	105.2(4)
C26	C25	C18	118.66(17)	C2b	C9	C1b	107.5(3)
C27	C26	C25	120.82(18)	C3A	C9	C1A	105.5(4)
C16	C27	N2	117.33(16)	C3A	C9	C2A	113.6(5)
C26	C27	N2	121.87(17)	C3b	C9	C1b	112.1(4)
C26	C27	C16	120.73(17)	C3b	C9	C2b	104.8(4)

[1]2-X,1-Y,1-Z

Table SI5 Hydrogen Atom Coordinates ($Å^2×10^4$) and Isotropic Displacement Parameters ($Å^2×10^3$)for Hardy012815_FINALCIF.

Atom	**x**	**y**	**z**	**U(eq)**
H1	4640(30)	6885(5)	2397(5)	49.7(5)

H2	3190(30)	7423(3)	3173(5)	53.6(6)
H4a	6413(14)	8192(4)	1432.5(12)	54.7(8)
H4b	5989(11)	8032(3)	1985(4)	54.7(8)
H4c	7739(5)	8516.3(15)	1878(4)	54.7(8)
H5a	8936(5)	7486(5)	2517.6(11)	48.4(8)
H5b	11131(13)	7327(4)	2284.7(12)	48.4(8)
H5c	10568(17)	7993.5(15)	2394(2)	48.4(8)
H6a	11658(12)	7580(3)	1434(4)	63.0(9)
H6b	9821(6)	7911(6)	1097.6(13)	63.0(9)
H6c	11096(17)	8247(3)	1544(3)	63.0(9)
H7	9548(3)	6940.4(8)	1032.1(7)	28.9(5)
H13	5315(3)	5646.6(8)	1192.0(7)	30.6(6)
H15	2962(3)	5658.4(8)	1845.8(7)	30.0(5)
H17	-281(3)	5505.4(8)	2032.5(7)	30.0(5)
H20	-6461(3)	4275.6(9)	2140.8(8)	40.0(6)
H21	-9216(3)	3952.5(9)	2582.3(8)	45.1(7)
H22	-9569(3)	4293.6(9)	3380.7(9)	46.2(7)
H23	-7176(3)	4962.3(9)	3740.3(8)	42.4(6)
H26	-948(3)	6180.3(8)	3637.7(7)	33.5(6)
H28	3133(3)	6205.1(9)	3834.0(7)	33.2(6)
H30	5844(3)	6448.3(9)	4470.5(7)	36.2(6)
H33a	6600(8)	6514(3)	5331(5)	76.5(10)
H33b	8310(20)	6154.0(15)	5047(3)	76.5(10)
H33c	8971(17)	6407(4)	5583(3)	76.5(10)
H34a	9280(20)	7897.6(18)	5298(2)	70.4(9)
H34b	7227(5)	7586(4)	5497(4)	70.4(9)
H34c	9589(19)	7427(3)	5730(2)	70.4(9)
H35a	11349(6)	6647(5)	4704(5)	85.0(11)
H35b	11707(9)	7335(3)	4777(6)	85.0(11)
H35c	12132(5)	6901(7)	5233.1(12)	85.0(11)
H36	8771(3)	8010.3(9)	4511.2(7)	36.4(6)
H39a	3723(7)	8682(3)	3485(4)	63.9(9)
H39b	4406(12)	8963(5)	4009.8(9)	63.9(9)
H39c	5073(7)	9277(3)	3522(5)	63.9(9)
H40a	8193(11)	8965(6)	4343.8(19)	65.6(9)
H40b	10026(7)	8682(3)	4043(5)	65.6(9)
H40c	8878(17)	9276(3)	3857(3)	65.6(9)
H41a	9148(11)	8281(5)	3224.1(9)	60.1(8)
H41b	6714(11)	8245(5)	2991.9(17)	60.1(8)
H41c	7900(20)	8864.3(10)	3050(2)	60.1(8)
H1Aa	10910(40)	5474(3)	1015(10)	75(3)
H1Ab	8710(20)	5109(8)	977(11)	75(3)
H1Ac	10160(50)	5132(9)	521(2)	75(3)
H1ba	11517(13)	6079(4)	802(12)	83(3)
H1bb	10696(12)	5456(12)	975(8)	83(3)
H1bc	11160(20)	5556(14)	416(4)	83(3)

H2Aa	9320(30)	6643(8)	222(14)	101(5)
H2Ab	11250(30)	6335(16)	544(6)	101(5)
H2Ac	10320(60)	6047(9)	37(9)	101(5)
H2ba	6865(12)	6505(10)	54(7)	68(3)
H2bb	9220(40)	6722(6)	246(4)	68(3)
H2bc	8940(40)	6194(4)	-136(4)	68(3)
H3Aa	5670(40)	5430(14)	448(5)	93(5)
H3Ab	5600(40)	6027(5)	144(13)	93(5)
H3Ac	7051(16)	5495(16)	-16(8)	93(5)
H3ba	7060(50)	5109(7)	635(7)	94(4)
H3bb	5460(17)	5567(5)	355(13)	94(4)
H3bc	7410(40)	5298(11)	85(8)	94(4)

Table SI6 Atomic Occupancy for Hardy012815FINALCIF

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
C44S	0.5	C45S	0.5	O46S	0.5
C1A	0.463(9)	H1Aa	0.463(9)	H1Ab	0.463(9)
H1Ac	0.463(9)	C1b	0.537(9)	H1ba	0.537(9)
H1bb	0.537(9)	H1bc	0.537(9)	C2A	0.463(9)
H2Aa	0.463(9)	H2Ab	0.463(9)	H2Ac	0.463(9)
C2b	0.537(9)	H2ba	0.537(9)	H2bb	0.537(9)
H2bc	0.537(9)	C3A	0.463(9)	H3Aa	0.463(9)
H3Ab	0.463(9)	H3Ac	0.463(9)	C3b	0.537(9)
H3ba	0.537(9)	H3bb	0.537(9)	H3bc	0.537(9)

Crystal Data for $C_{44}H_{54}N_4O_3$ (M =682.91): monoclinic, space group $P2_1/n$ (no. 14), a = 6.2424(2) Å, b = 22.8992(7) Å, c = 27.3834(8) Å, β = 94.704(1)°, V = 3901.2(2) Å^3, Z = 4, T = 180.45 K, μ(Mo Kα) = 0.073 mm^{-1}, *Dcalc* = 1.1626 g/mm^3, 75008 reflections measured (2.98 ≤ 2Θ ≤ 48.22), 6196 unique (R_{int} = 0.0492, R_{sigma}= 0.0308) which were used in all calculations. The final R_1 was 0.0453 (I>=2u(I)) and wR_2 was 0.1212 (all data).

VO[L^I]

Bam150

Table SI7 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for bam150_0mFINAL. Ueq is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
V1	4939.7(4)	5939.3(4)	1615.2(3)	22.73(14)
O2	4719.3(18)	6483.5(15)	2629.6(11)	27.7(4)
O1	4098.5(18)	4725.8(15)	2299.7(11)	29.1(4)
N2	6753(2)	6499.5(17)	1214.5(12)	22.1(5)
N1	6001(2)	4890.4(17)	831.5(12)	23.2(5)
N3	9707(2)	4809.8(19)	-1603.8(13)	29.5(5)
N4	10558(2)	6551.4(19)	-1162.3(13)	29.1(5)
C1	5222(3)	7259(2)	2790.0(16)	23.9(6)
C14	6405(3)	7634(2)	2265.4(16)	25.7(6)
C2	4609(3)	7717(2)	3525.2(16)	27.5(6)
C13	6959(3)	8438(2)	2469.0(17)	30.2(6)
C8	6384(3)	8890(2)	3163.4(17)	32.1(7)
C7	5209(3)	8503(2)	3675.6(17)	31.3(7)
C16	7600(2)	6128(2)	491.4(15)	21.9(6)
C27	7167(2)	5251(2)	262.2(15)	21.8(6)
C26	7855(3)	4842(2)	-431.6(16)	26.4(6)
C17	8725(3)	6537(2)	18.7(16)	25.5(6)
C25	9020(3)	5255(2)	-931.1(15)	24.8(6)
C18	9466(3)	6121(2)	-705.2(16)	24.9(6)
C24	10809(3)	5231(2)	-2054.8(16)	29.9(6)
C23	11592(3)	4785(3)	-2764.2(17)	36.8(7)
C20	12400(3)	6530(3)	-2350.6(18)	40.9(8)
C19	11235(3)	6119(2)	-1838.4(16)	30.1(6)
C22	12706(3)	5203(3)	-3227.8(18)	43.4(8)
C21	13109(3)	6085(3)	-3024.2(19)	45.7(8)
C29	4535(3)	3499(2)	1344.3(16)	26.0(6)
C30	4244(3)	2564(2)	1139.8(17)	30.9(6)
C28	5613(3)	3995(2)	785.9(16)	25.9(6)
C31	3293(3)	1971(2)	1660.2(18)	30.4(6)
O3	3977.2(18)	6714.2(15)	1084.7(11)	32.3(5)
C15	7120(3)	7201(2)	1543.2(16)	25.8(6)
C3	3326(3)	7339(2)	4111.1(17)	35.9(7)
C9	6926(3)	9782(3)	3409.9(19)	42.2(8)
C5	3601(4)	6135(3)	4464.9(19)	45.8(8)
C4	2211(3)	7544(3)	3646(2)	45.0(8)
C6	2828(4)	7951(3)	4852(2)	57.7(11)
C11	5886(4)	10791(3)	3438(2)	58.4(10)
C10	8206(4)	10081(4)	2795(3)	80.9(15)
C12	7220(5)	9375(3)	4273(3)	71.8(13)
C32	3005(3)	924(2)	1478(2)	36.5(7)

C34	1515(4)	855(3)	1728(3)	62.2(11)
C33	3475(4)	857(3)	560(2)	64.0(11)
C37	2869(3)	3233(2)	2666.7(17)	30.9(6)
C36	2642(3)	2337(2)	2416.2(18)	34.1(7)
C38	2157(3)	3530(3)	3528.8(18)	37.4(7)
C41	3182(3)	3358(3)	4051.2(19)	43.6(8)
C40	1493(3)	4712(3)	3458(2)	45.8(8)
C39	1078(4)	2811(3)	3988(2)	67.0(12)
C35	3718(5)	-29(3)	1969(4)	95.8(18)
C42	3834(3)	3861(2)	2104.0(16)	26.9(6)

Table SI8 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for bam150_0mFINAL. The Anisotropic displacement factor exponent takes the form: $2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Atom	$\mathbf{U_{11}}$	$\mathbf{U_{22}}$	$\mathbf{U_{33}}$	$\mathbf{U_{12}}$	$\mathbf{U_{13}}$	$\mathbf{U_{23}}$
V1	24.1(3)	25.3(3)	20.7(2)	-8.65(18)	-3.12(18)	-6.32(18)
O2	31.3(10)	30.9(11)	23.2(9)	-12.7(8)	-0.8(8)	-9.5(8)
O1	32.5(11)	31.4(11)	25.2(10)	-15.4(9)	0.4(8)	-8.6(8)
N2	24.4(12)	22.6(12)	19.3(11)	-4.6(9)	-2.7(9)	-5.4(9)
N1	25.7(12)	25.4(12)	19.1(11)	-10.3(10)	-2.8(9)	-2.5(9)
N3	28.6(13)	34.2(14)	23.0(12)	-3.5(10)	-2.4(10)	-4.7(10)
N4	25.1(12)	34.4(13)	25.1(12)	-7.8(10)	-2.9(10)	0.2(10)
C1	28.2(14)	21.3(14)	23.3(14)	-5.1(11)	-6.9(11)	-4.1(11)
C14	27.3(14)	25.0(14)	25.7(14)	-5.2(11)	-4.1(12)	-7.2(11)
C2	33.5(16)	27.8(15)	21.7(14)	-6.0(12)	-5.1(12)	-6.1(11)
C13	31.8(16)	28.6(15)	30.8(15)	-11.2(12)	-1.6(12)	-8.0(12)
C8	37.9(17)	29.6(16)	31.7(15)	-10.7(13)	-5.4(13)	-10.3(13)
C7	41.2(17)	28.7(16)	24.7(14)	-8.1(13)	-2.7(13)	-9.8(12)
C16	22.2(14)	24.2(14)	18.8(13)	-4.0(11)	-4.2(11)	-2.9(11)
C27	23.6(14)	21.0(14)	20.1(13)	-5.3(11)	-3.8(11)	-2.1(11)
C26	29.3(15)	26.9(15)	24.5(14)	-6.4(12)	-6.1(12)	-5.8(11)
C17	26.8(14)	24.9(14)	25.7(14)	-8.0(11)	-4.4(12)	-5.1(11)
C25	23.6(14)	28.2(15)	20.7(13)	-2.0(11)	-3.6(11)	-3.5(11)
C18	24.5(14)	25.2(15)	22.9(14)	-3.9(11)	-5.4(11)	0.7(11)
C24	26.0(15)	38.5(17)	19.7(14)	-0.3(13)	-4.0(12)	1.3(12)
C23	32.1(16)	47.4(19)	24.4(15)	5.2(14)	-3.4(13)	-5.6(13)
C20	31.0(17)	52(2)	33.7(17)	-11.3(15)	-0.8(14)	1.7(15)
C19	23.4(14)	39.1(17)	22.3(14)	-1.4(12)	-4.1(12)	2.5(12)
C22	32.2(17)	61(2)	24.5(16)	6.4(16)	-0.1(13)	0.0(15)
C21	28.8(17)	63(2)	32.2(17)	-5.5(16)	3.2(14)	5.0(16)
C29	26.9(14)	27.3(15)	24.1(14)	-10.1(12)	-4.1(11)	-2.1(11)
C30	32.6(16)	31.4(16)	30.3(15)	-9.5(13)	-5.4(13)	-7.2(12)
C28	28.7(15)	28.6(15)	22.6(14)	-7.2(12)	-4.7(12)	-7.7(11)
C31	31.2(15)	26.5(15)	35.2(16)	-9.3(12)	-10.6(13)	-0.7(12)
O3	31.3(11)	35.7(11)	31.3(11)	-4.8(9)	-8.8(9)	-6.5(9)

C15	25.9(14)	22.7(14)	29.0(14)	-7.9(11)	-3.0(12)	-5.5(11)
C3	40.4(17)	40.0(18)	27.4(15)	-15.0(14)	4.4(13)	-13.8(13)
C9	49(2)	41.5(19)	42.5(18)	-22.9(16)	0.4(15)	-20.7(15)
C5	61(2)	47(2)	28.9(16)	-25.2(17)	-1.3(15)	-3.0(14)
C4	34.2(17)	48(2)	53(2)	-10.8(15)	1.3(15)	-17.1(16)
C6	63(2)	68(2)	42.1(19)	-29(2)	18.1(17)	-31.1(18)
C11	79(3)	37(2)	63(2)	-21.5(18)	-5(2)	-21.3(18)
C10	73(3)	85(3)	98(3)	-53(2)	20(2)	-58(3)
C12	103(3)	67(3)	70(3)	-32(2)	-38(3)	-26(2)
C32	39.0(17)	23.3(15)	49.4(19)	-9.2(13)	-15.3(15)	-0.9(13)
C34	55(2)	58(2)	85(3)	-30.0(19)	-8(2)	-28(2)
C33	79(3)	49(2)	74(3)	-29(2)	-3(2)	-32(2)
C37	27.4(15)	34.8(16)	29.9(15)	-12.9(13)	-2.9(12)	-1.7(12)
C36	32.1(16)	33.9(17)	35.9(16)	-17.1(13)	-4.5(13)	1.0(13)
C38	36.7(17)	47.3(19)	28.3(15)	-21.0(15)	1.1(13)	-4.5(14)
C41	51(2)	47(2)	29.5(16)	-9.7(16)	-5.9(15)	-2.5(14)
C40	33.9(18)	64(2)	40.0(18)	-4.4(16)	-4.5(14)	-17.8(16)
C39	66(3)	87(3)	48(2)	-52(2)	20.9(19)	-22(2)
C35	131(4)	32(2)	158(5)	-16(2)	-104(4)	7(3)
C42	27.9(15)	26.3(15)	28.8(15)	-9.6(12)	-8.0(12)	-3.2(12)

Table SI9 Bond Lengths for bam150_0mFINAL.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
V1	O2	1.9299(17)	C25	C18	1.434(4)
V1	O1	1.9295(18)	C24	C23	1.426(4)
V1	N2	2.054(2)	C24	C19	1.440(4)
V1	N1	2.050(2)	C23	C22	1.355(4)
V1	O3	1.5958(19)	C20	C19	1.417(4)
O2	C1	1.311(3)	C20	C21	1.357(4)
O1	C42	1.313(3)	C22	C21	1.409(5)
N2	C16	1.422(3)	C29	C30	1.416(4)
N2	C15	1.310(3)	C29	C28	1.422(4)
N1	C27	1.426(3)	C29	C42	1.426(4)
N1	C28	1.306(3)	C30	C31	1.370(4)
N3	C25	1.351(3)	C31	C32	1.532(4)
N3	C24	1.342(3)	C31	C36	1.411(4)
N4	C18	1.341(3)	C3	C5	1.529(4)
N4	C19	1.345(3)	C3	C4	1.535(4)
C1	C14	1.420(4)	C3	C6	1.540(4)
C1	C2	1.431(4)	C9	C11	1.526(5)
C14	C13	1.412(4)	C9	C10	1.522(5)
C14	C15	1.417(4)	C9	C12	1.537(5)
C2	C7	1.379(4)	C32	C34	1.524(5)
C2	C3	1.536(4)	C32	C33	1.517(5)

C13	C8	1.364(4)	C32	C35	1.515(5)
C8	C7	1.413(4)	C37	C36	1.380(4)
C8	C9	1.537(4)	C37	C38	1.543(4)
C16	C27	1.442(3)	C37	C42	1.429(4)
C16	C17	1.364(4)	C38	C41	1.528(4)
C27	C26	1.357(4)	C38	C40	1.534(5)
C26	C25	1.412(4)	C38	C39	1.532(4)
C17	C18	1.416(4)			

Table SI10 Bond Angles for bam150_0mFINAL.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O1	V1	O2	86.90(7)	C19	C24	N3	121.8(2)
N2	V1	O2	87.31(8)	C19	C24	C23	118.8(3)
N2	V1	O1	141.41(9)	C22	C23	C24	120.2(3)
N1	V1	O2	148.02(9)	C21	C20	C19	120.6(3)
N1	V1	O1	86.94(8)	C24	C19	N4	121.4(2)
N1	V1	N2	78.27(8)	C20	C19	N4	120.0(3)
O3	V1	O2	108.55(9)	C20	C19	C24	118.6(3)
O3	V1	O1	111.11(9)	C21	C22	C23	121.0(3)
O3	V1	N2	106.90(9)	C22	C21	C20	120.8(3)
O3	V1	N1	102.94(9)	C28	C29	C30	116.5(2)
C1	O2	V1	131.78(16)	C42	C29	C30	120.7(2)
C42	O1	V1	130.98(17)	C42	C29	C28	122.6(2)
C16	N2	V1	115.02(15)	C31	C30	C29	121.8(3)
C15	N2	V1	124.87(17)	C29	C28	N1	126.5(2)
C15	N2	C16	120.0(2)	C32	C31	C30	123.0(3)
C27	N1	V1	115.17(15)	C36	C31	C30	116.0(2)
C28	N1	V1	124.23(18)	C36	C31	C32	120.8(2)
C28	N1	C27	120.3(2)	C14	C15	N2	126.8(2)
C24	N3	C25	116.6(2)	C5	C3	C2	109.4(3)
C19	N4	C18	116.8(2)	C4	C3	C2	110.4(2)
C14	C1	O2	121.5(2)	C4	C3	C5	110.4(3)
C2	C1	O2	120.1(2)	C6	C3	C2	111.6(2)
C2	C1	C14	118.4(2)	C6	C3	C5	107.4(3)
C13	C14	C1	120.5(2)	C6	C3	C4	107.5(3)
C15	C14	C1	122.9(2)	C11	C9	C8	109.4(3)
C15	C14	C13	116.6(2)	C10	C9	C8	111.7(2)
C7	C2	C1	117.4(2)	C10	C9	C11	108.7(3)
C3	C2	C1	120.3(2)	C12	C9	C8	109.1(3)
C3	C2	C7	122.3(2)	C12	C9	C11	109.6(3)
C8	C13	C14	122.0(3)	C12	C9	C10	108.3(3)
C7	C8	C13	116.4(2)	C34	C32	C31	111.0(3)
C9	C8	C13	124.4(3)	C33	C32	C31	111.7(3)
C9	C8	C7	119.2(2)	C33	C32	C34	107.1(3)

C8	C7	C2	125.2(2)	C35	C32	C31	108.5(3)
C27	C16	N2	114.2(2)	C35	C32	C34	109.2(3)
C17	C16	N2	125.8(2)	C35	C32	C33	109.2(3)
C17	C16	C27	119.9(2)	C38	C37	C36	122.0(2)
C16	C27	N1	113.3(2)	C42	C37	C36	117.2(3)
C26	C27	N1	126.2(2)	C42	C37	C38	120.8(2)
C26	C27	C16	120.5(2)	C37	C36	C31	126.0(3)
C25	C26	C27	120.5(2)	C41	C38	C37	108.8(2)
C18	C17	C16	120.7(2)	C40	C38	C37	111.5(2)
C26	C25	N3	119.1(2)	C40	C38	C41	109.1(3)
C18	C25	N3	121.4(2)	C39	C38	C37	111.4(2)
C18	C25	C26	119.5(2)	C39	C38	C41	108.1(3)
C17	C18	N4	119.1(2)	C39	C38	C40	107.8(3)
C25	C18	N4	121.9(2)	C29	C42	O1	121.2(2)
C25	C18	C17	118.9(2)	C37	C42	O1	120.6(2)
C23	C24	N3	119.4(3)	C37	C42	C29	118.2(2)

Table SI11 Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103) for bam150_0mFINAL.

Atom	**x**	**y**	**z**	**U(eq)**
H13	7739(3)	8666(2)	2119.0(17)	36.2(8)
H7	4808(3)	8803(2)	4152.3(17)	37.6(8)
H26	7557(3)	4286(2)	-579.0(16)	31.7(7)
H17	9008(3)	7095(2)	173.4(16)	30.6(7)
H23	11338(3)	4205(3)	-2909.1(17)	44.2(9)
H20	12682(3)	7110(3)	-2224.2(18)	49.1(9)
H22	13212(3)	4903(3)	-3687.7(18)	52(1)
H21	13870(3)	6365(3)	-3355.4(19)	54.8(10)
H30	4711(3)	2347(2)	638.7(17)	37.0(8)
H28	6090(3)	3648(2)	344.1(16)	31.1(7)
H15	7935(3)	7440(2)	1274.4(16)	30.9(7)
H5a	3930(20)	5731(3)	4016.7(19)	68.7(13)
H5b	4252(16)	6027(3)	4788(11)	68.7(13)
H5c	2791(6)	5891(5)	4812(11)	68.7(13)
H4a	2014(15)	8307(3)	3457(12)	67.6(12)
H4b	2495(9)	7174(15)	3178(8)	67.6(12)
H4c	1428(7)	7279(16)	4014(4)	67.6(12)
H6a	3512(10)	7849(17)	5150(9)	86.5(16)
H6b	2610(20)	8709(4)	4652(2)	86.5(16)
H6c	2048(15)	7676(15)	5217(9)	86.5(16)
H11a	5727(19)	11059(12)	2894(4)	87.6(15)
H11b	5072(9)	10612(5)	3822(12)	87.6(15)
H11c	6207(11)	11338(8)	3615(15)	87.6(15)
H10a	8866(11)	9450(7)	2769(15)	121(2)

H10b	8035(8)	10350(20)	2255(6)	121(2)
H10c	8524(19)	10630(20)	2974(12)	121(2)
H12a	6422(8)	9180(20)	4669(4)	107.7(19)
H12b	7890(20)	8752(15)	4250(5)	107.7(19)
H12c	7530(30)	9937(9)	4437(8)	107.7(19)
H34a	1194(6)	840(20)	2317(4)	93.4(16)
H34b	1056(5)	1477(11)	1438(13)	93.4(16)
H34c	1357(4)	209(11)	1587(15)	93.4(16)
H33a	3050(20)	1474(12)	246(3)	96.0(17)
H33b	4423(5)	850(20)	388(4)	96.0(17)
H33c	3250(20)	206(12)	466(4)	96.0(17)
H36	2002(3)	1937(2)	2779.3(18)	40.9(8)
H41a	3616(16)	2623(5)	4086(11)	65.4(12)
H41b	3831(13)	3842(12)	3796(7)	65.4(12)
H41c	2741(4)	3501(17)	4600(4)	65.4(12)
H40a	2165(3)	5183(3)	3251(13)	68.6(12)
H40b	917(17)	4844(5)	3083(11)	68.6(12)
H40c	980(18)	4848(6)	3996(3)	68.6(12)
H39a	416(15)	2913(17)	3673(9)	100.5(18)
H39b	1473(6)	2065(4)	4052(15)	100.5(18)
H39c	670(20)	3003(16)	4525(7)	100.5(18)
H35a	4661(6)	-8(17)	1794(17)	144(3)
H35b	3420(30)	8(17)	2551(4)	144(3)
H35c	3530(30)	-692(3)	1873(19)	144(3)

Table SI12 Solvent masks information for bam150_0mFINAL.

Number	X	Y	Z	Volume	Electron count
1	0.000	0.500	0.500	341.2	59.5
2	0.000	0.500	0.000	82.4	0.2

Crystal Data for $C_{42}H_{48}N_4O_3V$ (M =707.82): triclinic, space group P-1 (no. 2), a = 10.5213(4) Å, b = 12.7581(5) Å, c = 16.9448(7) Å, α = 77.715(1)°, β = 74.447(1)°,γ = 79.226(1)°, V = 2120.59(14) Å^3, Z = 2, T = 296.15 K, μ(Mo Kα) = 0.272 mm^{-1}, *Dcalc* = 1.1084 g/cm^3, 35450 reflections measured ($3.3 \leq 2\Theta \leq 49.42$), 7239 unique ($R_{int}$ = 0.0414, R_{sigma} = 0.0397) which were used in all calculations. The final R_1 was 0.0492 (I>=2u(I)) and wR_2 was 0.1405 (all data).

Zn[L^I](CH$_3$OH)

Table SI13 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Emily05222015_0mFinalCif. Ueq is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
Zn1	3184.2(3)	3244.4(2)	2731.92(18)	22.58(10)
O1	3995(2)	2082.2(12)	2815.9(11)	25.9(4)
O2	2306(2)	2779.8(13)	1514.3(11)	29.2(4)
O3	5039(2)	3993.9(14)	2623.7(12)	32.1(5)
N1	3529(2)	3706.8(13)	4061.3(12)	18.5(4)
N2	1606(2)	4185.7(13)	2895.9(12)	19.7(4)
N4	146(2)	6635.7(14)	5118.6(14)	26.5(5)
N3	2384(2)	6225.3(14)	6345.9(13)	23.5(5)
C15	4360(3)	3320.0(16)	4568.9(15)	20.2(5)
C6	5055(3)	2488.3(17)	4322.0(15)	20.9(5)
C1	4801(3)	1887.8(17)	3457.0(16)	20.5(5)
C2	5469(3)	1018.5(17)	3319.2(16)	22.7(5)
C3	6379(3)	854.5(17)	4006.9(17)	24.6(6)
C4	6674(3)	1443.6(17)	4860.3(16)	23.9(6)
C5	5986(3)	2242.6(18)	4997.0(16)	25.1(6)
C11	7718(3)	1162.3(19)	5564.2(18)	30.4(6)
C13	9277(3)	1179(2)	5377(2)	40.8(8)
C12	7727(4)	1811(2)	6458.7(18)	45.0(8)
C14	7258(3)	179(2)	5568(2)	41.2(8)
C7	5118(3)	301.0(17)	2426.8(16)	25.0(6)
C8	5627(3)	676(2)	1734.5(18)	33.7(7)
C9	3467(3)	27.1(19)	2164.3(18)	31.3(6)
C10	5881(4)	-581.9(19)	2436.2(19)	38.0(7)
C16	2798(3)	4494.4(16)	4390.4(15)	18.8(5)
C27	1696(3)	4734.9(16)	3751.0(15)	18.0(5)
C28	579(3)	4272.9(17)	2277.1(16)	22.6(5)
C29	332(3)	3750.0(17)	1394.1(15)	22.3(5)
C30	-860(3)	3990.3(19)	846.1(17)	28.3(6)
C31	-1264(3)	3521(2)	-9.3(17)	29.6(6)
C35	-2543(3)	3754(2)	-619.9(19)	41.6(8)
C37	-2050(4)	3876(2)	-1419.0(19)	46.4(8)
C38	-3746(4)	2973(4)	-885(4)	112(2)
C36	-3140(5)	4654(4)	-195(2)	103(2)
C32	-465(3)	2759.9(19)	-319.0(16)	28.6(6)
C33	705(3)	2480.5(18)	165.6(16)	24.8(6)
C39	1514(3)	1638(2)	-211.6(17)	31.1(6)
C42	786(4)	1120(2)	-1141.2(19)	44.4(8)
C41	1521(4)	953(2)	330(2)	48.0(9)
C40	3095(3)	1946(2)	-212.3(19)	40.9(8)
C34	1171(3)	3007.1(18)	1054.1(16)	22.8(6)

C26	858(3)	5450.8(17)	4011.1(16)	23.8(6)
C25	1033(3)	5962.8(16)	4888.3(16)	21.3(5)
C24	353(3)	7097.5(17)	5961.2(18)	26.7(6)
C19	1484(3)	6897.7(17)	6583.0(17)	26.3(6)
C18	2160(3)	5752.7(16)	5509.2(16)	20.2(5)
C17	3035(3)	5016.1(16)	5229.3(15)	19.9(5)
C20	1630(3)	7396.0(19)	7462.8(18)	33.8(7)
C21	701(3)	8056(2)	7705(2)	40.9(8)
C22	-396(3)	8266(2)	7096(2)	42.0(8)
C23	-579(3)	7805.4(19)	6244(2)	36.6(7)
C43	5261(4)	4059(3)	1810(2)	62.5(11)

Table SI14 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Emily05222015_0mFinalCif. 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}**
Zn1	26.03(18)	22.46(17)	17.66(16)	6.54(12)	3.51(12)	3.04(12)
O1	36.7(11)	21.2(9)	17.7(9)	10.2(8)	3.2(8)	2.7(7)
O2	32.0(11)	32.8(11)	17.7(9)	10.5(8)	1.2(8)	0.4(8)
O3	30.8(11)	40.0(12)	26.1(10)	-1.9(9)	3.1(9)	12.5(9)
N1	21.8(11)	15.6(10)	17.1(10)	4.2(8)	4.2(8)	2.3(8)
N2	23.0(11)	18.0(11)	18.3(10)	4.3(8)	4.2(9)	4.6(8)
N4	25.9(12)	17.7(11)	34.2(13)	4.7(9)	9.8(10)	1.9(10)
N3	26.3(12)	20.3(11)	21.4(11)	-0.6(9)	8.7(9)	-0.5(9)
C15	24.9(13)	18.8(13)	14.8(12)	1.7(10)	4(1)	1.4(10)
C6	24.1(13)	19.2(13)	21.1(13)	4.2(10)	6.4(10)	6.8(10)
C1	21.0(13)	20.4(13)	22.5(13)	2.5(10)	9.3(10)	6.8(10)
C2	25.0(14)	21.0(13)	23.8(13)	3.5(11)	10.0(11)	5.8(11)
C3	25.1(14)	19.5(13)	32.0(14)	9.2(11)	10.3(11)	8.0(11)
C4	23.5(14)	23.5(14)	26.0(14)	5.0(11)	4.9(11)	8.7(11)
C5	28.8(14)	26.0(14)	19.1(13)	5.7(11)	3.2(11)	4.6(11)
C11	29.7(15)	29.6(15)	33.1(15)	10.7(12)	2.9(12)	12.2(12)
C13	29.0(16)	44.4(19)	52(2)	8.5(14)	3.6(14)	21.2(16)
C12	52(2)	50(2)	29.0(16)	23.8(16)	-3.5(14)	9.3(14)
C14	43.3(19)	44.6(19)	40.8(18)	4.3(15)	1.4(14)	24.8(15)
C7	30.7(15)	19.9(13)	24.8(13)	6.7(11)	10.0(11)	3.7(11)
C8	42.1(17)	32.6(16)	27.8(15)	3.5(13)	17.1(13)	4.3(12)
C9	36.5(16)	26.1(15)	28.1(15)	1.0(12)	10.4(12)	0.1(12)
C10	50.6(19)	25.2(15)	35.5(16)	12.8(14)	12.0(14)	0.9(13)
C16	20.0(13)	15.0(12)	21.2(12)	0.9(10)	5.5(10)	4(1)
C27	18.8(12)	14.8(12)	20.1(12)	0.4(10)	5.6(10)	3.7(10)
C28	24.7(14)	21.3(13)	23.7(13)	6.4(11)	6.3(11)	7.9(11)
C29	23.0(13)	25.7(14)	19.1(12)	0.2(11)	2.8(10)	8.6(11)

C30	26.8(14)	35.0(16)	26.3(14)	8.4(12)	7.7(11)	11.6(12)
C31	19.4(14)	47.2(18)	25.0(14)	0.9(12)	2.9(11)	15.8(13)
C35	27.1(16)	73(2)	29.7(16)	8.5(15)	2.8(13)	24.2(16)
C37	47(2)	66(2)	28.7(16)	12.3(17)	1.0(14)	22.6(16)
C38	30(2)	179(5)	145(5)	-37(3)	-38(3)	114(4)
C36	105(4)	181(5)	36(2)	111(4)	13(2)	41(3)
C32	24.8(14)	40.0(16)	17.6(13)	-5.8(12)	3.5(11)	3.9(12)
C33	21.7(13)	32.4(15)	19.2(13)	-4.1(11)	4.2(10)	6.1(11)
C39	30.5(15)	35.7(16)	20.3(13)	1.1(12)	3.6(11)	-2.1(12)
C42	41.0(18)	50(2)	29.7(16)	3.7(15)	3.4(14)	-7.3(14)
C41	71(2)	26.8(16)	43.0(19)	6.4(16)	13.6(17)	1.7(14)
C40	31.1(16)	53(2)	30.6(16)	4.9(14)	7.3(13)	-2.1(14)
C34	20.8(13)	26.8(14)	21.4(13)	-3.4(11)	4.3(10)	8.1(11)
C26	24.1(14)	22.3(13)	22.0(13)	5.5(11)	0.7(10)	3.6(11)
C25	20.9(13)	13.9(12)	28.4(14)	-0.2(10)	7.2(11)	3.4(10)
C24	26.4(14)	17.7(13)	34.4(15)	-1.0(11)	13.9(12)	-0.1(11)
C19	26.5(14)	18.5(13)	32.8(15)	-3.7(11)	16.1(12)	-0.8(11)
C18	21.8(13)	15.1(12)	22.1(13)	-1.3(10)	7.5(10)	0.5(10)
C17	19.7(13)	20.2(13)	18.8(12)	2.7(10)	3(1)	4.2(10)
C20	38.0(17)	30.2(15)	29.2(15)	-1.3(13)	14.4(13)	-2.9(12)
C21	44.1(19)	32.9(17)	40.0(18)	-4.9(14)	26.4(15)	-9.8(14)
C22	35.1(17)	29.3(16)	57(2)	2.3(13)	28.0(16)	-7.7(15)
C23	30.5(16)	24.6(15)	52.6(19)	5.3(12)	18.2(14)	0.4(13)
C43	61(2)	91(3)	43(2)	-19(2)	7.3(18)	35(2)

Table SI15 Bond Lengths for Emily05222015_0mFinalCif.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	O1	1.9637(17)	C7	C9	1.534(4)
Zn1	O2	1.9499(17)	C7	C10	1.534(4)
Zn1	O3	2.1024(19)	C16	C27	1.463(3)
Zn1	N1	2.0713(19)	C16	C17	1.367(3)
Zn1	N2	2.075(2)	C27	C26	1.371(3)
O1	C1	1.291(3)	C28	C29	1.428(3)
O2	C34	1.299(3)	C29	C30	1.423(4)
O3	C43	1.421(4)	C29	C34	1.431(4)
N1	C15	1.305(3)	C30	C31	1.372(4)
N1	C16	1.415(3)	C31	C35	1.532(4)
N2	C27	1.413(3)	C31	C32	1.415(4)
N2	C28	1.306(3)	C35	C37	1.524(4)
N4	C25	1.345(3)	C35	C38	1.523(5)
N4	C24	1.349(3)	C35	C36	1.521(5)
N3	C19	1.355(3)	C32	C33	1.379(4)

N3	C18	1.344(3)	C33	C39	1.538(4)
C15	C6	1.424(3)	C33	C34	1.444(3)
C6	C1	1.440(3)	C39	C42	1.538(4)
C6	C5	1.424(3)	C39	C41	1.543(4)
C1	C2	1.450(3)	C39	C40	1.532(4)
C2	C3	1.374(4)	C26	C25	1.419(3)
C2	C7	1.545(3)	C25	C18	1.436(3)
C3	C4	1.419(4)	C24	C19	1.432(4)
C4	C5	1.367(4)	C24	C23	1.429(4)
C4	C11	1.537(4)	C19	C20	1.420(4)
C11	C13	1.538(4)	C18	C17	1.422(3)
C11	C12	1.530(4)	C20	C21	1.364(4)
C11	C14	1.542(4)	C21	C22	1.406(5)
C7	C8	1.544(4)	C22	C23	1.364(4)

Table SI16 Bond Angles for Emily05222015_0mFinalCif.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	Zn1	O1	94.93(7)	C17	C16	C27	119.7(2)
O3	Zn1	O1	101.34(8)	C16	C27	N2	115.0(2)
O3	Zn1	O2	98.66(8)	C26	C27	N2	125.7(2)
N1	Zn1	O1	89.46(7)	C26	C27	C16	119.4(2)
N1	Zn1	O2	164.37(8)	C29	C28	N2	127.0(2)
N1	Zn1	O3	95.17(8)	C30	C29	C28	115.8(2)
N2	Zn1	O1	152.16(8)	C34	C29	C28	124.2(2)
N2	Zn1	O2	89.89(8)	C34	C29	C30	120.0(2)
N2	Zn1	O3	105.01(8)	C31	C30	C29	122.2(3)
N2	Zn1	N1	79.46(8)	C35	C31	C30	123.8(3)
C1	O1	Zn1	130.08(16)	C32	C31	C30	116.6(2)
C34	O2	Zn1	131.72(16)	C32	C31	C35	119.5(2)
C43	O3	Zn1	120.97(19)	C37	C35	C31	110.7(2)
C15	N1	Zn1	123.74(16)	C38	C35	C31	108.8(3)
C16	N1	Zn1	114.68(15)	C38	C35	C37	109.3(3)
C16	N1	C15	121.6(2)	C36	C35	C31	111.2(3)
C27	N2	Zn1	114.74(15)	C36	C35	C37	106.8(3)
C28	N2	Zn1	124.29(17)	C36	C35	C38	109.9(4)
C28	N2	C27	121.0(2)	C33	C32	C31	125.0(2)
C24	N4	C25	116.9(2)	C39	C33	C32	122.2(2)

C18	N3	C19	117.2(2)	C34	C33	C32	118.0(2)
C6	C15	N1	127.0(2)	C34	C33	C39	119.8(2)
C1	C6	C15	123.6(2)	C42	C39	C33	112.3(2)
C5	C6	C15	116.0(2)	C41	C39	C33	110.0(2)
C5	C6	C1	120.3(2)	C41	C39	C42	107.3(2)
C6	C1	O1	123.1(2)	C40	C39	C33	109.8(2)
C2	C1	O1	119.5(2)	C40	C39	C42	108.0(2)
C2	C1	C6	117.4(2)	C40	C39	C41	109.3(3)
C3	C2	C1	117.9(2)	C29	C34	O2	122.8(2)
C7	C2	C1	120.0(2)	C33	C34	O2	119.1(2)
C7	C2	C3	122.0(2)	C33	C34	C29	118.0(2)
C4	C3	C2	125.7(2)	C25	C26	C27	121.4(2)
C5	C4	C3	116.2(2)	C26	C25	N4	119.3(2)
C11	C4	C3	119.6(2)	C18	C25	N4	121.6(2)
C11	C4	C5	124.2(2)	C18	C25	C26	119.1(2)
C4	C5	C6	122.4(2)	C19	C24	N4	121.8(2)
C13	C11	C4	108.9(2)	C23	C24	N4	119.2(3)
C12	C11	C4	111.9(2)	C23	C24	C19	118.9(2)
C12	C11	C13	108.9(2)	C24	C19	N3	121.0(2)
C14	C11	C4	110.3(2)	C20	C19	N3	119.8(3)
C14	C11	C13	108.5(2)	C20	C19	C24	119.2(2)
C14	C11	C12	108.2(2)	C25	C18	N3	121.5(2)
C8	C7	C2	111.4(2)	C17	C18	N3	119.7(2)
C9	C7	C2	110.2(2)	C17	C18	C25	118.9(2)
C9	C7	C8	109.3(2)	C18	C17	C16	121.3(2)
C10	C7	C2	111.3(2)	C21	C20	C19	119.9(3)
C10	C7	C8	107.5(2)	C22	C21	C20	121.2(3)
C10	C7	C9	107.0(2)	C23	C22	C21	121.0(3)
C27	C16	N1	114.6(2)	C22	C23	C24	119.8(3)
C17	C16	N1	125.7(2)				

Table SI17 Solvent masks information for Emily05222015_0m.

Number	X	Y	Z	Volume	Electron count
1	-0.267	-0.290	0.291	177.6	35.4
2	0.267	0.290	0.709	177.6	35.6
3	0.309	0.856	0.975	35.5	0.0

4	0.691	0.144	0.025	35.5	0.0

Crystal Data for $C_{43}H_{52}N_4O_3Zn$ (M =738.31): triclinic, space group P-1 (no. 2), a = 9.3102(5) Å, b = 15.1537(7) Å, c = 16.4769(8) Å, α = 105.875(2)°, β = 100.257(2)°, γ = 91.511(2)°, V = 2193.30(19) Å^3, Z = 2, T = 180.45 K, μ(Mo Kα) = 0.599 mm^{-1}, *Dcalc* = 1.1179 g/mm^3, 43775 reflections measured (3.26 ≤ 2Θ ≤ 51.44), 8341 unique (R_{int} = 0.0552, R_{sigma} = 0.0462) which were used in all calculations. The final R_1 was 0.0467 (I>=2u(I)) and wR_2 was 0.1186 (all data).

Fe[L^I]-O-Fe[L^I]

Eh004final

Table SI18 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Emily004final. Ueq is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Fe1	4556.95(17)	1191.69(6)	5962.7(3)	34.32(11)
O1	3331.3(8)	1335.7(3)	4939.8(14)	45.6(4)
O2	4945.8(9)	1531.0(3)	5457.2(15)	46.1(4)
O3	5000	1260.2(5)	7500	42.7(5)
N1	4030(1)	719.4(4)	5637.7(15)	33.4(4)
N2	5560.8(10)	903.4(4)	6183.4(16)	35.6(4)
N3	4978.0(12)	-405.8(4)	6352.1(16)	45.2(4)

N4	6722.6(12)	-189.4(4)	7265.8(18)	47.4(5)
C1	2673.7(12)	1231.3(5)	4922(2)	40.8(5)
C2	1998.2(13)	1449.5(5)	4687(2)	49.7(6)
C3	2070.8(15)	1811.8(6)	4546(3)	72.9(9)
C4	2048.9(19)	1873.3(7)	3440(3)	93.5(12)
C5	2946.6(18)	1942.6(6)	5732(4)	94.1(12)
C6	1292(2)	2003.9(7)	4340(4)	112.8(16)
C7	1306.9(14)	1321.9(6)	4638(2)	52.1(6)
C8	1204.1(13)	993.5(5)	4788(2)	45.4(5)
C9	386.4(16)	884.9(6)	4691(3)	58.7(6)
C10	295(2)	518.0(8)	4644(4)	108.4(14)
C11	-477.1(18)	1023.1(11)	3502(4)	120.8(15)
C12	467(3)	1018.7(9)	5773(4)	97.0(11)
C13	1863.8(13)	787.5(5)	5043(2)	42.3(5)
C14	2606.0(12)	898.8(5)	5124.9(19)	37.2(4)
C15	3266.4(12)	664.8(5)	5424.9(18)	35.5(4)
C16	4640.1(12)	463.6(5)	5966.5(17)	31.9(4)
C17	4477.4(12)	141.2(5)	5954.0(17)	36.2(4)
C18	5166.3(13)	-91.0(4)	6375.5(17)	36.3(4)
C19	5666.8(16)	-612.0(5)	6787(2)	47.7(6)
C20	5518.2(19)	-950.8(5)	6806(2)	65.7(8)
C21	6216(2)	-1162.5(6)	7212(3)	71.1(9)
C22	7055(2)	-1056.8(6)	7628(3)	73.2(8)
C23	7217.9(19)	-737.3(6)	7637(2)	62.1(7)
C24	6533.2(16)	-505.3(5)	7234(2)	47.2(5)
C25	6039.1(13)	17.8(5)	6832.9(18)	36.7(4)
C26	6187.2(13)	350.9(5)	6807.1(19)	37.5(4)
C27	5505.9(12)	569.6(4)	6346.6(18)	32.7(4)
C28	6203.4(13)	1012.6(5)	6184(2)	39.6(5)
C29	6318.1(13)	1338.1(5)	5963(2)	39.3(5)
C30	7084.7(13)	1402.2(5)	6032(2)	43.9(5)
C31	7248.4(13)	1701.8(5)	5798(2)	44.0(5)
C32	8057.9(14)	1781.4(6)	5844(2)	50.5(6)
C33	8617.4(17)	1480.4(7)	6080(3)	66.7(7)
C34	7731.1(18)	1926.5(7)	4610(3)	66.2(7)
C35	8655.3(17)	2028.1(7)	6871(3)	72.8(8)
C36	6629.9(14)	1947.8(5)	5509(2)	47.3(5)
C37	5865.8(13)	1904.7(5)	5407(2)	45.4(5)
C38	5214.1(15)	2185.6(5)	5089(3)	58.3(7)
C39	4289.4(16)	2115.3(6)	3861(3)	74.1(9)
C40	5142(2)	2231.1(6)	6123(3)	76.0(9)
C41	5549.3(18)	2506.0(6)	4949(3)	84.5(10)

C42	5686.3(13)	1587.0(5)	5613(2)	40.0(5)

Table SI19 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Emily004final. 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}**
Fe1	33.28(15)	21.59(16)	53.1(2)	7.29(12)	29.22(15)	4.61(10)
O1	33.7(7)	28.9(7)	70.4(10)	11.1(7)	30.3(7)	5.6(5)
O2	44.5(8)	28.8(7)	73.9(11)	17.7(7)	41.1(8)	9.3(6)
O3	49.0(11)	28.1(10)	60.4(14)	0	38.5(11)	0
N1	32.8(8)	24.4(8)	42.7(10)	3.9(7)	23.2(7)	3.5(6)
N2	38.6(8)	25.5(8)	49.3(10)	8.9(7)	30.5(8)	6.8(6)
N3	53.9(10)	26.1(9)	39(1)	2.4(8)	20.3(8)	4.9(7)
N4	56.6(11)	37.2(10)	57.5(12)	16.9(9)	39.8(10)	19.1(8)
C1	29.6(9)	33.2(11)	50.0(13)	1.1(9)	19.8(9)	2.2(7)
C2	32.8(10)	34.0(11)	67.3(15)	-3(1)	23.5(10)	2.0(8)
C3	41.8(12)	32.1(12)	128(3)	3.5(15)	43.9(15)	7.9(9)
C4	63.5(17)	51.4(17)	139(3)	41.7(19)	49.1(19)	16.8(13)
C5	57.7(16)	39.7(15)	155(3)	-26.5(18)	51.3(19)	-7.5(12)
C6	67.4(18)	40.7(15)	219(5)	0(2)	83(3)	13.9(13)
C7	33.8(10)	42.2(12)	73.5(16)	-8.8(11)	29.7(11)	2.9(9)
C8	33.1(10)	49.5(13)	52.4(13)	-10.6(10)	25.9(10)	-5.3(9)
C9	47.1(12)	64.5(16)	77.6(18)	-8.9(13)	45.2(13)	-7.3(11)
C10	102(2)	77(2)	207(4)	-43(2)	126(3)	-39.0(19)
C11	36.6(14)	185(4)	120(3)	33(3)	38.6(18)	-11.8(19)
C12	116(3)	98(3)	132(3)	-24(2)	104(3)	-16(2)
C13	39.6(10)	37.6(11)	50.9(13)	-5.8(10)	28.5(10)	-6.9(8)
C14	34.2(9)	30.7(10)	45.9(12)	-2.6(9)	24.3(9)	-2.2(7)
C15	40(1)	25.1(9)	42.2(11)	0.5(8)	25.7(9)	-1.2(7)
C16	37.1(9)	25.0(9)	33.4(10)	6.1(8)	21.7(8)	6.0(7)
C17	38.8(10)	27.5(10)	37.5(11)	1.6(8)	21.1(9)	1.6(7)
C18	49.5(11)	23.4(9)	29.6(10)	4.5(8)	21.3(9)	7.3(8)
C19	63.9(14)	27.7(11)	36.1(12)	5.0(9)	23.3(11)	13.7(9)
C20	76.0(17)	28.5(12)	56.6(16)	5.7(11)	23.1(13)	8.5(11)
C21	93(2)	25.1(12)	62.7(17)	10.5(11)	31.9(16)	20.4(12)
C22	86(2)	46.3(15)	80(2)	20.1(14)	47.7(17)	36.0(14)
C23	74.5(17)	43.9(14)	71.0(18)	22.1(12)	46.6(15)	30.3(12)
C24	61.8(13)	33.8(11)	48.1(13)	11(1)	35.0(11)	18.3(10)
C25	46.9(10)	31.7(10)	37.1(11)	9.8(9)	28.7(9)	12.8(8)
C26	41.7(10)	34.7(11)	44.0(12)	9.8(9)	30.4(9)	9.1(8)
C27	41.8(10)	25.1(9)	38.4(11)	5.8(8)	28.4(9)	5.9(7)

C28	38.3(10)	33.0(11)	54.2(13)	9.5(9)	31.9(10)	9.0(8)
C29	37.9(10)	32(1)	50.0(13)	8.3(9)	28.2(10)	2.8(8)
C30	37.6(10)	39.1(11)	56.6(14)	7.6(10)	30(1)	2.2(8)
C31	37.9(10)	41.5(12)	49.4(13)	3(1)	25.4(10)	-7.4(8)
C32	42.2(11)	50.7(13)	60.8(15)	1.4(11)	32.8(11)	-11.1(9)
C33	56.1(14)	68.2(17)	97(2)	9.8(15)	57.6(15)	-0.1(12)
C34	66.5(15)	63.6(17)	76.1(18)	1.3(14)	47.9(15)	-19.9(13)
C35	51.0(14)	84(2)	82(2)	-17.9(16)	40.2(14)	-26.0(13)
C36	43.2(11)	36.4(11)	55.4(14)	9.4(10)	27(1)	-5.6(9)
C37	41.5(10)	32.2(11)	57.0(14)	11.3(10)	27.7(10)	0.4(8)
C38	48.0(12)	30.0(11)	89.8(19)	20.2(12)	39.0(13)	5.9(9)
C39	48.8(13)	48.9(15)	99(2)	33.3(15)	33.2(14)	9.8(11)
C40	80.0(19)	38.3(14)	121(3)	9.2(15)	67.9(19)	17.3(12)
C41	66.6(16)	35.0(13)	141(3)	29.3(16)	59.0(19)	4.8(11)
C42	37.7(10)	32.7(11)	52.3(13)	10.6(9)	29.3(10)	4.2(8)

Table SI20 Bond Lengths for Eh004final.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Fe1	O1	1.9196(13)	C13	C14	1.416(3)
Fe1	O2	1.9074(13)	C14	C15	1.425(3)
Fe1	O3	1.7616(4)	C16	C17	1.366(3)
Fe1	N1	2.1107(15)	C16	C27	1.447(3)
Fe1	N2	2.1007(15)	C17	C18	1.422(3)
O1	C1	1.304(2)	C18	C25	1.430(3)
O2	C42	1.302(2)	C19	C20	1.432(3)
O3	Fe1[1]	1.7616(4)	C19	C24	1.420(3)
N1	C15	1.305(2)	C20	C21	1.383(4)
N1	C16	1.418(2)	C21	C22	1.384(4)
N2	C27	1.412(2)	C22	C23	1.355(4)
N2	C28	1.299(2)	C23	C24	1.421(3)
N3	C18	1.344(2)	C25	C26	1.410(3)
N3	C19	1.349(3)	C26	C27	1.369(3)
N4	C24	1.348(3)	C28	C29	1.426(3)
N4	C25	1.345(2)	C29	C30	1.420(3)
C1	C2	1.430(3)	C29	C42	1.418(3)
C1	C14	1.424(3)	C30	C31	1.364(3)
C2	C3	1.528(3)	C31	C32	1.531(3)
C2	C7	1.374(3)	C31	C36	1.410(3)
C3	C4	1.527(5)	C32	C33	1.533(3)
C3	C5	1.540(4)	C32	C34	1.533(4)

C3	C6	1.540(3)	C32	C35	1.534(3)
C7	C8	1.405(3)	C36	C37	1.377(3)
C8	C9	1.537(3)	C37	C38	1.547(3)
C8	C13	1.367(3)	C37	C42	1.429(3)
C9	C10	1.523(4)	C38	C39	1.536(4)
C9	C11	1.543(4)	C38	C40	1.531(4)
C9	C12	1.513(4)	C38	C41	1.532(3)

[1]1-X,+Y,3/2-Z

Table SI21 Bond Angles for Emily004final.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O1	Fe1	N1	86.13(6)	C17	C16	C27	119.77(16)
O1	Fe1	N2	148.95(7)	C16	C17	C18	120.72(18)
O2	Fe1	O1	93.85(6)	N3	C18	C17	118.74(19)
O2	Fe1	N1	147.27(7)	N3	C18	C25	122.16(17)
O2	Fe1	N2	87.14(6)	C17	C18	C25	119.08(17)
O3	Fe1	O1	107.24(6)	N3	C19	C20	118.6(2)
O3	Fe1	O2	108.74(7)	N3	C19	C24	122.4(2)
O3	Fe1	N1	102.43(7)	C24	C19	C20	118.9(2)
O3	Fe1	N2	101.73(6)	C21	C20	C19	118.5(3)
N2	Fe1	N1	76.86(6)	C20	C21	C22	122.2(2)
C1	O1	Fe1	128.11(13)	C23	C22	C21	120.6(2)
C42	O2	Fe1	133.73(12)	C22	C23	C24	120.5(3)
Fe1	O3	Fe1[1]	161.50(12)	N4	C24	C19	121.88(18)
C15	N1	Fe1	121.35(13)	N4	C24	C23	118.8(2)
C15	N1	C16	120.87(16)	C19	C24	C23	119.3(2)
C16	N1	Fe1	115.92(12)	N4	C25	C18	121.89(18)
C27	N2	Fe1	115.34(11)	N4	C25	C26	118.76(18)
C28	N2	Fe1	124.57(13)	C26	C25	C18	119.34(16)
C28	N2	C27	120.09(15)	C27	C26	C25	120.80(18)
C18	N3	C19	115.59(19)	N2	C27	C16	114.64(15)
C25	N4	C24	116.03(19)	C26	C27	N2	125.35(17)
O1	C1	C2	120.40(18)	C26	C27	C16	120.00(17)
O1	C1	C14	121.13(17)	N2	C28	C29	126.53(17)
C14	C1	C2	118.47(18)	C30	C29	C28	116.54(18)
C1	C2	C3	120.60(19)	C42	C29	C28	123.34(17)
C7	C2	C1	117.5(2)	C42	C29	C30	120.01(18)
C7	C2	C3	121.91(19)	C31	C30	C29	121.80(19)
C2	C3	C5	109.3(2)	C30	C31	C32	123.7(2)
C2	C3	C6	112.2(2)	C30	C31	C36	116.80(18)

C4	C3	C2	110.0(2)	C36	C31	C32	119.50(19)
C4	C3	C5	110.7(3)	C31	C32	C33	112.17(19)
C4	C3	C6	107.5(3)	C31	C32	C34	109.47(19)
C5	C3	C6	107.1(3)	C31	C32	C35	109.1(2)
C2	C7	C8	125.36(19)	C33	C32	C35	109.0(2)
C7	C8	C9	119.60(19)	C34	C32	C33	107.7(2)
C13	C8	C7	116.85(18)	C34	C32	C35	109.3(2)
C13	C8	C9	123.5(2)	C37	C36	C31	124.95(19)
C8	C9	C11	109.4(2)	C36	C37	C38	122.40(19)
C10	C9	C8	112.1(2)	C36	C37	C42	117.61(19)
C10	C9	C11	107.8(3)	C42	C37	C38	119.99(18)
C12	C9	C8	109.1(2)	C39	C38	C37	109.6(2)
C12	C9	C10	110.2(3)	C40	C38	C37	110.1(2)
C12	C9	C11	108.1(3)	C40	C38	C39	111.0(2)
C8	C13	C14	121.5(2)	C40	C38	C41	107.2(2)
C1	C14	C15	122.85(17)	C41	C38	C37	111.36(19)
C13	C14	C1	120.25(18)	C41	C38	C39	107.6(2)
C13	C14	C15	116.90(18)	O2	C42	C29	121.58(17)
N1	C15	C14	126.82(18)	O2	C42	C37	119.70(17)
N1	C16	C27	114.00(16)	C29	C42	C37	118.70(17)
C17	C16	N1	126.23(17)				

[1]1-X,+Y,3/2-Z

Crystal Data for $C_{90}H_{108}Fe_2N_8O_{6.5}$ (M =1529.56): monoclinic, space group C2/c (no. 15), a = 18.9491(3) Å, b = 41.3420(7) Å, c = 13.8422(2) Å, β = 128.2090(10)°, V = 8520.7(2) Å^3, Z = 4, T = 180(2) K, μ(MoKα) = 0.399 mm^{-1}, *Dcalc* = 1.192 g/mm^3, 50373 reflections measured (1.98 ≤ 2Θ ≤ 55.48), 9764 unique (R_{int} = 0.0354, R_{sigma} = 0.0364) which were used in all calculations. The final R_1 was 0.0457 (>2sigma(I)) and wR_2 was 0.1465 (all data).

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