Supporting Information for

N,N-dialkyl-N'-acylthioureas as modular ligands for deposition of transition metal sulphides

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X-ray analysis.

Raw data frames were read by program SAINT[1] and integrated using 3D profiling algorithms. The resulting data were reduced to produce hkl reflections and their intensities and estimated standard deviations. The data were corrected for Lorentz and polarization effects and numerical absorption corrections were applied based on indexed and measured faces.

Ni(L3)$_2$. The structure was solved and refined in *SHELXTL2014*, using full-matrix least-squares refinement. The non-H atoms were refined with anisotropic thermal parameters and all of the H atoms were calculated in idealized positions and refined riding on their parent atoms. The asymmetric unit consists of a half Ni complex located on a 2-fold rotational axis along the z-axis. In the final cycle of refinement, 5829 reflections (of which 5510 are observed with $I > 2\sigma(I)$) were used to refine 190 parameters and the resulting R_1, wR_2 and S (goodness of fit) were 2.00%, 4.85% and 1.029, respectively. The refinement was carried out by minimizing the wR_2 function using F^2 rather than F values. R_1 is calculated to provide a reference to the conventional R value but its function is not minimized.

Cu(L3)$_2$·THF. The structure was solved and refined in *SHELXTL2014*, using full-matrix least-squares refinement. The non-H atoms were refined with anisotropic thermal parameters and all of the H atoms were calculated in idealized positions and refined riding on their parent atoms. The asymmetric unit consists of two half complexes with each one located on an independent center of inversion, and a disordered tetrahydrofuran solvent molecule. One of the two complexes has a disorder in the coordination ring with the Cu, S and O refined in two parts with their site occupation factors dependently refined. The solvent molecule is disordered and also refined in two parts with their site occupation factors dependently refined. In the final cycle of refinement, 8897 reflections (of which 7375 are observed with $I > 2\sigma(I)$) were used to refine 450 parameters and the resulting R_1, wR_2 and S (goodness of fit) were 3.86%, 9.50% and 1.025, respectively. The refinement was carried out by minimizing the wR_2 function using F^2 rather than F values. R_1 is calculated to provide a reference to the conventional R value but its function is not minimized.

Co(L3)$_3$. The structure was solved and refined in *SHELXTL2014*, using full-matrix least-squares refinement. The non-H atoms were refined with anisotropic thermal parameters and all of the H atoms were calculated in idealized positions and refined riding on their parent atoms. The

asymmetric unit consists of the Co-complex with three coordinated ligands. One of the diisopropylamine groups is disordered and was refined in two parts with their site occupation factors dependently refined. In the final cycle of refinement, **18743** reflections (of which **12079** are observed with $I > 2\sigma(I)$) were used to refine **560** parameters and the resulting R_1, wR_2 and S (goodness of fit) were **5.82**%, **11.33**% and **1.106**, respectively. The refinement was carried out by minimizing the wR_2 function using F^2 rather than F values. R_1 is calculated to provide a reference to the conventional R value but its function is not minimized.

$Zn(L3)_2 \cdot NCCH_3$. The structure was solved and refined in *SHELXTL2014*, using full-matrix least-squares refinement. The non-H atoms were refined with anisotropic thermal parameters and all of the H atoms were calculated in idealized positions and refined riding on their parent atoms. In addition to the Zn complex, there is a molecule of acetonitrile solvent molecule in the asymmetric unit. In the final cycle of refinement, 8616 reflections (of which 3934 are observed with $I > 2\sigma(I)$) were used to refine 406 parameters and the resulting R_1, wR_2 and S (goodness of fit) were 4.98%, 8.92% and 0.829, respectively. The refinement was carried out by minimizing the wR_2 function using F^2 rather than F values. R_1 is calculated to provide a reference to the conventional R value but its function is not minimized.

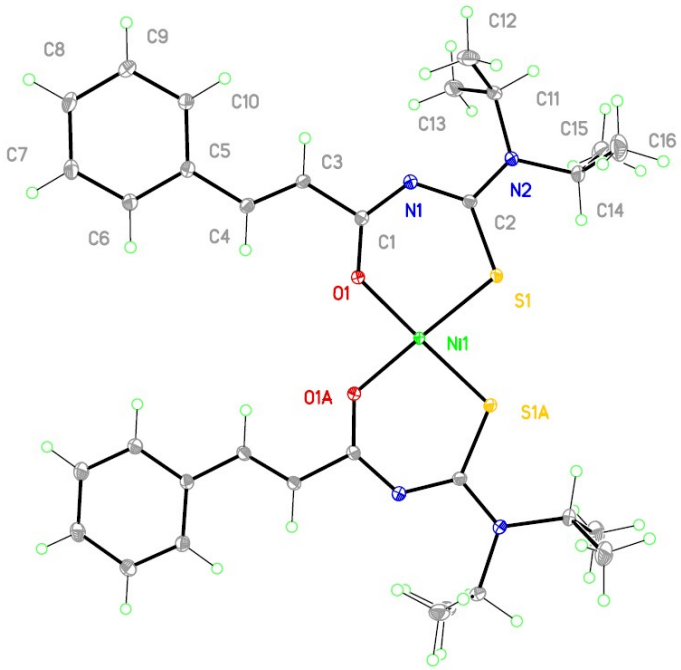


Figure S1. Full X-ray crystallographic structure for Ni(L3)$_2$

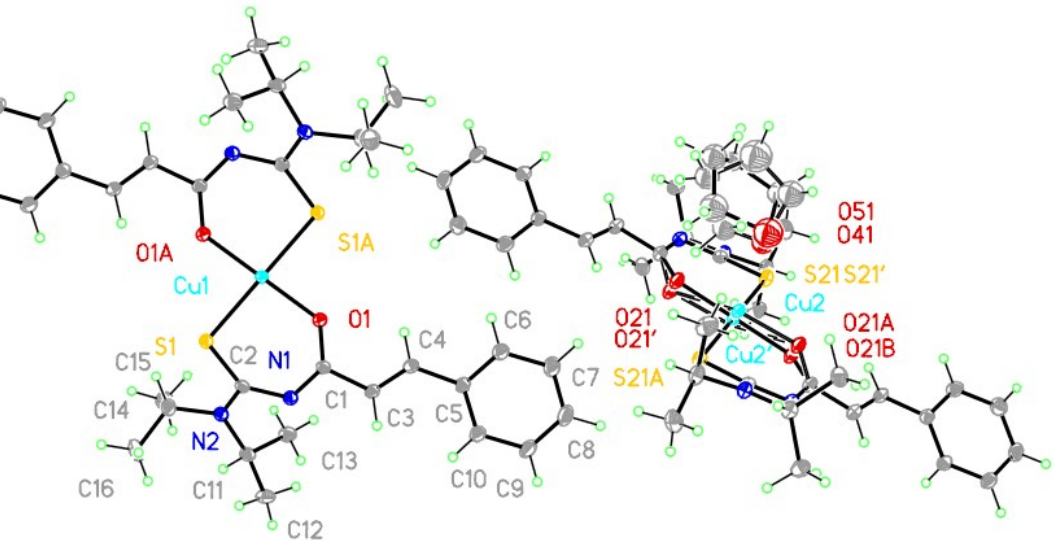


Figure S2. Full X-ray crystallographic structure for Cu(L3)2·TH

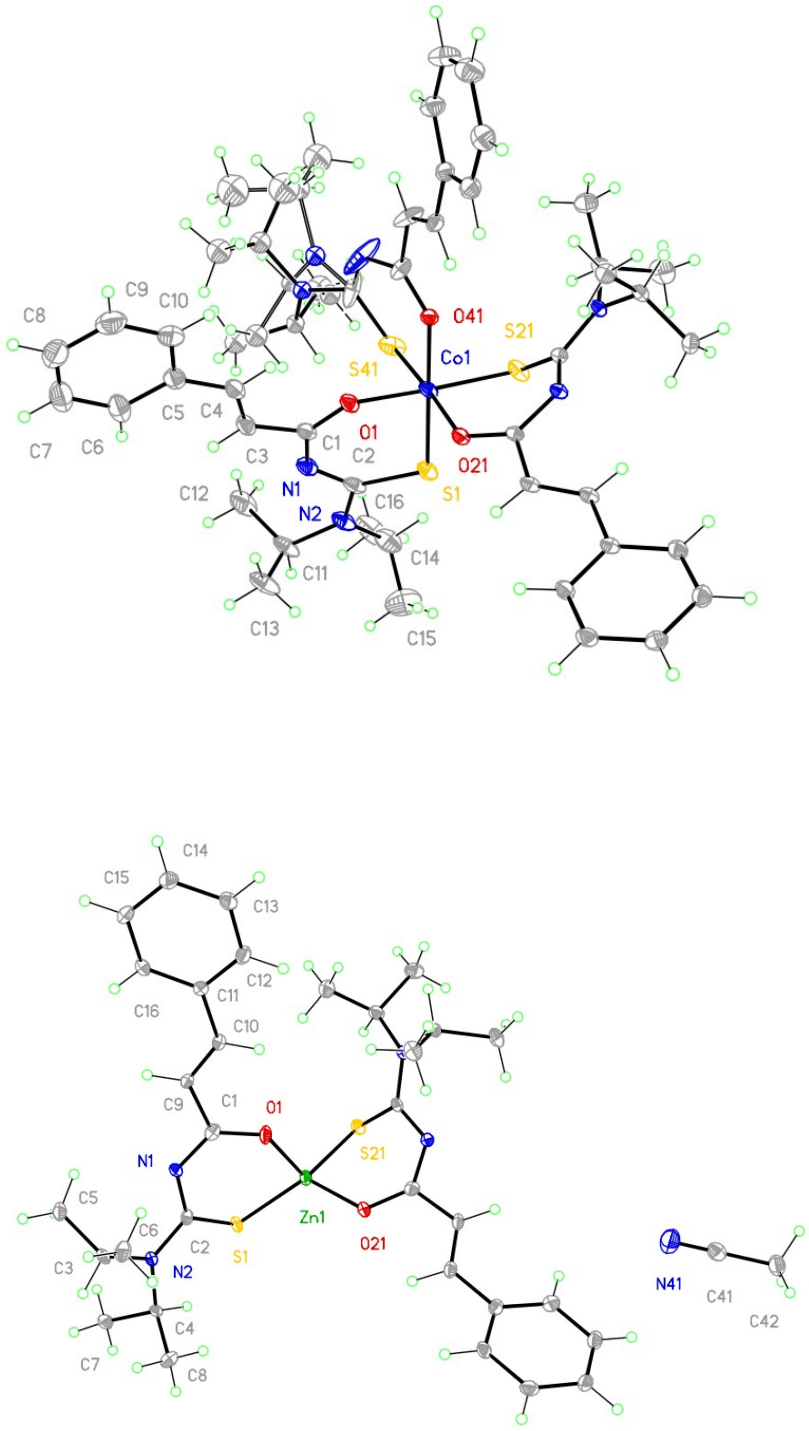


Figure S3. X-ray structure of Co(L3)3, showing the disorder on one of the amine sites.

Figure S4. X-ray structure of $Zn(L3)_2 \cdot NCCH_3$ with solvent molecule included.

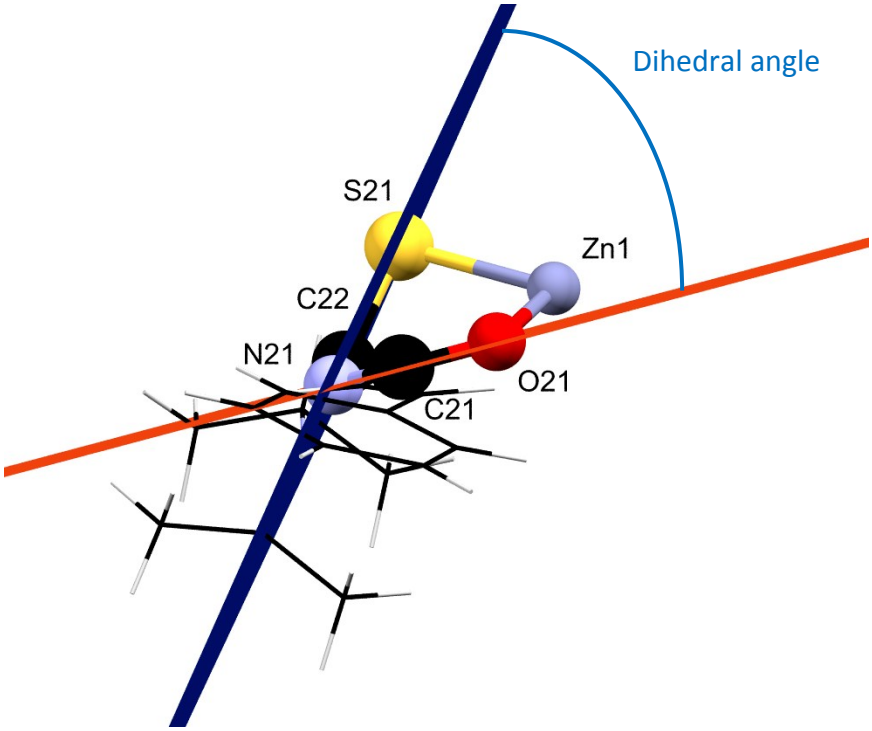
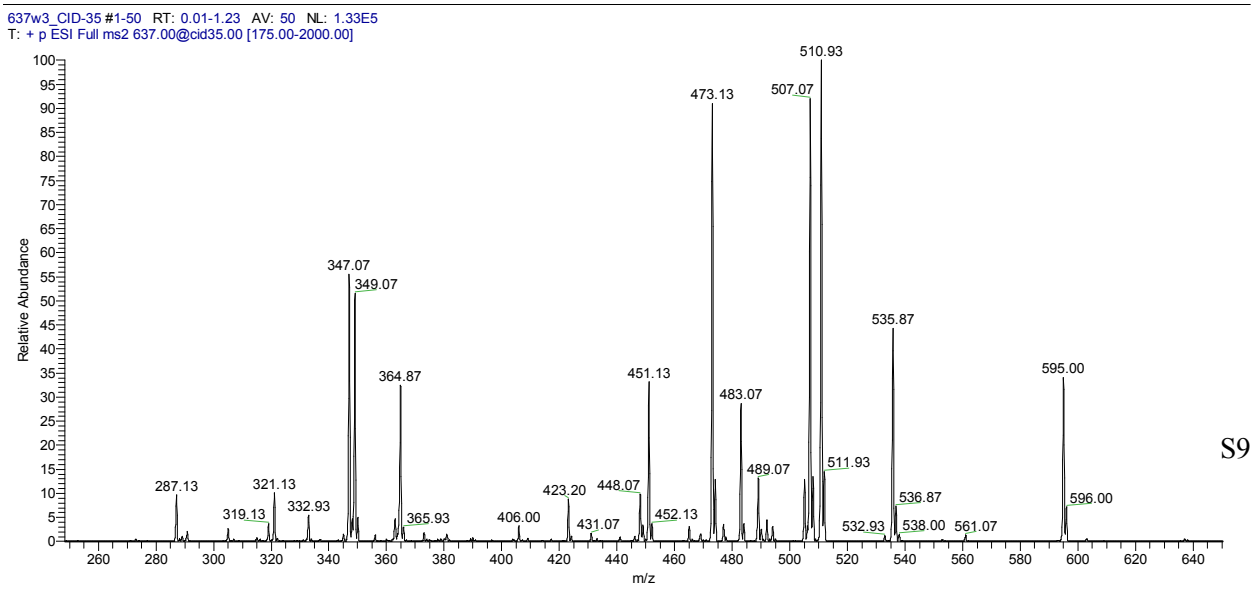


Figure S5. Example of the dihedral angle around N21 of $Zn(L3)_2 \cdot THF$ with the OCN plane (orange) and the SCN plane (dark blue).

Figure S6. Fragments observed in the tandem mass spectrometry experiments of $Ni(L3)_2$.



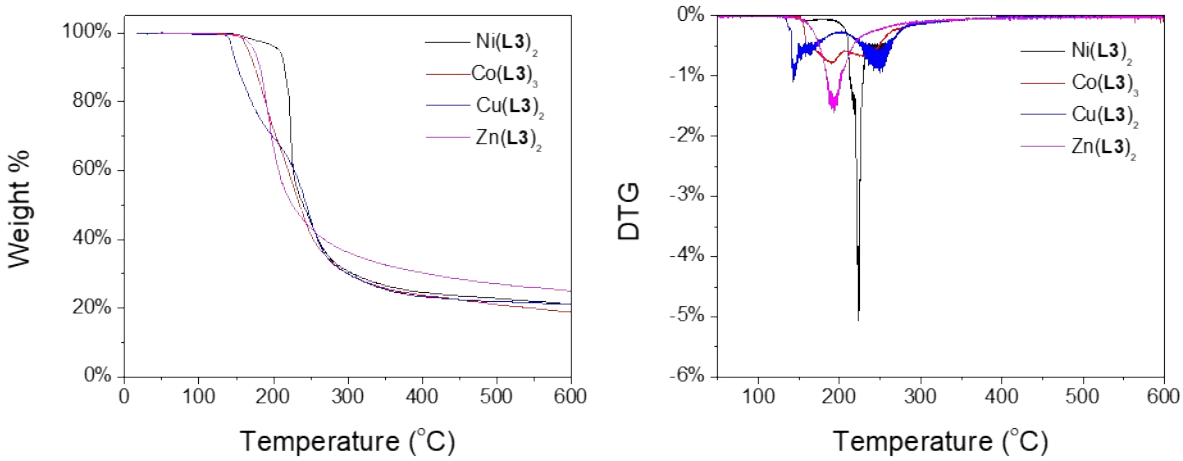


Figure S5. TGA and DTG curves of $Ni(L3)_2$, $Cu(L3)_2$, $Co(L3)_3$, and $Zn(L3)_2$.

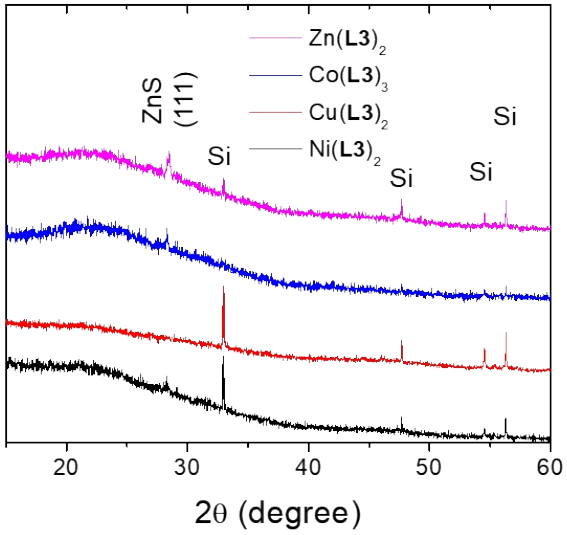


Figure S6. PXRD patterns of the deposits grown at 350 °C.

$Ni(L3)_2$ X-ray tables

Table S1. Crystal data and structure refinement for $Ni(\mathbf{L3})_2$.

Identification code	$Ni(\mathbf{L3})_2$	
Empirical formula	$C_{32}H_{42}N_4NiO_2S_2$	
Formula weight	637.52	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I-4	
Unit cell dimensions	a = 14.662(2) Å	α = 90°.
	b = 14.662(2) Å	β = 90°.
	c = 15.487(2) Å	γ = 90°.
Volume	3329.2(11) $Å^3$	
Z	4	
Density (calculated)	1.272 Mg/m^3	
Absorption coefficient	0.742 mm^{-1}	
F(000)	1352	
Crystal size	0.200 x 0.162 x 0.079 mm^3	
Theta range for data collection	1.913 to 32.828°.	
Index ranges	-22≤h≤20, -22≤k≤21, -23≤l≤22	
Reflections collected	36001	
Independent reflections	5829 [R(int) = 0.0226]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Integration	
Max. and min. transmission	0.9516 and 0.8848	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5829 / 0 / 190	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0200, wR2 = 0.0485 [5510]	
R indices (all data)	R1 = 0.0225, wR2 = 0.0491	
Absolute structure parameter	-0.0091(19)	
Largest diff. peak and hole	0.320 and -0.143 $e.Å^{-3}$	

$R1 = \sum(||F_o| - |F_c||) / \sum|F_o|$

$wR2 = [\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]]^{1/2}$ $S = [\sum[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$

$w= 1/[\sigma^2(F_O^2)+(m*p)^2+n*p]$, $p = [\max(F_O^2,0)+ 2* F_c^2]/3$, m & n are constants.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $Ni(L3)_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni1	5000	10000	5372(1)	10(1)
S1	5961(1)	9830(1)	6401(1)	20(1)
O1	5858(1)	9836(1)	4490(1)	12(1)
N1	7113(1)	9118(1)	5168(1)	13(1)
N2	7416(1)	8773(1)	6573(1)	14(1)
C1	6649(1)	9472(1)	4512(1)	11(1)
C2	6868(1)	9196(1)	6002(1)	12(1)
C3	7156(1)	9405(1)	3688(1)	12(1)
C4	6884(1)	9787(1)	2947(1)	13(1)
C5	7395(1)	9773(1)	2132(1)	13(1)
C6	6945(1)	10006(1)	1366(1)	18(1)
C7	7400(1)	9993(1)	576(1)	22(1)
C8	8316(1)	9747(1)	541(1)	21(1)
C9	8772(1)	9516(1)	1297(1)	20(1)
C10	8323(1)	9533(1)	2088(1)	16(1)
C11	8283(1)	8320(1)	6299(1)	16(1)
C12	8960(1)	8984(1)	5889(1)	24(1)
C13	8109(1)	7468(1)	5757(1)	22(1)
C14	7222(1)	8790(1)	7514(1)	17(1)
C15	7272(1)	7840(1)	7916(1)	30(1)
C16	7843(1)	9468(1)	7972(1)	33(1)

Table S3. Bond lengths [Å] and angles [°] for Ni(**L3**)$_2$.

Ni1-O1	1.8719(9)
Ni1-O1#1	1.8719(9)
Ni1-S1	2.1424(4)
Ni1-S1#1	2.1424(4)
S1-C2	1.7370(13)
O1-C1	1.2771(15)
N1-C1	1.3283(16)
N1-C2	1.3441(16)
N2-C2	1.3458(16)
N2-C14	1.4852(18)
N2-C11	1.4963(17)
C1-C3	1.4806(17)
C3-C4	1.3376(17)
C3-H3A	0.9500
C4-C5	1.4672(17)
C4-H4A	0.9500
C5-C6	1.4002(18)
C5-C10	1.4077(19)
C6-C7	1.3927(19)
C6-H6A	0.9500
C7-C8	1.392(2)
C7-H7A	0.9500
C8-C9	1.391(2)
C8-H8A	0.9500
C9-C10	1.3911(18)
C9-H9A	0.9500
C10-H10A	0.9500
C11-C13	1.526(2)
C11-C12	1.529(2)
C11-H11A	1.0000
C12-H12A	0.9800
C12-H12B	0.9800
C12-H12C	0.9800

C13-H13A	0.9800
C13-H13B	0.9800
C13-H13C	0.9800
C14-C16	1.523(2)
C14-C15	1.528(2)
C14-H14A	1.0000
C15-H15A	0.9800
C15-H15B	0.9800
C15-H15C	0.9800
C16-H16A	0.9800
C16-H16B	0.9800
C16-H16C	0.9800

O1-Ni1-O1#1	86.34(5)
O1-Ni1-S1	94.92(3)
O1#1-Ni1-S1	178.62(3)
O1-Ni1-S1#1	178.62(3)
O1#1-Ni1-S1#1	94.92(3)
S1-Ni1-S1#1	83.83(2)
C2-S1-Ni1	107.51(4)
C1-O1-Ni1	130.12(8)
C1-N1-C2	124.36(11)
C2-N2-C14	121.56(11)
C2-N2-C11	121.66(11)
C14-N2-C11	116.64(10)
O1-C1-N1	130.46(12)
O1-C1-C3	117.40(11)
N1-C1-C3	112.13(11)
N1-C2-N2	115.66(11)
N1-C2-S1	126.28(10)
N2-C2-S1	117.97(10)
C4-C3-C1	124.25(12)
C4-C3-H3A	117.9
C1-C3-H3A	117.9
C3-C4-C5	125.44(12)
C3-C4-H4A	117.3

C5-C4-H4A	117.3
C6-C5-C10	118.39(12)
C6-C5-C4	119.03(12)
C10-C5-C4	122.58(12)
C7-C6-C5	121.04(13)
C7-C6-H6A	119.5
C5-C6-H6A	119.5
C8-C7-C6	120.01(13)
C8-C7-H7A	120.0
C6-C7-H7A	120.0
C9-C8-C7	119.60(13)
C9-C8-H8A	120.2
C7-C8-H8A	120.2
C10-C9-C8	120.65(13)
C10-C9-H9A	119.7
C8-C9-H9A	119.7
C9-C10-C5	120.31(13)
C9-C10-H10A	119.8
C5-C10-H10A	119.8
N2-C11-C13	112.13(11)
N2-C11-C12	112.77(11)
C13-C11-C12	113.69(12)
N2-C11-H11A	105.8
C13-C11-H11A	105.8
C12-C11-H11A	105.8
C11-C12-H12A	109.5
C11-C12-H12B	109.5
H12A-C12-H12B	109.5
C11-C12-H12C	109.5
H12A-C12-H12C	109.5
H12B-C12-H12C	109.5
C11-C13-H13A	109.5
C11-C13-H13B	109.5
H13A-C13-H13B	109.5
C11-C13-H13C	109.5
H13A-C13-H13C	109.5

H13B-C13-H13C	109.5
N2-C14-C16	110.74(12)
N2-C14-C15	112.01(12)
C16-C14-C15	112.11(13)
N2-C14-H14A	107.2
C16-C14-H14A	107.2
C15-C14-H14A	107.2
C14-C15-H15A	109.5
C14-C15-H15B	109.5
H15A-C15-H15B	109.5
C14-C15-H15C	109.5
H15A-C15-H15C	109.5
H15B-C15-H15C	109.5
C14-C16-H16A	109.5
C14-C16-H16B	109.5
H16A-C16-H16B	109.5
C14-C16-H16C	109.5
H16A-C16-H16C	109.5
H16B-C16-H16C	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,z

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Ni(**L3**)$_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni1	11(1)	13(1)	7(1)	0	0	3(1)
S1	19(1)	31(1)	9(1)	-5(1)	-3(1)	13(1)
O1	11(1)	16(1)	10(1)	0(1)	0(1)	2(1)
N1	13(1)	16(1)	11(1)	0(1)	0(1)	2(1)
N2	14(1)	16(1)	11(1)	2(1)	-1(1)	3(1)
C1	12(1)	10(1)	11(1)	-1(1)	1(1)	-1(1)
C2	11(1)	12(1)	13(1)	-1(1)	-1(1)	1(1)
C3	11(1)	13(1)	12(1)	-1(1)	1(1)	1(1)
C4	13(1)	14(1)	13(1)	-1(1)	2(1)	0(1)
C5	15(1)	12(1)	12(1)	0(1)	1(1)	0(1)
C6	18(1)	20(1)	14(1)	2(1)	1(1)	5(1)
C7	26(1)	27(1)	13(1)	4(1)	1(1)	6(1)
C8	24(1)	26(1)	14(1)	3(1)	6(1)	0(1)
C9	15(1)	27(1)	17(1)	1(1)	4(1)	0(1)
C10	14(1)	22(1)	13(1)	1(1)	0(1)	-1(1)
C11	13(1)	18(1)	15(1)	2(1)	-1(1)	4(1)
C12	14(1)	28(1)	29(1)	8(1)	1(1)	1(1)
C13	22(1)	20(1)	24(1)	-3(1)	-2(1)	8(1)
C14	19(1)	22(1)	10(1)	2(1)	0(1)	4(1)
C15	38(1)	31(1)	20(1)	11(1)	4(1)	4(1)
C16	41(1)	38(1)	20(1)	-10(1)	-6(1)	-2(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Ni(**L3**)$_2$.

	x	y	z	U(eq)
H3A	7709	9068	3685	15
H4A	6314	10094	2949	16
H6A	6320	10175	1385	21
H7A	7084	10153	62	26
H8A	8627	9737	3	25
H9A	9397	9344	1273	24
H10A	8645	9382	2601	20
H11A	8579	8101	6842	19
H12A	9561	8694	5848	35
H12B	9006	9534	6246	35
H12C	8749	9150	5309	35
H13A	8679	7126	5691	33
H13B	7881	7647	5187	33
H13C	7655	7084	6046	33
H14A	6582	9012	7587	21
H15A	7017	7858	8500	45
H15B	7910	7642	7943	45
H15C	6923	7410	7562	45
H16A	7675	9501	8584	49
H16B	7775	10071	7708	49
H16C	8478	9267	7920	49

Cu(L3)$_2$·THF X-ray tables

Table S6. Crystal data and structure refinement for Cu(**L3**)$_2$·THF.

Identification code	Cu(**L3**)$_2$·THF	
Empirical formula	$C_{36}H_{50}CuN_4O_3S_2$	
Formula weight	634.31	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.5648(7) Å	α = 79.6830(10)°.
	b = 11.9358(8) Å	β = 72.2510(10)°.
	c = 15.2248(10) Å	γ = 84.0150(10)°.
Volume	1796.4(2) Å^3	
Z	2	
Density (calculated)	1.173 Mg/m^3	
Absorption coefficient	0.698 mm^{-1}	
F(000)	670	
Crystal size	0.259 x 0.176 x 0.108 mm^3	
Theta range for data collection	1.737 to 28.287°.	
Index ranges	-14≤h≤14, -15≤k≤15, -20≤l≤20	
Reflections collected	36766	
Independent reflections	8897 [R(int) = 0.0210]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Multi	
Max. and min. transmission	0.5633 and 0.5089	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8897 / 0 / 450	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0386, wR2 = 0.0950 [7375]	
R indices (all data)	R1 = 0.0514, wR2 = 0.1040	
Largest diff. peak and hole	1.162 and -0.518 e.Å^{-3}	

$R1 = \sum(||F_o| - |F_c||) / \sum|F_o|$

$wR2 = [\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]]^{1/2}$

$S = [\sum[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$

$W = 1/[\sigma^2(F_o^2)+(m*p)^2+n*p]$, $p = [\max(F_o^2,0)+ 2* F_c^2]/3$, m & n are constants.

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Cu(**L3**)$_2$·THF. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu1	0	0	0	16(1)
S1	896(1)	-1632(1)	-568(1)	21(1)
O1	1147(1)	-93(1)	770(1)	24(1)
N1	2743(2)	-1588(1)	364(1)	19(1)
N2	3473(2)	-2309(1)	-1003(1)	20(1)
C1	2053(2)	-845(2)	903(1)	18(1)
C2	2470(2)	-1821(1)	-395(1)	18(1)
C3	2472(2)	-848(2)	1745(1)	19(1)
C4	1882(2)	-163(2)	2374(1)	19(1)
C5	2290(2)	-31(2)	3185(1)	21(1)
C6	1614(2)	790(2)	3735(2)	29(1)
C7	2043(3)	1018(2)	4460(2)	41(1)
C8	3145(3)	414(2)	4652(2)	39(1)
C9	3804(2)	-421(2)	4131(2)	32(1)
C10	3388(2)	-645(2)	3402(1)	26(1)
C11	4828(2)	-2576(2)	-869(1)	22(1)
C12	4850(2)	-3409(2)	12(2)	28(1)
C13	5547(2)	-1499(2)	-962(2)	26(1)
C14	3309(2)	-2660(2)	-1854(2)	27(1)
C15	4358(2)	-2171(2)	-2740(2)	35(1)
C16	3281(2)	-3957(2)	-1726(2)	36(1)
Cu2	5000	5000	5000	24(1)
S21	5899(2)	6744(2)	4553(1)	8(1)
O21	4660(20)	4980(18)	3843(16)	24(2)
Cu2'	4774(6)	5106(3)	5103(4)	29(1)
S21'	5917(5)	6749(4)	4545(3)	44(2)
O21'	4450(30)	5130(20)	3895(19)	31(4)
N21	5277(2)	6786(1)	2924(1)	20(1)
N22	7144(2)	7680(1)	2802(1)	20(1)

C21	4541(2)	5884(2)	3221(1)	20(1)
C22	6129(2)	7059(2)	3355(1)	18(1)
C23	3637(2)	5809(2)	2660(1)	21(1)
C24	2975(2)	4879(2)	2765(1)	21(1)
C25	2157(2)	4675(2)	2188(1)	21(1)
C26	1788(2)	3566(2)	2245(2)	28(1)
C27	1052(2)	3326(2)	1690(2)	32(1)
C28	670(2)	4196(2)	1071(2)	30(1)
C29	1023(2)	5306(2)	1010(2)	28(1)
C30	1764(2)	5541(2)	1562(1)	22(1)
C31	7443(2)	7932(2)	1762(1)	22(1)
C32	7667(2)	6863(2)	1304(1)	28(1)
C33	6448(2)	8803(2)	1439(1)	29(1)
C34	8111(2)	8106(2)	3182(1)	24(1)
C35	9474(2)	7485(2)	2871(2)	36(1)
C36	8187(2)	9399(2)	2930(2)	32(1)
O41	1618(5)	5807(4)	6305(4)	77(2)
C42	2159(6)	7196(4)	5658(4)	43(1)
C43	1477(4)	7325(4)	4923(3)	32(1)
C44	298(7)	6676(5)	5259(5)	56(2)
C45	843(8)	5644(7)	5594(5)	71(2)
O51	2563(4)	5998(4)	5828(3)	44(1)
C52	1831(9)	7099(7)	6054(7)	64(2)
C53	1136(12)	7466(10)	5411(9)	95(3)
C54	838(9)	6391(7)	5092(6)	55(2)
C55	1354(8)	5473(6)	5719(5)	52(2)

Table S8. Bond lengths [Å] and angles [°] for Cu(**L3**)$_2$·THF.

Cu1-O1	1.9093(13)
Cu1-O1#1	1.9093(13)
Cu1-S1#1	2.2709(4)
Cu1-S1	2.2709(4)
S1-C2	1.7473(18)
O1-C1	1.280(2)
N1-C1	1.323(2)
N1-C2	1.354(2)
N2-C2	1.335(2)
N2-C14	1.493(2)
N2-C11	1.501(2)
C1-C3	1.478(2)
C3-C4	1.336(3)
C3-H3A	0.9500
C4-C5	1.465(2)
C4-H4A	0.9500
C5-C6	1.398(3)
C5-C10	1.401(3)
C6-C7	1.391(3)
C6-H6A	0.9500
C7-C8	1.385(3)
C7-H7A	0.9500
C8-C9	1.383(3)
C8-H8A	0.9500
C9-C10	1.387(3)
C9-H9A	0.9500
C10-H10A	0.9500
C11-C13	1.523(3)
C11-C12	1.524(3)
C11-H11A	1.0000
C12-H12A	0.9800
C12-H12B	0.9800
C12-H12C	0.9800
C13-H13A	0.9800

C13-H13B	0.9800
C13-H13C	0.9800
C14-C15	1.526(3)
C14-C16	1.527(3)
C14-H14A	1.0000
C15-H15A	0.9800
C15-H15B	0.9800
C15-H15C	0.9800
C16-H16A	0.9800
C16-H16B	0.9800
C16-H16C	0.9800
Cu2-O21	1.91(2)
Cu2-O21#2	1.91(2)
Cu2-S21#2	2.283(2)
Cu2-S21	2.283(2)
S21-C22	1.741(3)
O21-C21	1.33(2)
Cu2'-Cu2'#2	0.551(12)
Cu2'-O21'#2	1.91(3)
Cu2'-O21'	1.97(3)
Cu2'-S21'	2.301(6)
Cu2'-S21'#2	2.323(6)
S21'-C22	1.732(5)
S21'-Cu2'#2	2.323(6)
O21'-C21	1.22(3)
O21'-Cu2'#2	1.91(3)
N21-C21	1.324(2)
N21-C22	1.359(2)
N22-C22	1.342(2)
N22-C34	1.488(2)
N22-C31	1.497(2)
C21-C23	1.480(2)
C23-C24	1.334(3)
C23-H23A	0.9500
C24-C25	1.470(2)
C24-H24A	0.9500

C25-C30	1.396(3)
C25-C26	1.399(3)
C26-C27	1.390(3)
C26-H26A	0.9500
C27-C28	1.387(3)
C27-H27A	0.9500
C28-C29	1.393(3)
C28-H28A	0.9500
C29-C30	1.388(3)
C29-H29A	0.9500
C30-H30A	0.9500
C31-C32	1.525(3)
C31-C33	1.526(3)
C31-H31A	1.0000
C32-H32A	0.9800
C32-H32B	0.9800
C32-H32C	0.9800
C33-H33A	0.9800
C33-H33B	0.9800
C33-H33C	0.9800
C34-C36	1.526(3)
C34-C35	1.528(3)
C34-H34A	1.0000
C35-H35A	0.9800
C35-H35B	0.9800
C35-H35C	0.9800
C36-H36A	0.9800
C36-H36B	0.9800
C36-H36C	0.9800
O41-C45	1.591(9)
O41-C42	1.821(8)
C42-C43	1.485(7)
C42-H42A	0.9900
C42-H42B	0.9900
C43-C44	1.443(8)
C43-H43A	0.9900

C43-H43B	0.9900
C44-C45	1.383(10)
C44-H44A	0.9900
C44-H44B	0.9900
C45-H45A	0.9900
C45-H45B	0.9900
O51-C52	1.493(9)
O51-C55	1.545(9)
C52-C53	1.382(14)
C52-H52A	0.9900
C52-H52B	0.9900
C53-C54	1.543(14)
C53-H53A	0.9900
C53-H53B	0.9900
C54-C55	1.492(11)
C54-H54A	0.9900
C54-H54B	0.9900
C55-H55A	0.9900
C55-H55B	0.9900

O1-Cu1-O1#1	180.0
O1-Cu1-S1#1	86.27(4)
O1#1-Cu1-S1#1	93.73(4)
O1-Cu1-S1	93.72(4)
O1#1-Cu1-S1	86.27(4)
S1#1-Cu1-S1	180.0
C2-S1-Cu1	104.71(6)
C1-O1-Cu1	130.77(12)
C1-N1-C2	125.10(16)
C2-N2-C14	122.05(16)
C2-N2-C11	122.78(15)
C14-N2-C11	115.15(15)
O1-C1-N1	129.50(17)
O1-C1-C3	116.35(15)
N1-C1-C3	114.00(15)
N2-C2-N1	115.81(16)

N2-C2-S1	119.55(14)
N1-C2-S1	124.43(14)
C4-C3-C1	122.46(16)
C4-C3-H3A	118.8
C1-C3-H3A	118.8
C3-C4-C5	126.66(17)
C3-C4-H4A	116.7
C5-C4-H4A	116.7
C6-C5-C10	118.18(18)
C6-C5-C4	119.03(17)
C10-C5-C4	122.66(17)
C7-C6-C5	121.01(19)
C7-C6-H6A	119.5
C5-C6-H6A	119.5
C8-C7-C6	119.9(2)
C8-C7-H7A	120.1
C6-C7-H7A	120.1
C9-C8-C7	119.8(2)
C9-C8-H8A	120.1
C7-C8-H8A	120.1
C8-C9-C10	120.5(2)
C8-C9-H9A	119.7
C10-C9-H9A	119.7
C9-C10-C5	120.53(19)
C9-C10-H10A	119.7
C5-C10-H10A	119.7
N2-C11-C13	111.98(15)
N2-C11-C12	114.51(16)
C13-C11-C12	112.36(17)
N2-C11-H11A	105.7
C13-C11-H11A	105.7
C12-C11-H11A	105.7
C11-C12-H12A	109.5
C11-C12-H12B	109.5
H12A-C12-H12B	109.5
C11-C12-H12C	109.5

H12A-C12-H12C	109.5
H12B-C12-H12C	109.5
C11-C13-H13A	109.5
C11-C13-H13B	109.5
H13A-C13-H13B	109.5
C11-C13-H13C	109.5
H13A-C13-H13C	109.5
H13B-C13-H13C	109.5
N2-C14-C15	111.94(17)
N2-C14-C16	109.97(18)
C15-C14-C16	112.88(17)
N2-C14-H14A	107.2
C15-C14-H14A	107.2
C16-C14-H14A	107.2
C14-C15-H15A	109.5
C14-C15-H15B	109.5
H15A-C15-H15B	109.5
C14-C15-H15C	109.5
H15A-C15-H15C	109.5
H15B-C15-H15C	109.5
C14-C16-H16A	109.5
C14-C16-H16B	109.5
H16A-C16-H16B	109.5
C14-C16-H16C	109.5
H16A-C16-H16C	109.5
H16B-C16-H16C	109.5
O21-Cu2-O21#2	180.0(2)
O21-Cu2-S21#2	85.3(7)
O21#2-Cu2-S21#2	94.7(7)
O21-Cu2-S21	94.7(7)
O21#2-Cu2-S21	85.3(7)
S21#2-Cu2-S21	180.00(5)
C22-S21-Cu2	105.16(12)
C21-O21-Cu2	126.0(14)
Cu2'#2-Cu2'-O21'#2	87.9(13)
Cu2'#2-Cu2'-O21'	75.9(11)

O21'#2-Cu2'-O21'	163.7(4)
Cu2'#2-Cu2'-S21'	85.4(9)
O21'#2-Cu2'-S21'	87.5(8)
O21'-Cu2'-S21'	91.1(8)
Cu2'#2-Cu2'-S21'#2	80.9(8)
O21'#2-Cu2'-S21'#2	92.0(8)
O21'-Cu2'-S21'#2	85.5(8)
S21'-Cu2'-S21'#2	166.3(3)
C22-S21'-Cu2'	107.7(3)
C22-S21'-Cu2'#2	102.0(3)
Cu2'-S21'-Cu2'#2	13.7(3)
C21-O21'-Cu2'#2	132.9(17)
C21-O21'-Cu2'	131.9(17)
Cu2'#2-O21'-Cu2'	16.3(4)
C21-N21-C22	124.28(16)
C22-N22-C34	121.66(15)
C22-N22-C31	123.16(15)
C34-N22-C31	115.06(15)
O21'-C21-N21	130.9(11)
N21-C21-O21	128.2(10)
O21'-C21-C23	115.1(11)
N21-C21-C23	113.93(16)
O21-C21-C23	117.0(10)
N22-C22-N21	115.38(16)
N22-C22-S21'	119.7(2)
N21-C22-S21'	124.7(2)
N22-C22-S21	120.30(15)
N21-C22-S21	124.14(15)
C24-C23-C21	122.17(17)
C24-C23-H23A	118.9
C21-C23-H23A	118.9
C23-C24-C25	126.45(17)
C23-C24-H24A	116.8
C25-C24-H24A	116.8
C30-C25-C26	118.41(18)
C30-C25-C24	122.58(17)

C26-C25-C24	118.98(17)
C27-C26-C25	121.03(19)
C27-C26-H26A	119.5
C25-C26-H26A	119.5
C28-C27-C26	119.9(2)
C28-C27-H27A	120.1
C26-C27-H27A	120.1
C27-C28-C29	119.73(19)
C27-C28-H28A	120.1
C29-C28-H28A	120.1
C30-C29-C28	120.22(19)
C30-C29-H29A	119.9
C28-C29-H29A	119.9
C29-C30-C25	120.72(19)
C29-C30-H30A	119.6
C25-C30-H30A	119.6
N22-C31-C32	113.33(16)
N22-C31-C33	113.13(16)
C32-C31-C33	112.66(17)
N22-C31-H31A	105.6
C32-C31-H31A	105.6
C33-C31-H31A	105.6
C31-C32-H32A	109.5
C31-C32-H32B	109.5
H32A-C32-H32B	109.5
C31-C32-H32C	109.5
H32A-C32-H32C	109.5
H32B-C32-H32C	109.5
C31-C33-H33A	109.5
C31-C33-H33B	109.5
H33A-C33-H33B	109.5
C31-C33-H33C	109.5
H33A-C33-H33C	109.5
H33B-C33-H33C	109.5
N22-C34-C36	111.49(17)
N22-C34-C35	110.70(17)

C36-C34-C35	112.23(17)
N22-C34-H34A	107.4
C36-C34-H34A	107.4
C35-C34-H34A	107.4
C34-C35-H35A	109.5
C34-C35-H35B	109.5
H35A-C35-H35B	109.5
C34-C35-H35C	109.5
H35A-C35-H35C	109.5
H35B-C35-H35C	109.5
C34-C36-H36A	109.5
C34-C36-H36B	109.5
H36A-C36-H36B	109.5
C34-C36-H36C	109.5
H36A-C36-H36C	109.5
H36B-C36-H36C	109.5
C45-O41-C42	92.1(4)
C43-C42-O41	100.5(4)
C43-C42-H42A	111.7
O41-C42-H42A	111.7
C43-C42-H42B	111.7
O41-C42-H42B	111.7
H42A-C42-H42B	109.4
C44-C43-C42	109.8(4)
C44-C43-H43A	109.7
C42-C43-H43A	109.7
C44-C43-H43B	109.7
C42-C43-H43B	109.7
H43A-C43-H43B	108.2
C45-C44-C43	99.3(6)
C45-C44-H44A	111.9
C43-C44-H44A	111.9
C45-C44-H44B	111.9
C43-C44-H44B	111.9
H44A-C44-H44B	109.6
C44-C45-O41	110.9(6)

C44-C45-H45A	109.5
O41-C45-H45A	109.5
C44-C45-H45B	109.5
O41-C45-H45B	109.5
H45A-C45-H45B	108.0
C52-O51-C55	94.7(5)
C53-C52-O51	107.6(8)
C53-C52-H52A	110.2
O51-C52-H52A	110.2
C53-C52-H52B	110.2
O51-C52-H52B	110.2
H52A-C52-H52B	108.5
C52-C53-C54	106.8(9)
C52-C53-H53A	110.4
C54-C53-H53A	110.4
C52-C53-H53B	110.4
C54-C53-H53B	110.4
H53A-C53-H53B	108.6
C55-C54-C53	101.0(7)
C55-C54-H54A	111.6
C53-C54-H54A	111.6
C55-C54-H54B	111.6
C53-C54-H54B	111.6
H54A-C54-H54B	109.4
C54-C55-O51	103.4(6)
C54-C55-H55A	111.1
O51-C55-H55A	111.1
C54-C55-H55B	111.1
O51-C55-H55B	111.1
H55A-C55-H55B	109.1

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x+1,-y+1,-z+1

Table S9. Anisotropic displacement parameters ($Å^2$x 10^3) for Cu(**L3**)$_2$·THF. The anisotropicdisplacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu1	16(1)	16(1)	17(1)	-4(1)	-6(1)	2(1)
S1	18(1)	21(1)	27(1)	-10(1)	-10(1)	3(1)
O1	27(1)	24(1)	26(1)	-11(1)	-15(1)	8(1)
N1	17(1)	19(1)	22(1)	-5(1)	-6(1)	1(1)
N2	19(1)	21(1)	23(1)	-7(1)	-7(1)	3(1)
C1	15(1)	17(1)	20(1)	-3(1)	-5(1)	-1(1)
C2	18(1)	14(1)	21(1)	-2(1)	-6(1)	0(1)
C3	16(1)	21(1)	22(1)	-3(1)	-8(1)	1(1)
C4	16(1)	20(1)	20(1)	-2(1)	-6(1)	0(1)
C5	19(1)	24(1)	18(1)	-3(1)	-5(1)	-1(1)
C6	29(1)	34(1)	28(1)	-11(1)	-13(1)	9(1)
C7	43(1)	54(2)	35(1)	-26(1)	-20(1)	18(1)
C8	41(1)	56(2)	29(1)	-20(1)	-20(1)	11(1)
C9	29(1)	45(1)	27(1)	-10(1)	-15(1)	9(1)
C10	25(1)	32(1)	24(1)	-8(1)	-10(1)	7(1)
C11	17(1)	21(1)	27(1)	-7(1)	-6(1)	4(1)
C12	23(1)	22(1)	35(1)	-1(1)	-9(1)	4(1)
C13	21(1)	25(1)	32(1)	-2(1)	-8(1)	-1(1)
C14	25(1)	33(1)	28(1)	-17(1)	-10(1)	6(1)
C15	40(1)	39(1)	26(1)	-10(1)	-10(1)	6(1)
C16	34(1)	36(1)	41(1)	-22(1)	-4(1)	-3(1)
Cu2	39(2)	21(2)	19(2)	20(1)	-26(1)	-29(1)
S21	10(2)	10(2)	3(2)	4(1)	-1(1)	-8(1)
O21	30(4)	19(4)	24(2)	4(2)	-15(3)	-2(2)
Cu2'	24(1)	33(2)	30(2)	-13(2)	-5(1)	13(2)
S21'	43(3)	51(4)	42(3)	-9(2)	-15(2)	-5(2)
O21'	41(8)	26(7)	37(6)	9(4)	-31(6)	-15(5)
N21	17(1)	23(1)	19(1)	-1(1)	-6(1)	-3(1)
N22	19(1)	22(1)	18(1)	-2(1)	-6(1)	-4(1)
C21	20(1)	23(1)	17(1)	1(1)	-7(1)	-3(1)

C22	16(1)	17(1)	20(1)	-1(1)	-4(1)	0(1)
C23	20(1)	26(1)	18(1)	0(1)	-8(1)	-3(1)
C24	18(1)	25(1)	20(1)	-1(1)	-8(1)	-1(1)
C25	16(1)	25(1)	21(1)	-5(1)	-5(1)	-1(1)
C26	24(1)	27(1)	34(1)	-2(1)	-14(1)	-2(1)
C27	28(1)	30(1)	42(1)	-12(1)	-15(1)	-2(1)
C28	24(1)	41(1)	32(1)	-14(1)	-14(1)	1(1)
C29	24(1)	36(1)	26(1)	-5(1)	-12(1)	3(1)
C30	19(1)	25(1)	24(1)	-3(1)	-8(1)	-1(1)
C31	20(1)	25(1)	19(1)	-1(1)	-3(1)	-6(1)
C32	26(1)	34(1)	25(1)	-10(1)	-3(1)	-2(1)
C33	31(1)	28(1)	24(1)	3(1)	-8(1)	-3(1)
C34	22(1)	30(1)	22(1)	-1(1)	-7(1)	-11(1)
C35	24(1)	39(1)	47(1)	-1(1)	-16(1)	-7(1)
C36	37(1)	30(1)	29(1)	-5(1)	-6(1)	-14(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Cu(**L3**)$_2$·THF.

	x	y	z	U(eq)
H3A	3187	-1357	1843	23
H4A	1119	285	2286	23
H6A	850	1199	3612	35
H7A	1581	1585	4822	49
H8A	3447	574	5142	47
H9A	4548	-845	4273	39
H10A	3851	-1219	3048	31
H11A	5358	-2970	-1403	26
H12A	5761	-3727	-47	41
H12B	4263	-4027	94	41
H12C	4542	-3008	553	41
H13A	6461	-1708	-944	39
H13B	5080	-1083	-446	39
H13C	5561	-1015	-1557	39
H14A	2422	-2337	-1913	33
H15A	4133	-2312	-3287	52
H15B	5232	-2540	-2740	52
H15C	4384	-1348	-2761	52
H16A	3127	-4178	-2273	54
H16B	2563	-4220	-1167	54
H16C	4134	-4304	-1657	54
H23A	3526	6444	2211	25
H24A	3038	4289	3262	25
H26A	2044	2968	2670	33
H27A	813	2568	1735	38
H28A	169	4035	690	36
H29A	755	5904	591	33
H30A	2006	6299	1512	27
H31A	8314	8304	1530	27

H32A	8223	6295	1589	43
H32B	8114	7058	634	43
H32C	6807	6549	1393	43
H33A	6309	9456	1774	43
H33B	5600	8450	1571	43
H33C	6797	9063	767	43
H34A	7780	7923	3878	29
H35A	9379	6660	3043	53
H35B	10072	7722	3178	53
H35C	9846	7675	2192	53
H36A	7287	9759	3104	48
H36B	8599	9602	2257	48
H36C	8722	9665	3269	48
H42A	1857	7804	6053	52
H42B	3139	7193	5388	52
H43A	1229	8139	4753	38
H43B	2086	7051	4358	38
H44A	-395	7005	5761	67
H44B	-76	6608	4750	67
H45A	1465	5307	5065	85
H45B	126	5111	5912	85
H52A	1210	6987	6694	77
H52B	2466	7672	6017	77
H53A	1674	7979	4871	114
H53B	296	7887	5699	114
H54A	-127	6343	5194	66
H54B	1320	6365	4426	66
H55A	1627	4771	5432	63
H55B	675	5291	6330	63

Co(L3)$_3$ X-ray tables

Table S11. Crystal data and structure refinement for Co(**L3**)$_3$.

Identification code	Co(**L3**)$_3$	
Empirical formula	$C_{48}H_{63}CoN_6O_3S_3$	
Formula weight	927.15	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 9.6733(4) Å	α = 90°.
	b = 26.7438(10) Å	β = 92.5405(9)°.
	c = 18.9117(7) Å	γ = 90°.
Volume	4887.7(3) Å^3	
Z	4	
Density (calculated)	1.260 Mg/m^3	
Absorption coefficient	0.525 mm^{-1}	
F(000)	1968	
Crystal size	0.265 x 0.060 x 0.052 mm^3	
Theta range for data collection	1.523 to 34.023°.	
Index ranges	-15≤h≤15, -42≤k≤38, -27≤l≤29	
Reflections collected	114933	
Independent reflections	18743 [R(int) = 0.0601]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Multi	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18743 / 0 / 560	
Goodness-of-fit on F^2	1.016	
Final R indices [I>2sigma(I)]	R1 = 0.0582, wR2 = 0.1133 [12079]	
R indices (all data)	R1 = 0.1105, wR2 = 0.1310	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.970 and -0.805 e.Å^{-3}	

$R1 = \sum(||F_o| - |F_c||) / \sum|F_o|$

$wR2 = [\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]]^{1/2}$

$S = [\sum[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$

$w= 1/[\sigma^2(F_O^2)+(m*p)^2+n*p]$, $p = [\max(F_O^2,0)+ 2* F_c^2]/3$, m & n are constants.

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Co(**L3**)$_3$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co1	2118(1)	3247(1)	3019(1)	19(1)
S1	891(1)	2619(1)	3421(1)	27(1)
O1	642(1)	3488(1)	2408(1)	23(1)
N1	-802(2)	2784(1)	2228(1)	28(1)
N2	-1020(2)	2042(1)	2792(1)	30(1)
C1	-358(2)	3249(1)	2117(1)	24(1)
C2	-361(2)	2485(1)	2758(1)	25(1)
C3	-1194(2)	3523(1)	1569(1)	29(1)
C4	-894(2)	3988(1)	1378(1)	28(1)
C5	-1644(2)	4302(1)	853(1)	31(1)
C6	-2834(2)	4139(1)	472(1)	40(1)
C7	-3496(3)	4443(1)	-24(2)	49(1)
C8	-2998(3)	4916(1)	-153(1)	52(1)
C9	-1831(3)	5088(1)	222(2)	48(1)
C10	-1161(2)	4782(1)	722(1)	38(1)
C11	-2319(2)	1940(1)	2355(1)	36(1)
C12	-2069(3)	1880(1)	1570(2)	50(1)
C13	-3464(2)	2312(1)	2504(2)	43(1)
C14	-594(3)	1647(1)	3301(2)	43(1)
C15	-1585(4)	1615(1)	3899(2)	68(1)
C16	-406(3)	1143(1)	2944(2)	62(1)
S21	3900(1)	3009(1)	3723(1)	24(1)
O21	1410(1)	3676(1)	3752(1)	19(1)
N21	3425(1)	3882(1)	4428(1)	16(1)
N22	5677(2)	3700(1)	4222(1)	17(1)
C21	2060(2)	3861(1)	4284(1)	16(1)
C22	4336(2)	3579(1)	4136(1)	16(1)
C23	1175(2)	4113(1)	4798(1)	18(1)
C24	1629(2)	4284(1)	5430(1)	18(1)

C25	837(2)	4556(1)	5954(1)	17(1)
C26	1510(2)	4710(1)	6587(1)	22(1)
C27	832(2)	5000(1)	7074(1)	25(1)
C28	-536(2)	5138(1)	6942(1)	23(1)
C29	-1226(2)	4975(1)	6324(1)	22(1)
C30	-555(2)	4690(1)	5836(1)	21(1)
C31	6805(2)	3400(1)	3918(1)	24(1)
C32	7748(2)	3178(1)	4504(1)	39(1)
C33	7593(2)	3707(1)	3394(1)	36(1)
C34	6144(2)	4156(1)	4612(1)	18(1)
C35	5641(2)	4635(1)	4256(1)	24(1)
C36	5860(2)	4131(1)	5398(1)	23(1)
S41	2805(1)	2726(1)	2203(1)	32(1)
O41	3163(1)	3804(1)	2679(1)	20(1)
N41	3588(4)	3564(1)	1518(1)	63(1)
C41	3662(2)	3859(1)	2084(1)	25(1)
C42	3128(3)	3092(1)	1495(1)	45(1)
C43	4395(3)	4334(1)	1957(1)	35(1)
C44	4318(2)	4729(1)	2375(1)	22(1)
C45	4982(2)	5216(1)	2288(1)	22(1)
C46	5952(2)	5307(1)	1776(1)	30(1)
C47	6570(3)	5771(1)	1726(1)	40(1)
C48	6236(2)	6157(1)	2180(1)	38(1)
C49	5283(2)	6072(1)	2690(1)	31(1)
C50	4660(2)	5609(1)	2743(1)	26(1)
N42	2572(4)	2832(1)	900(2)	22(1)
C51	2114(4)	2298(2)	891(2)	25(1)
C52	3414(9)	1986(3)	765(5)	49(2)
C53	908(5)	2202(2)	371(3)	35(1)
C54	2779(5)	3071(2)	207(2)	32(1)
C55	4099(10)	3239(4)	109(5)	66(3)
C56	1763(5)	3486(2)	27(3)	40(1)
N42'	3389(4)	2929(1)	813(2)	26(1)
C51'	2782(4)	2446(1)	572(2)	19(1)
C52'	3436(7)	1973(2)	922(4)	31(2)
C53'	1238(5)	2418(2)	618(3)	36(1)

C54'	4332(7)	3182(3)	232(4)	36(1)
C55'	3267(8)	3331(3)	-357(4)	72(2)
C56'	5459(7)	2893(3)	78(4)	59(2)

Table S13. Bond lengths [Å] and angles [°] for Co(**L3**)$_3$.

Co1-O1	1.9080(14)
Co1-O41	1.9255(13)
Co1-O21	1.9463(13)
Co1-S41	2.2032(6)
Co1-S1	2.2106(6)
Co1-S21	2.2243(5)
S1-C2	1.741(2)
O1-C1	1.265(2)
N1-C1	1.335(3)
N1-C2	1.339(3)
N2-C2	1.349(3)
N2-C14	1.475(3)
N2-C11	1.497(3)
C1-C3	1.481(3)
C3-C4	1.332(3)
C3-H3A	0.9500
C4-C5	1.466(3)
C4-H4A	0.9500
C5-C10	1.393(3)
C5-C6	1.401(3)
C6-C7	1.379(4)
C6-H6A	0.9500
C7-C8	1.379(4)
C7-H7A	0.9500
C8-C9	1.384(4)
C8-H8A	0.9500
C9-C10	1.389(4)
C9-H9A	0.9500
C10-H10A	0.9500
C11-C12	1.523(4)
C11-C13	1.524(3)
C11-H11A	1.0000
C12-H12A	0.9800
C12-H12B	0.9800

C12-H12C	0.9800
C13-H13A	0.9800
C13-H13B	0.9800
C13-H13C	0.9800
C14-C15	1.517(4)
C14-C16	1.521(4)
C14-H14A	1.0000
C15-H15A	0.9800
C15-H15B	0.9800
C15-H15C	0.9800
C16-H16A	0.9800
C16-H16B	0.9800
C16-H16C	0.9800
S21-C22	1.7543(18)
O21-C21	1.264(2)
N21-C22	1.335(2)
N21-C21	1.337(2)
N22-C22	1.340(2)
N22-C34	1.486(2)
N22-C31	1.488(2)
C21-C23	1.485(2)
C23-C24	1.335(3)
C23-H23A	0.9500
C24-C25	1.472(2)
C24-H24A	0.9500
C25-C26	1.398(2)
C25-C30	1.402(2)
C26-C27	1.390(3)
C26-H26A	0.9500
C27-C28	1.386(3)
C27-H27A	0.9500
C28-C29	1.389(3)
C28-H28A	0.9500
C29-C30	1.382(3)
C29-H29A	0.9500
C30-H30A	0.9500

C31-C33	1.517(3)
C31-C32	1.525(3)
C31-H31A	1.0000
C32-H32A	0.9800
C32-H32B	0.9800
C32-H32C	0.9800
C33-H33A	0.9800
C33-H33B	0.9800
C33-H33C	0.9800
C34-C35	1.517(3)
C34-C36	1.525(3)
C34-H34A	1.0000
C35-H35A	0.9800
C35-H35B	0.9800
C35-H35C	0.9800
C36-H36A	0.9800
C36-H36B	0.9800
C36-H36C	0.9800
S41-C42	1.700(3)
O41-C41	1.253(2)
N41-C41	1.329(3)
N41-C42	1.336(4)
C41-C43	1.480(3)
C42-N42'	1.395(4)
C42-N42	1.409(4)
C43-C44	1.324(3)
C43-H43A	0.9500
C44-C45	1.465(3)
C44-H44A	0.9500
C45-C46	1.398(3)
C45-C50	1.401(3)
C46-C47	1.383(3)
C46-H46A	0.9500
C47-C48	1.388(4)
C47-H47A	0.9500
C48-C49	1.383(3)

C48-H48A	0.9500
C49-C50	1.382(3)
C49-H49A	0.9500
C50-H50A	0.9500
N42-C54	1.478(6)
N42-C51	1.496(5)
C51-C53	1.514(6)
C51-C52	1.536(10)
C51-H51A	1.0000
C52-H52A	0.9800
C52-H52B	0.9800
C52-H52C	0.9800
C53-H53A	0.9800
C53-H53B	0.9800
C53-H53C	0.9800
C54-C55	1.374(10)
C54-C56	1.513(7)
C54-H54A	1.0000
C55-H55A	0.9800
C55-H55B	0.9800
C55-H55C	0.9800
C56-H56A	0.9800
C56-H56B	0.9800
C56-H56C	0.9800
N42'-C51'	1.483(5)
N42'-C54'	1.609(8)
C51'-C53'	1.502(6)
C51'-C52'	1.547(8)
C51'-H51B	1.0000
C52'-H52D	0.9800
C52'-H52E	0.9800
C52'-H52F	0.9800
C53'-H53D	0.9800
C53'-H53E	0.9800
C53'-H53F	0.9800
C54'-C56'	1.378(9)

C54'-C55'	1.536(10)
C54'-H54B	1.0000
C55'-H55D	0.9800
C55'-H55E	0.9800
C55'-H55F	0.9800
C56'-H56D	0.9800
C56'-H56E	0.9800
C56'-H56F	0.9800

O1-Co1-O41	85.84(6)
O1-Co1-O21	87.45(6)
O41-Co1-O21	89.38(5)
O1-Co1-S41	91.70(4)
O41-Co1-S41	94.32(4)
O21-Co1-S41	176.13(4)
O1-Co1-S1	93.75(4)
O41-Co1-S1	178.85(4)
O21-Co1-S1	89.53(4)
S41-Co1-S1	86.76(2)
O1-Co1-S21	176.68(5)
O41-Co1-S21	90.93(4)
O21-Co1-S21	91.74(4)
S41-Co1-S21	89.31(2)
S1-Co1-S21	89.47(2)
C2-S1-Co1	106.06(8)
C1-O1-Co1	129.12(14)
C1-N1-C2	125.53(17)
C2-N2-C14	122.68(18)
C2-N2-C11	121.4(2)
C14-N2-C11	115.73(18)
O1-C1-N1	130.3(2)
O1-C1-C3	115.99(19)
N1-C1-C3	113.71(17)
N1-C2-N2	115.15(18)
N1-C2-S1	127.15(15)
N2-C2-S1	117.62(17)

C4-C3-C1	122.29(18)
C4-C3-H3A	118.9
C1-C3-H3A	118.9
C3-C4-C5	127.66(19)
C3-C4-H4A	116.2
C5-C4-H4A	116.2
C10-C5-C6	118.1(2)
C10-C5-C4	119.2(2)
C6-C5-C4	122.7(2)
C7-C6-C5	120.8(3)
C7-C6-H6A	119.6
C5-C6-H6A	119.6
C8-C7-C6	120.4(3)
C8-C7-H7A	119.8
C6-C7-H7A	119.8
C7-C8-C9	119.9(3)
C7-C8-H8A	120.1
C9-C8-H8A	120.1
C8-C9-C10	119.9(3)
C8-C9-H9A	120.1
C10-C9-H9A	120.1
C9-C10-C5	120.9(2)
C9-C10-H10A	119.5
C5-C10-H10A	119.5
N2-C11-C12	113.01(18)
N2-C11-C13	112.31(18)
C12-C11-C13	113.4(2)
N2-C11-H11A	105.8
C12-C11-H11A	105.8
C13-C11-H11A	105.8
C11-C12-H12A	109.5
C11-C12-H12B	109.5
H12A-C12-H12B	109.5
C11-C12-H12C	109.5
H12A-C12-H12C	109.5
H12B-C12-H12C	109.5

C11-C13-H13A	109.5
C11-C13-H13B	109.5
H13A-C13-H13B	109.5
C11-C13-H13C	109.5
H13A-C13-H13C	109.5
H13B-C13-H13C	109.5
N2-C14-C15	111.0(2)
N2-C14-C16	112.3(2)
C15-C14-C16	111.9(2)
N2-C14-H14A	107.1
C15-C14-H14A	107.1
C16-C14-H14A	107.1
C14-C15-H15A	109.5
C14-C15-H15B	109.5
H15A-C15-H15B	109.5
C14-C15-H15C	109.5
H15A-C15-H15C	109.5
H15B-C15-H15C	109.5
C14-C16-H16A	109.5
C14-C16-H16B	109.5
H16A-C16-H16B	109.5
C14-C16-H16C	109.5
H16A-C16-H16C	109.5
H16B-C16-H16C	109.5
C22-S21-Co1	100.51(6)
C21-O21-Co1	128.24(11)
C22-N21-C21	123.69(15)
C22-N22-C34	121.97(14)
C22-N22-C31	123.06(15)
C34-N22-C31	114.94(14)
O21-C21-N21	129.09(16)
O21-C21-C23	114.68(15)
N21-C21-C23	116.13(15)
N21-C22-N22	117.21(15)
N21-C22-S21	124.13(13)
N22-C22-S21	118.39(13)

C24-C23-C21	124.37(16)
C24-C23-H23A	117.8
C21-C23-H23A	117.8
C23-C24-C25	127.71(16)
C23-C24-H24A	116.1
C25-C24-H24A	116.1
C26-C25-C30	117.96(16)
C26-C25-C24	119.04(15)
C30-C25-C24	122.94(16)
C27-C26-C25	121.05(17)
C27-C26-H26A	119.5
C25-C26-H26A	119.5
C28-C27-C26	120.26(18)
C28-C27-H27A	119.9
C26-C27-H27A	119.9
C27-C28-C29	119.15(18)
C27-C28-H28A	120.4
C29-C28-H28A	120.4
C30-C29-C28	120.86(17)
C30-C29-H29A	119.6
C28-C29-H29A	119.6
C29-C30-C25	120.69(17)
C29-C30-H30A	119.7
C25-C30-H30A	119.7
N22-C31-C33	111.07(17)
N22-C31-C32	110.77(17)
C33-C31-C32	112.60(18)
N22-C31-H31A	107.4
C33-C31-H31A	107.4
C32-C31-H31A	107.4
C31-C32-H32A	109.5
C31-C32-H32B	109.5
H32A-C32-H32B	109.5
C31-C32-H32C	109.5
H32A-C32-H32C	109.5
H32B-C32-H32C	109.5

C31-C33-H33A	109.5
C31-C33-H33B	109.5
H33A-C33-H33B	109.5
C31-C33-H33C	109.5
H33A-C33-H33C	109.5
H33B-C33-H33C	109.5
N22-C34-C35	112.91(14)
N22-C34-C36	112.50(15)
C35-C34-C36	113.73(16)
N22-C34-H34A	105.6
C35-C34-H34A	105.6
C36-C34-H34A	105.6
C34-C35-H35A	109.5
C34-C35-H35B	109.5
H35A-C35-H35B	109.5
C34-C35-H35C	109.5
H35A-C35-H35C	109.5
H35B-C35-H35C	109.5
C34-C36-H36A	109.5
C34-C36-H36B	109.5
H36A-C36-H36B	109.5
C34-C36-H36C	109.5
H36A-C36-H36C	109.5
H36B-C36-H36C	109.5
C42-S41-Co1	105.06(8)
C41-O41-Co1	128.31(13)
C41-N41-C42	126.3(2)
O41-C41-N41	130.1(2)
O41-C41-C43	116.92(18)
N41-C41-C43	112.88(19)
N41-C42-N42'	104.6(3)
N41-C42-N42	127.3(2)
N41-C42-S41	126.15(17)
N42'-C42-S41	126.5(2)
N42-C42-S41	105.6(2)
C44-C43-C41	123.30(19)

C44-C43-H43A	118.3
C41-C43-H43A	118.3
C43-C44-C45	127.31(19)
C43-C44-H44A	116.3
C45-C44-H44A	116.3
C46-C45-C50	117.93(19)
C46-C45-C44	122.95(19)
C50-C45-C44	119.11(18)
C47-C46-C45	120.6(2)
C47-C46-H46A	119.7
C45-C46-H46A	119.7
C46-C47-C48	120.7(2)
C46-C47-H47A	119.6
C48-C47-H47A	119.6
C49-C48-C47	119.3(2)
C49-C48-H48A	120.4
C47-C48-H48A	120.4
C50-C49-C48	120.3(2)
C50-C49-H49A	119.8
C48-C49-H49A	119.8
C49-C50-C45	121.1(2)
C49-C50-H50A	119.4
C45-C50-H50A	119.4
C42-N42-C54	115.7(3)
C42-N42-C51	125.6(3)
C54-N42-C51	117.0(3)
N42-C51-C53	112.9(4)
N42-C51-C52	106.0(4)
C53-C51-C52	114.8(4)
N42-C51-H51A	107.6
C53-C51-H51A	107.6
C52-C51-H51A	107.6
C51-C52-H52A	109.5
C51-C52-H52B	109.5
H52A-C52-H52B	109.5
C51-C52-H52C	109.5

H52A-C52-H52C	109.5
H52B-C52-H52C	109.5
C51-C53-H53A	109.5
C51-C53-H53B	109.5
H53A-C53-H53B	109.5
C51-C53-H53C	109.5
H53A-C53-H53C	109.5
H53B-C53-H53C	109.5
C55-C54-N42	115.1(5)
C55-C54-C56	109.1(6)
N42-C54-C56	113.8(4)
C55-C54-H54A	106.0
N42-C54-H54A	106.0
C56-C54-H54A	106.0
C54-C55-H55A	109.5
C54-C55-H55B	109.5
H55A-C55-H55B	109.5
C54-C55-H55C	109.5
H55A-C55-H55C	109.5
H55B-C55-H55C	109.5
C54-C56-H56A	109.5
C54-C56-H56B	109.5
H56A-C56-H56B	109.5
C54-C56-H56C	109.5
H56A-C56-H56C	109.5
H56B-C56-H56C	109.5
C42-N42'-C51'	118.2(3)
C42-N42'-C54'	129.1(4)
C51'-N42'-C54'	112.7(4)
N42'-C51'-C53'	114.0(3)
N42'-C51'-C52'	115.6(4)
C53'-C51'-C52'	108.8(4)
N42'-C51'-H51B	105.9
C53'-C51'-H51B	105.9
C52'-C51'-H51B	105.9
C51'-C52'-H52D	109.5

C51'-C52'-H52E	109.5
H52D-C52'-H52E	109.5
C51'-C52'-H52F	109.5
H52D-C52'-H52F	109.5
H52E-C52'-H52F	109.5
C51'-C53'-H53D	109.5
C51'-C53'-H53E	109.5
H53D-C53'-H53E	109.5
C51'-C53'-H53F	109.5
H53D-C53'-H53F	109.5
H53E-C53'-H53F	109.5
C56'-C54'-C55'	120.2(6)
C56'-C54'-N42'	112.7(5)
C55'-C54'-N42'	102.8(5)
C56'-C54'-H54B	106.8
C55'-C54'-H54B	106.8
N42'-C54'-H54B	106.8
C54'-C55'-H55D	109.5
C54'-C55'-H55E	109.5
H55D-C55'-H55E	109.5
C54'-C55'-H55F	109.5
H55D-C55'-H55F	109.5
H55E-C55'-H55F	109.5
C54'-C56'-H56D	109.5
C54'-C56'-H56E	109.5
H56D-C56'-H56E	109.5
C54'-C56'-H56F	109.5
H56D-C56'-H56F	109.5
H56E-C56'-H56F	109.5

Symmetry transformations used to generate equivalent atoms:

Table S14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Co(**L3**)$_3$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co1	14(1)	19(1)	25(1)	-8(1)	3(1)	-3(1)
S1	22(1)	23(1)	35(1)	-3(1)	-1(1)	-8(1)
O1	18(1)	27(1)	24(1)	-9(1)	1(1)	-4(1)
N1	22(1)	32(1)	30(1)	-12(1)	3(1)	-9(1)
N2	22(1)	24(1)	45(1)	-13(1)	5(1)	-7(1)
C1	18(1)	33(1)	22(1)	-12(1)	4(1)	-6(1)
C2	18(1)	26(1)	34(1)	-13(1)	7(1)	-6(1)
C3	21(1)	41(1)	26(1)	-10(1)	-2(1)	-6(1)
C4	18(1)	41(1)	24(1)	-11(1)	2(1)	-1(1)
C5	24(1)	43(1)	26(1)	-7(1)	5(1)	3(1)
C6	32(1)	49(2)	39(1)	-8(1)	-7(1)	4(1)
C7	38(1)	65(2)	44(2)	-5(1)	-7(1)	12(1)
C8	44(1)	76(2)	37(1)	11(1)	10(1)	26(2)
C9	43(1)	56(2)	47(2)	13(1)	20(1)	10(1)
C10	29(1)	48(1)	37(1)	1(1)	10(1)	2(1)
C11	19(1)	29(1)	59(2)	-20(1)	4(1)	-7(1)
C12	35(1)	56(2)	57(2)	-34(1)	1(1)	-14(1)
C13	23(1)	30(1)	76(2)	-16(1)	7(1)	-7(1)
C14	36(1)	26(1)	66(2)	-4(1)	1(1)	-10(1)
C15	83(2)	45(2)	76(2)	11(2)	25(2)	-10(2)
C16	37(1)	32(1)	114(3)	-18(2)	-6(2)	2(1)
S21	17(1)	16(1)	40(1)	-9(1)	-2(1)	2(1)
O21	14(1)	21(1)	22(1)	-4(1)	1(1)	-1(1)
N21	13(1)	15(1)	21(1)	-2(1)	2(1)	0(1)
N22	13(1)	17(1)	22(1)	-4(1)	1(1)	1(1)
C21	15(1)	13(1)	20(1)	0(1)	3(1)	-1(1)
C22	15(1)	15(1)	18(1)	0(1)	2(1)	-1(1)
C23	13(1)	18(1)	25(1)	-2(1)	4(1)	0(1)
C24	13(1)	17(1)	25(1)	-1(1)	3(1)	0(1)
C25	14(1)	15(1)	21(1)	-2(1)	3(1)	0(1)

C26	16(1)	25(1)	23(1)	-2(1)	1(1)	3(1)
C27	23(1)	32(1)	21(1)	-5(1)	-1(1)	2(1)
C28	22(1)	24(1)	22(1)	-3(1)	6(1)	3(1)
C29	16(1)	25(1)	26(1)	-2(1)	4(1)	4(1)
C30	15(1)	24(1)	23(1)	-5(1)	0(1)	0(1)
C31	16(1)	25(1)	32(1)	-10(1)	4(1)	4(1)
C32	28(1)	38(1)	52(2)	2(1)	3(1)	18(1)
C33	26(1)	51(1)	31(1)	-6(1)	11(1)	5(1)
C34	14(1)	18(1)	21(1)	-3(1)	0(1)	-1(1)
C35	26(1)	18(1)	27(1)	1(1)	1(1)	-2(1)
C36	22(1)	26(1)	19(1)	-3(1)	-2(1)	4(1)
S41	31(1)	21(1)	44(1)	-17(1)	15(1)	-8(1)
O41	18(1)	25(1)	18(1)	-6(1)	3(1)	-6(1)
N41	152(3)	20(1)	20(1)	0(1)	26(1)	16(1)
C41	36(1)	23(1)	18(1)	3(1)	6(1)	12(1)
C42	85(2)	28(1)	21(1)	-11(1)	-17(1)	30(1)
C43	52(1)	25(1)	29(1)	10(1)	24(1)	12(1)
C44	18(1)	30(1)	18(1)	5(1)	2(1)	4(1)
C45	19(1)	26(1)	22(1)	5(1)	0(1)	4(1)
C46	28(1)	33(1)	30(1)	5(1)	9(1)	4(1)
C47	36(1)	37(1)	48(1)	11(1)	17(1)	-1(1)
C48	34(1)	29(1)	51(2)	11(1)	4(1)	0(1)
C49	29(1)	28(1)	36(1)	2(1)	-2(1)	6(1)
C50	22(1)	31(1)	25(1)	2(1)	1(1)	4(1)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Co(**L3**)$_3$.

	x	y	z	U(eq)
H3A	-1972	3361	1346	35
H4A	-101	4135	1608	34
H6A	-3190	3814	557	49
H7A	-4300	4326	-280	59
H8A	-3455	5124	-497	62
H9A	-1489	5415	137	57
H10A	-363	4903	978	45
H11A	-2660	1608	2517	43
H12A	-2939	1789	1317	74
H12B	-1382	1616	1507	74
H12C	-1726	2196	1382	74
H13A	-4334	2200	2270	64
H13B	-3219	2642	2321	64
H13C	-3576	2334	3015	64
H14A	328	1746	3516	52
H15A	-1271	1355	4234	102
H15B	-2514	1532	3705	102
H15C	-1612	1938	4143	102
H16A	14	907	3286	92
H16B	198	1183	2545	92
H16C	-1309	1016	2771	92
H23A	223	4157	4668	22
H24A	2574	4222	5557	22
H26A	2446	4615	6685	26
H27A	1309	5103	7499	30
H28A	-996	5341	7270	27
H29A	-2170	5062	6237	27
H30A	-1043	4583	5416	25
H31A	6361	3116	3651	29

H32A	8474	2979	4294	59
H32B	7203	2963	4807	59
H32C	8171	3448	4789	59
H33A	8325	3501	3201	53
H33B	8006	3999	3635	53
H33C	6956	3818	3008	53
H34A	7175	4161	4587	21
H35A	6111	4922	4483	35
H35B	4640	4668	4301	35
H35C	5849	4626	3753	35
H36A	6317	4412	5645	34
H36B	6220	3815	5595	34
H36C	4860	4149	5458	34
H43A	4949	4356	1556	42
H44A	3772	4693	2777	26
H46A	6187	5048	1460	36
H47A	7231	5827	1378	48
H48A	6658	6476	2140	45
H49A	5055	6332	3005	37
H50A	4002	5556	3094	32
H51A	1804	2215	1375	30
H52A	3187	1630	792	73
H52B	4135	2068	1127	73
H52C	3749	2063	296	73
H53A	494	1877	473	52
H53B	1235	2202	-112	52
H53C	213	2465	417	52
H54A	2598	2804	-156	38
H55A	4285	3227	-396	99
H55B	4764	3025	373	99
H55C	4190	3584	279	99
H56A	828	3378	136	60
H56B	1790	3565	-478	60
H56C	2013	3784	306	60
H51B	2967	2420	57	23
H52D	3104	1675	665	46

H52E	3171	1953	1415	46
H52F	4446	1993	907	46
H53D	883	2132	341	54
H53E	819	2726	430	54
H53F	1004	2376	1114	54
H54B	4703	3500	444	43
H55D	2446	3472	-146	108
H55E	3002	3034	-637	108
H55F	3674	3580	-665	108
H56D	6003	2820	516	88
H56E	6036	3074	-249	88
H56F	5141	2579	-141	88

$Zn(L3)_2 \cdot NCCH_3$ X-ray tables

Table S16. Crystal data and structure refinement for $Zn(\mathbf{L3})_2 \cdot NCCH_3$.

Identification code	$Zn(\mathbf{L3})_2 \cdot NCCH_3$	
Empirical formula	$C_{34}H_{45}ZnN_5O_2S_2$	
Formula weight	685.24	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 13.8922(16) Å	α = 90°.
	b = 7.4030(9) Å	β = 99.859(2)°.
	c = 34.250(4) Å	γ = 90°.
Volume	3470.4(7) $Å^3$	
Z	4	
Density (calculated)	1.312 Mg/m^3	
Absorption coefficient	0.865 mm^{-1}	
F(000)	1448	
Crystal size	0.304 x 0.036 x 0.035 mm^3	
Theta range for data collection	1.207 to 28.323°.	
Index ranges	-15≤h≤18, -9≤k≤9, -45≤l≤43	
Reflections collected	34093	
Independent reflections	8616 [R(int) = 0.1359]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Integration	
Max. and min. transmission	0.9788 and 0.8661	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8616 / 0 / 406	
Goodness-of-fit on F^2	0.829	
Final R indices [I>2sigma(I)]	R1 = 0.0498, wR2 = 0.0892 [3934]	
R indices (all data)	R1 = 0.1435, wR2 = 0.1210	
Largest diff. peak and hole	1.188 and -0.545 $e.Å^{-3}$	

$R1 = \sum(||F_o| - |F_c||) / \sum|F_o|$

$wR2 = [\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]]^{1/2}$

$S = [\sum[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$

w= $1/[\sigma^2(F_o^2)+(m*p)^2+n*p]$, p = $[\max(F_o^2,0)+ 2* F_c^2]/3$, m & n are constants.

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Zn(**L3**)$_2$·$NCCH_3$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zn1	8273(1)	4928(1)	4347(1)	18(1)
S1	8665(1)	5853(2)	4986(1)	17(1)
S2	8518(1)	1987(2)	4162(1)	19(1)
O1	6888(2)	5639(4)	4245(1)	22(1)
O2	8715(2)	6125(4)	3899(1)	19(1)
N1	11116(3)	4921(6)	2138(1)	40(1)
N2	6741(2)	6987(4)	4851(1)	16(1)
N3	7837(2)	8813(4)	5233(1)	14(1)
N4	8425(2)	3716(5)	3454(1)	16(1)
N5	7247(2)	1558(4)	3478(1)	15(1)
C1	12116(3)	4762(6)	1563(1)	29(1)
C2	11554(3)	4851(7)	1886(1)	26(1)
C3	6414(3)	6149(6)	4513(1)	17(1)
C4	5338(3)	5917(5)	4426(1)	16(1)
C5	4886(3)	5417(5)	4070(1)	15(1)
C6	3837(3)	5243(5)	3923(1)	13(1)
C7	3127(3)	5413(5)	4165(1)	17(1)
C8	2145(3)	5290(5)	4010(1)	19(1)
C9	1853(3)	4948(7)	3607(1)	24(1)
C10	2539(3)	4757(6)	3364(1)	25(1)
C11	3522(3)	4902(6)	3520(1)	22(1)
C12	7684(3)	7314(5)	5009(1)	14(1)
C13	8821(3)	9329(5)	5448(1)	14(1)
C14	8835(3)	9447(6)	5896(1)	21(1)
C15	9175(3)	11064(6)	5285(1)	23(1)
C16	7040(3)	10101(6)	5278(1)	18(1)
C17	6247(3)	9276(6)	5485(1)	21(1)
C18	6613(3)	11029(6)	4887(1)	23(1)

C19	8796(3)	5285(6)	3580(1)	16(1)
C20	9319(3)	6193(6)	3295(1)	16(1)
C21	9569(3)	7931(6)	3322(1)	18(1)
C22	10100(3)	8915(6)	3053(1)	19(1)
C23	10641(3)	8017(6)	2806(1)	21(1)
C24	11144(3)	8955(7)	2558(1)	22(1)
C25	11104(3)	10816(7)	2544(1)	22(1)
C26	10568(3)	11742(6)	2783(1)	22(1)
C27	10077(3)	10795(6)	3041(1)	19(1)
C28	8005(3)	2493(5)	3669(1)	16(1)
C29	6785(3)	80(6)	3672(1)	20(1)
C30	6641(3)	-1608(6)	3417(1)	26(1)
C31	5831(3)	758(6)	3791(1)	28(1)
C32	6752(3)	2043(6)	3069(1)	17(1)
C33	6396(3)	3995(6)	3036(1)	25(1)
C34	7368(3)	1538(6)	2756(1)	24(1)

Table S18. Bond lengths [Å] and angles [°] for Zn(**L3**)$_2$·NCCH$_3$.

Zn1-O2	1.959(3)
Zn1-O1	1.968(3)
Zn1-S1	2.2706(11)
Zn1-S2	2.3083(12)
S1-C12	1.752(4)
S2-C28	1.759(4)
O1-C3	1.274(4)
O2-C19	1.277(4)
N1-C2	1.140(5)
N2-C3	1.324(5)
N2-C12	1.351(5)
N3-C12	1.345(5)
N3-C16	1.488(5)
N3-C13	1.489(5)
N4-C19	1.313(5)
N4-C28	1.359(5)
N5-C28	1.333(5)
N5-C29	1.483(5)
N5-C32	1.495(5)
C1-C2	1.460(5)
C1-H1	0.9800
C1-H2	0.9800
C1-H3	0.9800
C3-C4	1.482(5)
C4-C5	1.326(5)
C4-H10	0.9500
C5-C6	1.463(5)
C5-H4	0.9500
C6-C11	1.397(5)
C6-C7	1.398(5)
C7-C8	1.380(5)
C7-H5	0.9500
C8-C9	1.393(5)
C8-H6	0.9500

C9-C10	1.377(5)
C9-H9	0.9500
C10-C11	1.383(5)
C10-H7	0.9500
C11-H8	0.9500
C13-C15	1.516(5)
C13-C14	1.532(5)
C13-H14	1.0000
C14-H13	0.9800
C14-H11	0.9800
C14-H12	0.9800
C15-H16	0.9800
C15-H15	0.9800
C15-H17	0.9800
C16-C18	1.530(5)
C16-C17	1.537(5)
C16-H21	1.0000
C17-H19	0.9800
C17-H20	0.9800
C17-H18	0.9800
C18-H24	0.9800
C18-H23	0.9800
C18-H22	0.9800
C19-C20	1.476(5)
C20-C21	1.332(5)
C20-H31	0.9500
C21-C22	1.469(5)
C21-H25	0.9500
C22-C23	1.391(5)
C22-C27	1.393(5)
C23-C24	1.378(5)
C23-H30	0.9500
C24-C25	1.379(5)
C24-H29	0.9500
C25-C26	1.380(6)
C25-H28	0.9500

C26-C27	1.395(6)
C26-H27	0.9500
C27-H26	0.9500
C29-C30	1.518(6)
C29-C31	1.536(5)
C29-H38	1.0000
C30-H34	0.9800
C30-H33	0.9800
C30-H32	0.9800
C31-H35	0.9800
C31-H37	0.9800
C31-H36	0.9800
C32-C33	1.525(6)
C32-C34	1.529(5)
C32-H39	1.0000
C33-H42	0.9800
C33-H40	0.9800
C33-H41	0.9800
C34-H44	0.9800
C34-H43	0.9800
C34-H45	0.9800

O2-Zn1-O1	99.70(11)
O2-Zn1-S1	124.32(9)
O1-Zn1-S1	98.94(8)
O2-Zn1-S2	97.58(8)
O1-Zn1-S2	112.89(9)
S1-Zn1-S2	121.76(4)
C12-S1-Zn1	99.71(13)
C28-S2-Zn1	90.45(13)
C3-O1-Zn1	124.2(2)
C19-O2-Zn1	122.2(3)
C3-N2-C12	126.8(3)
C12-N3-C16	122.7(3)
C12-N3-C13	122.4(3)
C16-N3-C13	114.9(3)

C19-N4-C28	126.4(3)
C28-N5-C29	122.1(3)
C28-N5-C32	122.1(3)
C29-N5-C32	115.6(3)
C2-C1-H1	109.5
C2-C1-H2	109.5
H1-C1-H2	109.5
C2-C1-H3	109.5
H1-C1-H3	109.5
H2-C1-H3	109.5
N1-C2-C1	179.9(5)
O1-C3-N2	128.7(4)
O1-C3-C4	116.7(4)
N2-C3-C4	114.4(3)
C5-C4-C3	121.2(4)
C5-C4-H10	119.4
C3-C4-H10	119.4
C4-C5-C6	128.9(4)
C4-C5-H4	115.5
C6-C5-H4	115.5
C11-C6-C7	117.9(3)
C11-C6-C5	118.7(3)
C7-C6-C5	123.3(3)
C8-C7-C6	121.1(4)
C8-C7-H5	119.4
C6-C7-H5	119.4
C7-C8-C9	119.6(4)
C7-C8-H6	120.2
C9-C8-H6	120.2
C10-C9-C8	120.3(4)
C10-C9-H9	119.8
C8-C9-H9	119.8
C9-C10-C11	119.7(4)
C9-C10-H7	120.2
C11-C10-H7	120.2
C10-C11-C6	121.3(3)

C10-C11-H8	119.4
C6-C11-H8	119.4
N3-C12-N2	115.1(3)
N3-C12-S1	119.1(3)
N2-C12-S1	125.5(3)
N3-C13-C15	111.2(3)
N3-C13-C14	111.3(3)
C15-C13-C14	111.8(3)
N3-C13-H14	107.4
C15-C13-H14	107.4
C14-C13-H14	107.4
C13-C14-H13	109.5
C13-C14-H11	109.5
H13-C14-H11	109.5
C13-C14-H12	109.5
H13-C14-H12	109.5
H11-C14-H12	109.5
C13-C15-H16	109.5
C13-C15-H15	109.5
H16-C15-H15	109.5
C13-C15-H17	109.5
H16-C15-H17	109.5
H15-C15-H17	109.5
N3-C16-C18	112.4(3)
N3-C16-C17	113.4(3)
C18-C16-C17	112.4(3)
N3-C16-H21	105.9
C18-C16-H21	105.9
C17-C16-H21	105.9
C16-C17-H19	109.5
C16-C17-H20	109.5
H19-C17-H20	109.5
C16-C17-H18	109.5
H19-C17-H18	109.5
H20-C17-H18	109.5
C16-C18-H24	109.5

C16-C18-H23	109.5
H24-C18-H23	109.5
C16-C18-H22	109.5
H24-C18-H22	109.5
H23-C18-H22	109.5
O2-C19-N4	128.6(4)
O2-C19-C20	117.9(4)
N4-C19-C20	113.3(3)
C21-C20-C19	123.1(4)
C21-C20-H31	118.4
C19-C20-H31	118.4
C20-C21-C22	126.1(4)
C20-C21-H25	117.0
C22-C21-H25	117.0
C23-C22-C27	118.2(4)
C23-C22-C21	121.7(4)
C27-C22-C21	120.1(4)
C24-C23-C22	121.1(4)
C24-C23-H30	119.4
C22-C23-H30	119.4
C23-C24-C25	120.2(4)
C23-C24-H29	119.9
C25-C24-H29	119.9
C24-C25-C26	119.9(4)
C24-C25-H28	120.1
C26-C25-H28	120.1
C25-C26-C27	119.9(4)
C25-C26-H27	120.0
C27-C26-H27	120.0
C22-C27-C26	120.6(4)
C22-C27-H26	119.7
C26-C27-H26	119.7
N5-C28-N4	117.3(3)
N5-C28-S2	121.0(3)
N4-C28-S2	121.3(3)
N5-C29-C30	112.0(3)

N5-C29-C31	109.7(4)
C30-C29-C31	112.8(3)
N5-C29-H38	107.4
C30-C29-H38	107.4
C31-C29-H38	107.4
C29-C30-H34	109.5
C29-C30-H33	109.5
H34-C30-H33	109.5
C29-C30-H32	109.5
H34-C30-H32	109.5
H33-C30-H32	109.5
C29-C31-H35	109.5
C29-C31-H37	109.5
H35-C31-H37	109.5
C29-C31-H36	109.5
H35-C31-H36	109.5
H37-C31-H36	109.5
N5-C32-C33	112.9(3)
N5-C32-C34	112.0(3)
C33-C32-C34	113.1(3)
N5-C32-H39	106.0
C33-C32-H39	106.0
C34-C32-H39	106.0
C32-C33-H42	109.5
C32-C33-H40	109.5
H42-C33-H40	109.5
C32-C33-H41	109.5
H42-C33-H41	109.5
H40-C33-H41	109.5
C32-C34-H44	109.5
C32-C34-H43	109.5
H44-C34-H43	109.5
C32-C34-H45	109.5
H44-C34-H45	109.5
H43-C34-H45	109.5

Table S19. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Zn(\mathbf{L3})_2 \cdot NCCH_3$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn1	18(1)	23(1)	13(1)	-4(1)	5(1)	-1(1)
S1	19(1)	20(1)	12(1)	-5(1)	2(1)	3(1)
S2	22(1)	20(1)	14(1)	-1(1)	1(1)	1(1)
O1	18(2)	39(2)	12(1)	-5(1)	5(1)	2(1)
O2	23(2)	21(2)	15(2)	-6(1)	6(1)	-4(1)
N1	53(3)	32(2)	42(2)	2(2)	23(2)	2(3)
N2	15(2)	20(2)	12(2)	-5(2)	1(1)	-2(2)
N3	15(2)	14(2)	12(2)	-2(2)	3(1)	1(2)
N4	16(2)	18(2)	13(2)	-1(2)	3(1)	-3(2)
N5	16(2)	16(2)	12(2)	-2(2)	2(1)	-1(2)
C1	32(3)	35(3)	21(2)	-3(2)	7(2)	0(2)
C2	31(2)	22(3)	25(2)	-2(2)	3(2)	1(2)
C3	16(2)	18(2)	19(2)	6(2)	4(2)	3(2)
C4	15(2)	17(2)	18(2)	-2(2)	6(2)	-1(2)
C5	14(2)	16(3)	16(2)	1(2)	5(2)	2(2)
C6	15(2)	9(2)	15(2)	3(2)	2(2)	1(2)
C7	21(2)	17(3)	14(2)	-2(2)	1(2)	1(2)
C8	16(2)	17(3)	25(2)	3(2)	8(2)	1(2)
C9	17(2)	30(3)	23(2)	-1(2)	1(2)	0(2)
C10	18(2)	41(3)	14(2)	-6(2)	-3(2)	2(2)
C11	16(2)	29(3)	21(2)	-1(2)	7(2)	2(2)
C12	16(2)	17(2)	11(2)	2(2)	4(2)	1(2)
C13	12(2)	15(2)	15(2)	-4(2)	1(2)	-2(2)
C14	23(2)	23(3)	16(2)	-4(2)	2(2)	-4(2)
C15	19(2)	26(3)	24(2)	4(2)	6(2)	-3(2)
C16	18(2)	15(2)	19(2)	-7(2)	2(2)	3(2)
C17	20(2)	27(3)	17(2)	-3(2)	6(2)	3(2)
C18	18(2)	29(3)	24(2)	1(2)	6(2)	7(2)
C19	10(2)	20(3)	16(2)	1(2)	-1(2)	2(2)
C20	13(2)	26(3)	11(2)	-2(2)	3(2)	2(2)

C21	13(2)	31(3)	11(2)	-1(2)	3(2)	0(2)
C22	15(2)	28(3)	12(2)	0(2)	1(2)	-3(2)
C23	20(2)	20(3)	23(2)	1(2)	4(2)	-1(2)
C24	21(2)	29(3)	16(2)	1(2)	5(2)	-1(2)
C25	22(2)	28(3)	15(2)	0(2)	6(2)	-6(2)
C26	26(3)	16(2)	23(2)	0(2)	2(2)	-5(2)
C27	17(2)	28(3)	11(2)	-5(2)	0(2)	-1(2)
C28	17(2)	15(2)	17(2)	-6(2)	5(2)	0(2)
C29	25(2)	18(2)	18(2)	-2(2)	4(2)	-6(2)
C30	29(3)	20(3)	29(3)	0(2)	3(2)	-4(2)
C31	31(3)	29(3)	24(2)	-3(2)	11(2)	-6(2)
C32	19(2)	22(2)	10(2)	0(2)	1(2)	-4(2)
C33	25(3)	26(3)	23(2)	-1(2)	1(2)	5(2)
C34	31(3)	29(3)	11(2)	-1(2)	1(2)	1(2)

Table S20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $Zn(\mathbf{L3})_2 \cdot NCCH_3$.

	x	y	z	U(eq)
H1	12766	4265	1663	44
H2	12183	5978	1458	44
H3	11778	3982	1352	44
H10	4966	6130	4630	20
H4	5299	5134	3885	18
H5	3325	5618	4441	21
H6	1671	5438	4177	23
H9	1178	4846	3500	28
H7	2338	4526	3089	30
H8	3992	4768	3351	26
H14	9285	8349	5403	17
H13	8468	10516	5954	31
H11	9512	9541	6034	31
H12	8534	8361	5985	31
H16	9144	10945	4998	34
H15	9850	11299	5412	34
H17	8758	12068	5339	34
H21	7353	11079	5457	21
H19	5816	8509	5298	32
H20	5864	10245	5579	32
H18	6555	8546	5711	32
H24	7144	11527	4765	35
H23	6177	12008	4939	35
H22	6244	10148	4707	35
H31	9485	5505	3082	20
H25	9387	8597	3535	22
H30	10663	6734	2809	25
H29	11520	8319	2396	26
H28	11445	11459	2370	26
H27	10534	13023	2772	26

H26	9723	11439	3210	23
H38	7239	-240	3922	25
H34	6119	-1399	3190	40
H33	6461	-2620	3575	40
H32	7250	-1894	3322	40
H35	5965	1838	3957	41
H37	5558	-187	3940	41
H36	5361	1055	3552	41
H39	6152	1274	3014	21
H42	6083	4289	3264	37
H40	5923	4146	2791	37
H41	6952	4804	3033	37
H44	7945	2321	2784	36
H43	6979	1695	2492	36
H45	7576	276	2792	36