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Heterotrimetallic Sandwich Complexes Supported by Sulfonamido Ligands

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Supplementary Information

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Materials and Methods

Elemental analyses were performed by Atlantic Microlabs in Norcross, GA. IR spectra were obtained using a Nicolet 380 FT-IR with Smart Orbit Diamond ATR attachment. All room temperature ^{1}H-NMR and ^{13}C-NMR spectra were obtained on a 400MHz or 500MHz instrument and referenced to residual solvent. Mass spectrometric analysis was collected by Emory University Mass Spectrometry Center using electrospray ionization on a Thermo Finnigan LTQ-FTMS instrument. Magnetic susceptibility was measured with Evan's method on a 500MHz NMR spectrometer. X-ray crystallographic data was collected and analyzed by the Emory University Department of Chemistry X-Ray Crystallography Center. All reactions sensitive to air and/or moisture were carried out in an MBraun UNIlab glovebox under a nitrogen atmosphere. Solvents for use in the glovebox were degassed by evacuation and purging with nitrogen and dried using 3Å molecular sieves. Reagents were purchased from Sigma-Aldrich, Fisher Scientific, Acros Organics, Oakwood Chemicals, or Strem Chemicals and used without further purification. H_3Ts_3tren[1] and 15-crown-5•$Mg(OTf)_2$[2] were synthesized using previously published methods. *tert*-butyl *tert*-butanethiosulfinate was synthesized according literature procedure[3] with the following change: after drying the solution of thiosulfinate in dichloromethane with sodium sulfate, the solvent was removed under vacuum. This thiosulfinate was then used to make *tert*-butylsulfinyl chloride according to another published procedure[4].

Synthesis

Bus_3H_3tren:

An oven-dried 250 mL flask was charged with a dry stir bar, cooled under vaccum, and filled with 100 mL of anhydrous dichloromethane under nitrogen. To this flask, *tert*-butyl sulfinyl chloride (33.7g, 240mmol) was added via cannula at –78˚C. Tris(2-aminoethyl)amine (H_6tren) (11.6 mL, 77mmol) and triethylamine (35.6 mL, 255mmol) were mixed in anhydrous dichloromethane (40 mL) in a separate dry flask under nitrogen and added to the reaction vessel via cannula. After addition, the flask was stirred overnight under nitrogen and allowed to slowly warm to room temperature. The organic mixture was then washed with saturated aqueous sodium bicarbonate solution (3×200 mL), brine (200 mL), and dried over magnesium sulfate. The drying agent was filtered away and the filtrate concentrated via rotary evaporation. Pentane was added to precipitate the sulfinamide product. Yield: 34%. The proton NMR spectrum of this product indicates asymmetry consistent with the presence of three chiral sulfur centers in the same molecule, where the relative stereochemistry at each sulfur is random. Mass spectrometry of the precipitated product indicated the correct mass (ESMS: Exact mass calcd for $C_{18}H_{43}N_4O_3S_3^+$ [M + H], 459.24918. Found: 459.24877 (Δ = 0.9 ppm)) and this product was used in the next step without further purification. The crude mixture can be recrystallized with dichloromethane and pentane to afford a crystalline isomer(s) with a complex but well-defined splitting pattern (see page S8). The trisulfinamide product (4.9g, 10.6mmol) was stirred in 40 mL dichloromethane at 0˚C open to the air. To this stirred solution, 3-chloroperbenzoic acid (*m*-CPBA, 10.7g, 77% mixture, 48mmol active oxidant) was added carefully to control bubbling. The reaction was stirred for 5 minutes and was quenched with 40% aqueous sodium bisulfite solution and stirred for another 5 minutes. This mixture was extracted with dichloromethane and the organic layer was washed with aqueous sodium bicarbonate (2×100 mL), brine (100 mL), and dried over magnesium sulfate. The drying agent was filtered away and the filtrate

concentrated to dryness under rotary evaporation. Drying further under vacuum yielded an off-white solid. Yield: 4.0g, 75%. IR (FT-ATR) $\bar{\nu}$/cm^{-1}: 3262 (ν_{NH}), 2944, 2811, 1455, 1431, 1398, 1367, 1292, 1207, 1110, 1078, 1050, 1028, 950, 927, 894, 825, 814, 793, 732, 662, 565. δH(500 MHz; CDCl3) 1.39 (27 H, s, tBu), 2.59 (6 H, t, NCH_2), 3.27 (6 H, s, $BusNCH_2$) and 5.7 (3 H, t, NH). δC(125 MHz; CDCl3) 24.2, 42.0, 55.0, 60.0. ESMS: Exact mass calcd for $C_{18}H_{43}N_4O_6S_3^+$ [M + H], 507.23392. Found: 507.23400 (Δ = 0.2 ppm).

$Sr(OTf)_2•H_2O$

According to a literature procedure[5], triflic acid (10 mL, 113mmol) was diluted in 125 mL of water and added slowly to a vigorously stirred solution of $SrCO_3$ (9.2g, 62.2mmol) in water at 0˚C. After addition, the solution was allowed to slowly warm to room temperature. The solution was filtered to remove any unreacted carbonate and the water was removed under reduced pressure. Drying under vacuum at 100˚C afforded monohydrate product. Yield: 18.8g, 79%. Anal. Calcd for $C_2H_2F_6O_7S_2Sr$: C, 5.95; H, 0.5; F, 28.2%. Found: C, 6.0; H, 0.4; F, 28.0.

[^{n}Bu_4N][1-OH_2]

In a two-neck flask, Ts_3H_3tren (8.56g, 14.1mmol) and $CoCl_2$ (1.83g, 14.1mmol) were stirred in 40 mL DMA under nitrogen. KH (1.75g, 43.6mmol) was added in portions carefully, which causes the solution to change from blue to purple. After stirring overnight, Bu_4NBr (4.53g, 14.1mmol) was added with a few drops of methanol to quench any residual hydride base. The reaction mixture was diluted with CH_2Cl_2 (200 mL) and washed with water (3×200 mL) and brine (200 mL). The organic layer was dried with Na_2SO_4, filtered and concentrated under rotary evaporation. Addition of diethyl ether afforded purple crystals. Yield: 9.99g, 77%. Vapor diffusion of ether into a CH_2Cl_2 solution of the product afforded X-ray quality purple crystals (see note on S9) Anal. Calcd for $C_{43}H_{71}CoN_5O_7S_3$: C, 55.8; H, 7.7; N, 7.6%. Found: C, 55.9; H, 7.7; N, 7.5. λ_{max}(TFE)/nm 222 (ε/dm^3 mol^{-1} cm^{-1} 7 220), 528 (44) and 1571 (36). IR (FT-ATR) $\bar{\nu}$/cm^{-1}: 3293 (ν_{OH}), 3058, 2959, 2894, 2854, 1586, 1483, 1465, 1442, 1367, 1350, 1290, 1275, 1240, 1129, 1105, 1080, 1042, 1019, 970, 932, 871, 813, 753, 727, 709, 692, 663, 598, 569, 548, 530. ESMS: Exact mass calcd for $C_{27}H_{33}CoN_4O_6S_3^-$ [ML$^-$], 664.08997. Found: 664.08929 (Δ = 1.0 ppm). Magnetic susceptibility (Evan's method, $CDCl_3$): μ_{obs} = 3.46 μ_B.

[^{n}Bu_4N][1-OH_2] dehydration to form [^{n}Bu_4N][1]

In a glovebox, [^{n}Bu_4N][**1-OH_2**] was dissolved in dichloromethane with 3Å molecular sieves. After sitting overnight the solution was filtered through celite and layered under ether. Blue crystals were formed which were suitable for analysis by X-ray crystallography. λ_{max}(CH_2Cl_2)/nm 248sh (ε/dm^3 mol^{-1} cm^{-1} 14 100), 270sh (11 800), 408 (17), 567 (51), 746 (7) and 1483 (59). Magnetic susceptibility (Evan's method, $CDCl_3$): μ_{obs} = 4.29 μ_B.

$Ca1_2$

Under nitrogen, [^{n}Bu_4N][**1-OH_2**] (2.05g, 2.2mmol) was dissolved in 10 mL glyme with a few drops of methanol and dried overnight with 3Å molecular sieves. This solution was filtered into a vial and $Ca(OTf)_2$ (488mg, 1.4mmol) in methanol was added. The tightly-capped vial was heated to 85˚C, while periodically releasing pressure manually as blue crystals formed and the supernatant lightened. When most of the color of the solution had bleached, the supernatant was decanted and the crystals washed with glyme and ether. The crystals were then dried under vacuum. A few crystals taken from the mixture

after washing with ether and before drying were found suitable for analysis by X-ray crystallography. Yield: 1.06g, 70%. Anal. Calcd for $C_{54}H_{66}CaCo_2N_8O_{12}S_6$: C, 47.4; H, 4.9; N, 8.2%. Found: C, 47.5; H, 4.75; N, 8.05. λ_{max}(TFE)/nm 222 (ε/dm^3 mol^{-1} cm^{-1} 58 800), 406 (25), 561 (89), 700 (26) and 1439 (94). IR (FT-ATR) $\bar{\nu}$/cm^{-1}: 2903, 2858, 1560, 1496, 1446, 1400, 1342, 1253, 1116, 1081, 1035, 972, 916, 868, 810, 735, 708, 664, 606, 549. ESMS: Exact mass calcd for $C_{27}H_{35}CaCoN_4O_7S_3^+$ [ML$^-$ + H_2O + Ca^{2+}], 722.06203. Found: 722.06202 (Δ = 0.01 ppm). Exact mass calcd for $C_{27}H_{37}CaCoN_4O_8S_3^+$ [ML$^-$ + 2H_2O + Ca^{2+}], 740.07259. Found: 740.07259 (Δ = 0.0 ppm). Magnetic susceptibility (Evan's method, TFE-d_3): μ_{obs} = 5.82 μ_B.

$Sr1_2$•$(OH_2)_{1.5}$

[^{n}Bu$_4$N][**1-OH_2**] (85mg, 0.092mmol) and Sr(OTf)•H_2O (18mg, 0.046mmol) were mixed in 2 mL of acetone and evaporated to dryness. The pink residue was dissolved in 2 mL of acetonitrile with minimal methanol and heated to 80˚C overnight. The purple crystals were washed with dichloromethane, acetonitrile, and ether and dried under vacuum to yield purple crystalline product. Yield: 15mg, 23%. Anal. Calcd for $C_{54}H_{69}Co_2N_8O_{13.5}S_6Sr$: C, 44.92; H, 4.82; N, 7.76. Found: C, 44.54; H, 4.76; N, 7.74. λ_{max}(TFE)/nm 222 (ε/dm^3 mol^{-1} cm^{-1} 52 900), 411 (26), 561 (91), 690 (20) and 1421 (107). IR (FT-ATR) $\bar{\nu}$/cm^{-1}: 2911, 2856, 1600, 1496, 1446, 1398, 1246, 1126, 1079, 1040, 1020, 979, 928, 873, 811, 734, 708, 663, 601, 580, 549. ESMS: Exact mass calcd for $C_{27}H_{33}CoN_4O_6S_3^-$ [ML$^-$], 664.08997. Found: 664.08670 (Δ = 4.9 ppm).

$Ba1_2$•$3H_2O$

[^{n}Bu$_4$N][**1-OH_2**] (493mg, 0.53mmol) and $Ba(OTf)_2$ (116mg, 0.27mmol) were dissolved separately in acetone. The barium-containing solution was added to the cobalt solution and solution left open to air. A pink powder precipitated from solution, which was collected by filtration, washed with cold acetone and ether, and dried on the filter to afford pink BaCoTs•$(H_2O)_3$ (235mg, 58%). Anal. Calcd for $C_{54}H_{66}BaCo_2N_8O_{12}S_6$: C, 42.65; H, 4.77; N, 7.37. Found: C, 42.36; H, 4.69; N, 7.24. λ_{max}(TFE)/nm 222 (ε/dm^3 mol^{-1} cm^{-1} 56 400), 404 (29), 563 (103), 694 (18) and 1391 (103). IR (FT-ATR) $\bar{\nu}$/cm^{-1}: 3514 (ν_{OH}), 2954, 2904, 2856, 1599, 1495, 1447, 1399, 1352, 1246, 1220, 1207, 1139, 1115, 1073, 1038, 970, 933, 879, 812, 742, 708, 661, 600. ESMS: Exact mass calcd for $C_{18}H_{39}CoN_4O_6S_3^-$ [ML$^-$], 664.08997 (Δ =). Found: 664.08997 (Δ = 0.0 ppm). Magnetic susceptibility (Evan's method, TFE-d_3): μ_{obs} = 6.03 μ_B.

Dehydration of $Ba1_2$•$3H_2O$ and crystallization of $Ba1_2$ dimer

In a glovebox, **BaCoTs•$3H_2O$** was dissolved in dichloromethane containing 3Å molecular sieves. After sitting overnight the solution was filtered through celite and layered under ether, forming blue X-ray quality crystals.

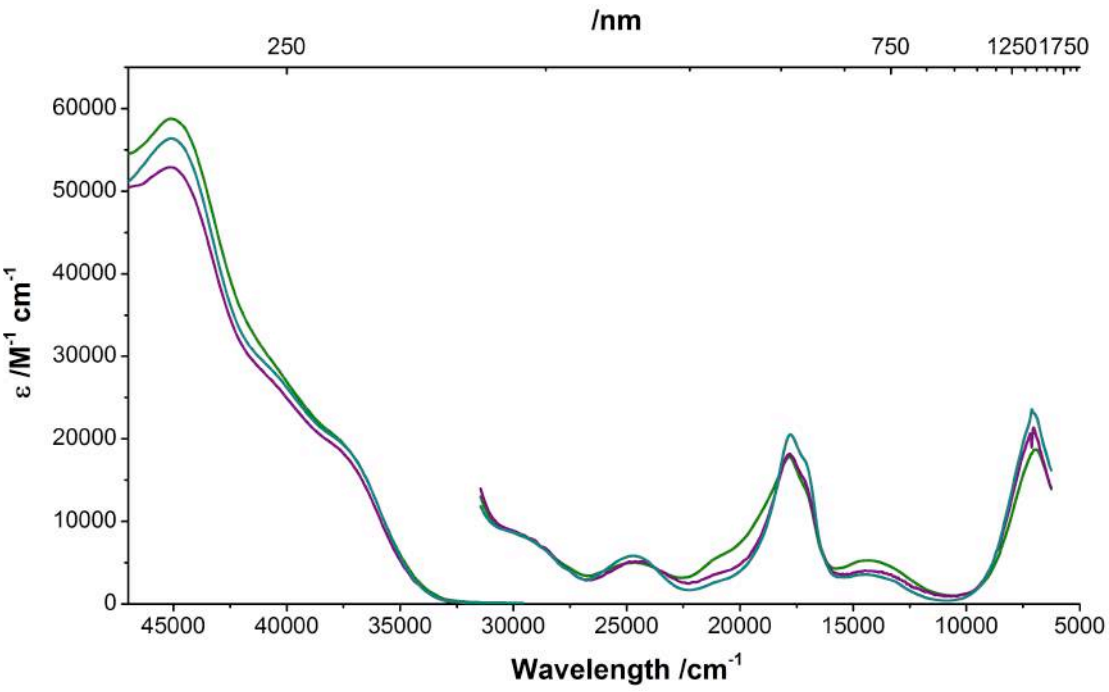


Figure S1. Absorption spectra of **Ca1$_2$** (—), **Sr1$_2$•(OH$_2$)$_{1.5}$** (—), and **Ba1$_2$•(OH$_2$)$_3$** (—) in trifluoroethanol.

[^{n}Bu$_4$N][2-OH$_2$]

In a schlenck flask, Bus$_3$H$_3$tren (5.27g, 10.4mmol) and $CoCl_2$ (1.35g, 10.4mmol) were stirred in 40 mL DMA under nitrogen. KH (1.29g, 32.2mmol) was added in portions carefully to keep bubbling to a minimum, and the solution turned from blue to turquoise. After stirring overnight, the solution had turned purple, and [Bu$_4$N][Br] (3.36g, 10.4mmol) was added with a few drops of methanol to quench any residual hydride base. The reaction mixture was diluted with CH_2Cl_2 (200 mL), and washed with water (3×200 mL) and brine (200 mL). The organic layer was dried with Na_2SO_4, filtered and concentrated under rotary evaporation. Addition of diethyl ether afforded purple flaky product. Yield: 4.0g, 47%. Vapor diffusion of ether into a CH_2Cl_2 solution of the product afforded flaky purple crystals suitable for X-ray diffraction analysis. Anal. Calcd for $C_{34}H_{77}CoN_5O_7S_3$: C, 49.6; H, 9.4; N, 8.5%. Found: C, 49.9; H, 8.3; N, 8.3. λ_{max}(TFE)/nm 260 (ε/dm^3 mol^{-1} cm^{-1} 3071), 527 (47) and 1587 (31). IR (FT-ATR) $\bar{\nu}$/cm^{-1}: 3332 (ν_{OH}), 2960, 2874, 1479, 1455, 1386, 1358, 1277, 1229, 1161, 1121, 1105, 1079, 1063, 1038, 971, 959, 922, 887, 858, 813, 799, 737, 667, 590, 542. ESMS: Exact mass calcd for $C_{18}H_{39}CoN_4O_6S_3^-$ [ML$^-$], 562.13692. Found: 562.13708 (Δ = 0.3 ppm). Exact mass calcd for $C_{52}H_{114}Co_2N_9O_{12}S_6^-$ [2ML$^-$ + Bu$_4$N$^+$], 1366.55807. Found: 1366.55703 (Δ = 0.8 ppm). Exact mass calcd for $C_{18}H_{39}CoN_4O_6S_3^-$ [ML$^-$ + Bu$_4$N$^+$ + H_2O – e$^-$], 822.43116. Found: 822.43413 (Δ = 3.6 ppm). Exact mass calcd for $C_{50}H_{111}CoN_6O_6S_3^+$ [ML$^-$ + 2Bu$_4$N$^+$], 1046.70537. Found: 1046.70848 (Δ = 3.0 ppm). Magnetic susceptibility (Evan's method, $CDCl_3$): μ_{obs} = 4.12 μ_B.

[^{n}Bu$_4$N][2-OH$_2$] dehydration to form [^{n}Bu$_4$N][2]

In a glovebox, [^{n}Bu$_4$N][**2-OH$_2$**] was dissolved in dichloromethane with 3Å molecular sieves. After sitting

overnight the solution was filtered through celite and layered under ether. Blue crystals were formed which were suitable for X-ray diffraction analysis. $\lambda_{max}(CH_2Cl_2)$/nm 267 (ε/dm^3 mol^{-1} cm^{-1} 6 030), 414 (15), 571 (37), 741 (7) and 1543 (52). Magnetic susceptibility (Evan's method, $CDCl_3$): μ_{obs} = 4.40 μ_B.

Mg2$_2$

[^{n}Bu$_4$N][**2-OH$_2$**] (72mg, 0.088mmol) and 15-crown-5 Mg(OTf)$_2$ adduct (24mg, 0.044mmol) were stirred in acetonitrile at 65˚C. Crystals slowly formed as the solution lightened in color. When the solution stopped lightening, the supernatant was decanted from the crystals and the crystals were washed with dichloromethane and dried under vacuum to yield blue crystalline product. Although these crystals were found to be insoluble in traditional organic solvents, some of the crystals were found to be suitable for X-ray diffraction analysis. Yield: 33mg, 65%. IR (FT-ATR) ν̄/cm^{-1}: 2909, 2865, 1478, 1461, 1393, 1365, 1333, 1274, 1244, 1224, 1141, 1080, 1032, 964, 913, 857, 816, 805, 726, 669, 614, 559, 542.

Ca2$_2$

[^{n}Bu$_4$N][**2-OH$_2$**] (478mg, 0.58mmol) was dissolved in 120 mL methanol at 60˚C, and Ca(OTf)$_2$ (98mg, 0.29mmol) was dissolved separately in 5 mL methanol at 60˚C. The calcium solution was added dropwise into the cobalt solution without stirring. The reaction solution was maintained at 60˚C, promoting formation of crystals concomitant bleaching of the supernatant. When the solution stopped losing color, the supernatant was decanted and the remaining blue crystals were washed with ether and dried under vacuum. Before drying, some blue crystals were examined by X-ray crystallography. If the methanol solution was too concentrated or too cool, a blue powder came out of solution. This powder has the same composition as the crystalline samples as shown by elemental analysis. Yield: 280mg, 83%. Anal. Calcd for $C_{36}H_{78}CaCo_2N_8O_{12}S_6$: C, 47.4; H, 4.9; N, 8.2%. Found: C, 47.5; H, 4.75; N, 8.05. λ_{max}(TFE)/nm 240 (ε/dm^3 mol^{-1} cm^{-1} 6 560), 260 (11 200), 401 (38), 560 (129) and 1405 (136). IR (FT-ATR) ν̄/cm^{-1}: 2906, 2864, 1479, 1393, 1363, 1335, 1272, 1244, 1227, 1133, 1075, 1032, 966, 914, 860, 815, 727, 673, 611, 561. ESMS: Exact mass calcd for $C_{18}H_{41}CaCoN_4O_7S_3^+$ [$ML^- + H_2O + Ca^{2+}$], 620.10898. Found: 620.10939 (Δ = 0.7 ppm). Magnetic susceptibility (Evan's method, TFE-d_3): μ_{obs} = 6.18 μ_B.

Sr2$_2$

[^{n}Bu$_4$N][**2-OH$_2$**] (119mg, 0.15mmol) and Sr(OTf)$_2$•H_2O (29mg, 0.07mmol) were dissolved separately in acetone, and these solutions were mixed. A blue powder formed, which was allowed to settle. This blue powder was triturated with methanol and ether, and then dried under vacuum. Vapor diffusion of ether into a solution of this solid in dichloromethane and methanol afforded X-ray quality crystals. Yield: 81mg, 92%. Anal. Calcd for $C_{36}H_{78}Co_2N_8O_{12}S_6Sr$: C, 35.65; H, 6.48; N, 9.24. Found: C, 35.65; H, 6.43; N, 9.12. λ_{max}(TFE)/nm 240sh (ε/dm^3 mol^{-1} cm^{-1} 5 550), 262 (9 760), 401 (49), 565 (138) and 1405 (122). IR (FT-ATR) ν̄/cm^{-1}: 2966, 2901, 2864, 1470, 1455, 1392, 1363, 1335, 1272, 1229, 1129, 1072, 1033, 965, 918, 861, 815, 739, 728, 675, 666, 607, 594, 563. ESMS: Exact mass calcd for $C_{18}H_{39}CoN_4O_6S_3Sr^+$ [$ML^- + Sr^{2+}$], 650.04144. Found: 650.04186 (Δ = 0.6 ppm). Exact mass calcd for $C_{18}H_{41}CoN_4O_7S_3Sr^+$ [$ML^- + H_2O + Sr^{2+}$], 668.05200. Found: 668.05233 (Δ = 0.5 ppm). Magnetic susceptibility (Evan's method, TFE-d_3): μ_{obs} = 6.12 μ_B.

Ba2$_2$

[^{n}Bu$_4$N][**2-OH$_2$**] (97.0mg, 0.12mmol) and Ba(OTf)$_2$ (25.7mg, 0.06mmol) were dissolved in acetone and

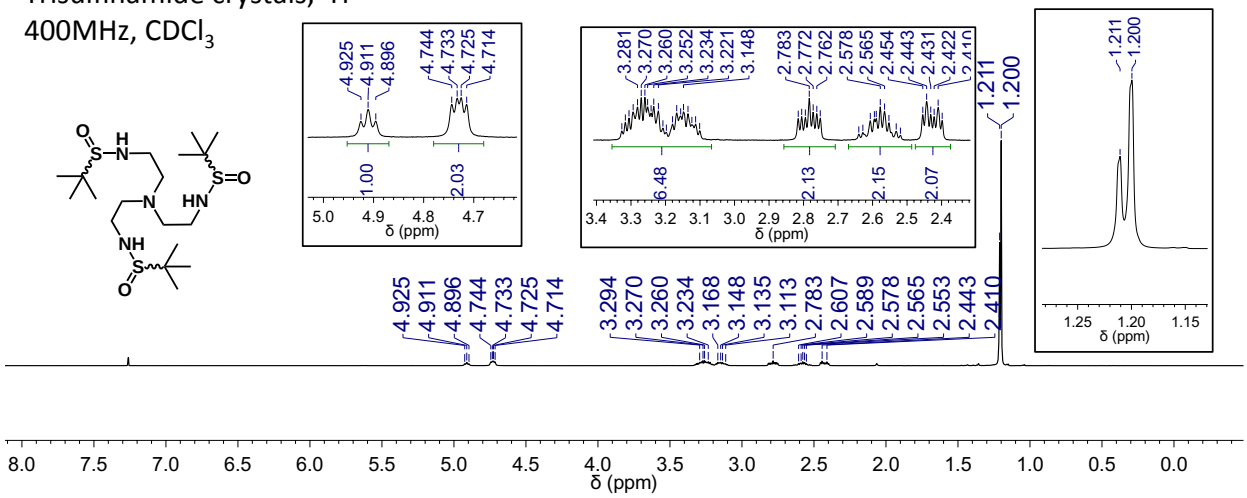
heated to 65˚C until supernatant stopped lightening and blue crystals stopped forming. The supernatant was decanted away, and the crystals were washed with ether and dried under vacuum to yield blue crystalline product. Vapor diffusion of ether into a solution of **Ba2$_2$** in dichloromethane and methanol yielded crystals suitable for X-ray crystallography. Yield: 57.0 mg, 75%. Anal. calcd for $C_{108}H_{138}Co_4N_{16}O_{27}S_{12}Sr_2$: C, 44.92; H, 4.82; N, 7.76. Found: C, 44.54; H, 4.76; N, 7.74. λ_{max}(TFE)/nm 241 (ε/dm^3 mol^{-1} cm^{-1} 5 220), 263 (8 930), 406 (36), 567 (109) and 1446 (102). IR (FT-ATR) $\tilde{\nu}$/cm^{-1}: 2967, 2900, 2859, 1471, 1393, 1363, 1233, 1123, 1070, 1040, 966, 924, 862, 814, 739, 665, 593, 563. ESMS: Exact mass calcd for $C_{18}H_{39}CoN_4O_6S_3^-$ [ML$^-$], 562.13692. Found: 562.13584 (Δ = 1.9 ppm). Magnetic susceptibility (Evan's method, TFE-d$_3$): μ_{obs} = 6.10 μ_B.

Electrochemistry

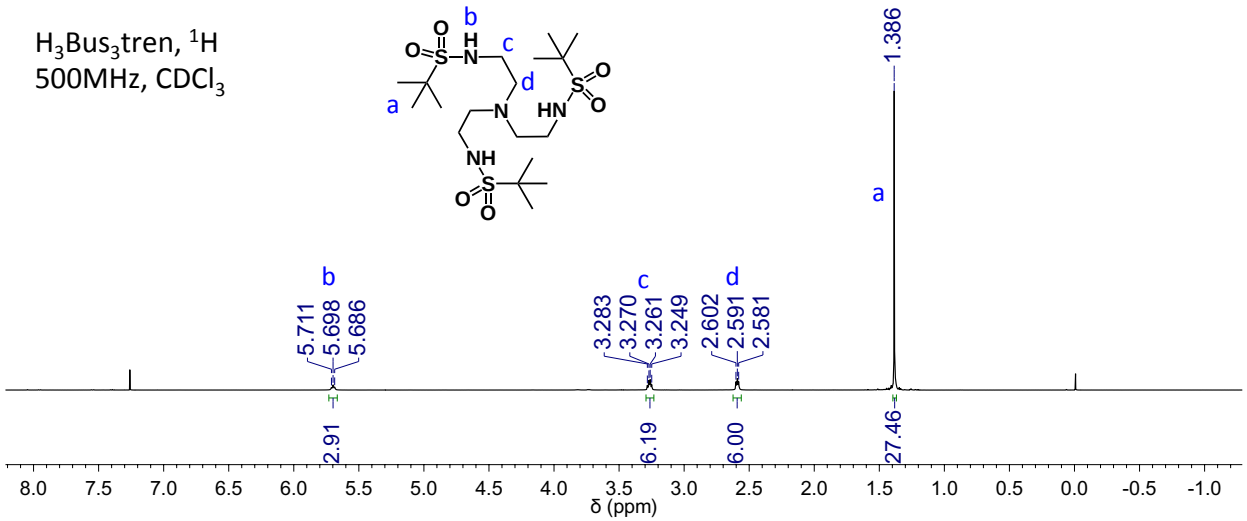
Cyclic voltammetric experiments were conducted in trifluoroethanol (TFE) or dichloromethane with 0.1M tetrabutylammonium hexafluorophosphate as supporting electrolyte and a glassy carbon working electrode. The reference electrode solution was made with Ag(PF_6) in TFE or Ag(NO_3) in acetonitrile for the dichloromethane solutions. For [^{n}Bu$_4$N][**1**] and [^{n}Bu$_4$N][**2**], the experiments were performed inside a glovebox using anhydrous dichloromethane. The potential window was scanned at 0.1 V/s.

NMR Spectra

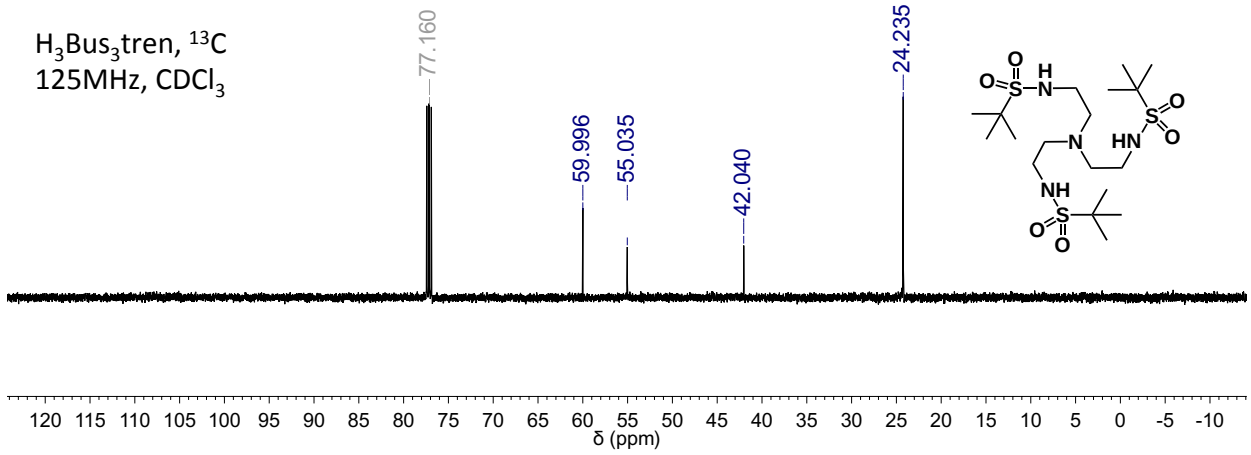
Trisulfinamide crystals, ^{1}H
400MHz, $CDCl_3$



H_3Bus_3tren, ^1H
500MHz, $CDCl_3$



H_3Bus_3tren, ^{13}C
125MHz, $CDCl_3$



Water Titration

Trifluoroethanol (TFE) was freshly distilled from calcium sulfate and sodium carbonate under nitrogen and degassed prior to use. Sandwich complexes were weighed out in a glovebox, dissolved in TFE and diluted to 5mL in volumetric flasks. A gas-tight syringe was used to dispense 3.5mL of each solution into a quartz cuvette fitted with a septum cap. Water was added to the cuvette in 5µL, 10µL, or 20µL increments from a gas-tight syringe. Each solution was scanned initially and inverted several times after each addition of water. For each complex, four wavelengths were chosen for data workup. For each wavelength, the smallest absorbance value was subtracted from the series of data points and these values were divided by the concentration of the sandwich complex in solution. These data were plotted versus equivalents of water added. The curves for **Ca2$_2$** and **Sr2$_2$** were fit to sigmoidal logistic functions using OriginPro 8.6. The data for **Ca1$_2$** and **Ba2$_2$** could not be reasonably modeled.

Slogistic1 Function: $y = \frac{a}{1+e^{-k(x-c)}}$

	a		c		k		Statistics	
	Value	Standard Error	Value	Standard Error	Value	Standard Error	Reduced Chi-Sqr	Adj. R-Square
Ca2$_2$	27.9487	0.18493	208.70663	1.30343	-0.01927	3.74532E-4	0.08362	0.99931
Sr2$_2$	35.98668	0.89708	115.94357	3.7926	-0.01887	8.122E-4	0.40771	0.99738

Ca2$_2$ halfway point: 209eq
Sr2$_2$ halfway point: 116eq

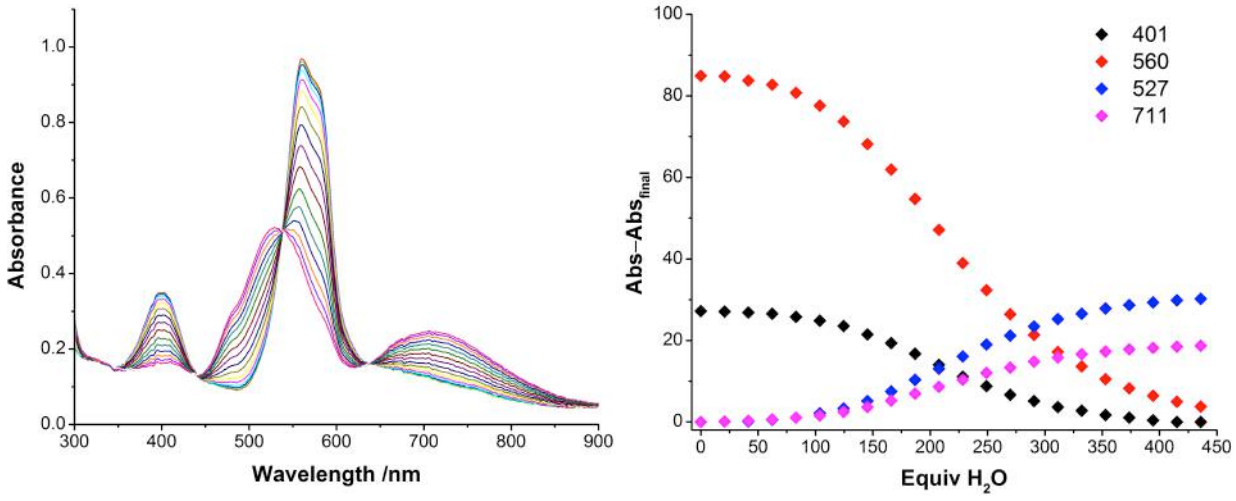


Figure S2. Ca2$_2$ UV-Vis traces (left) and titration curves (right)

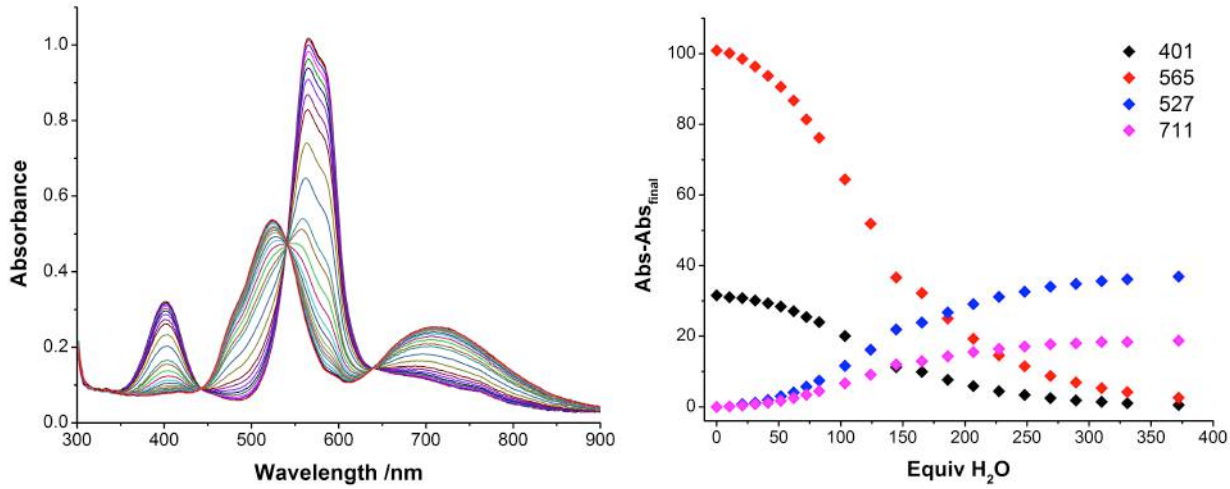


Figure S3. $Sr2_2$ UV-Vis traces (left) and titration curves (right)

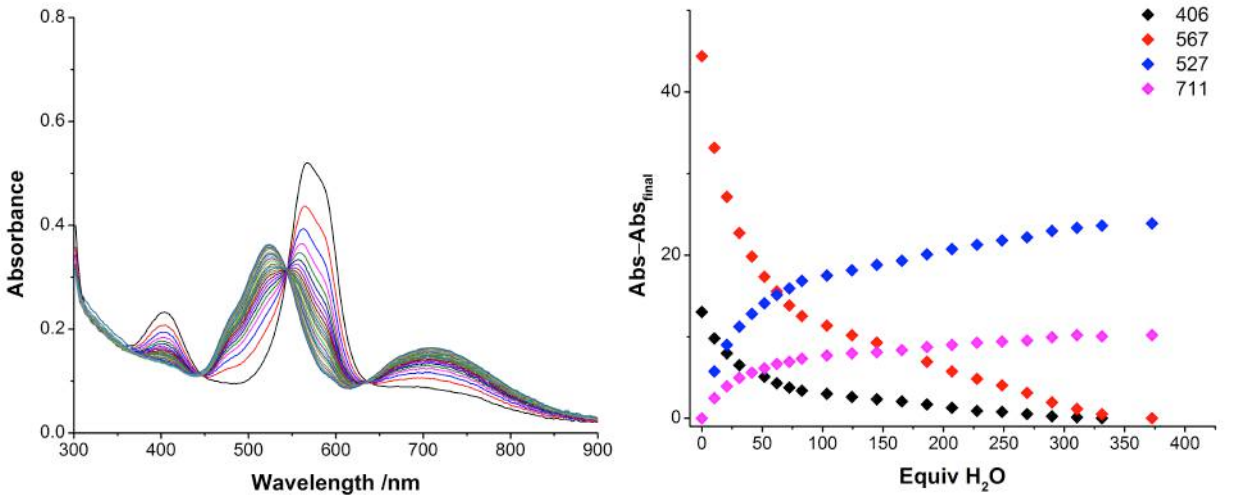


Figure S4. **$Ba2_2$** UV-Vis traces (left) and titration curves (right)

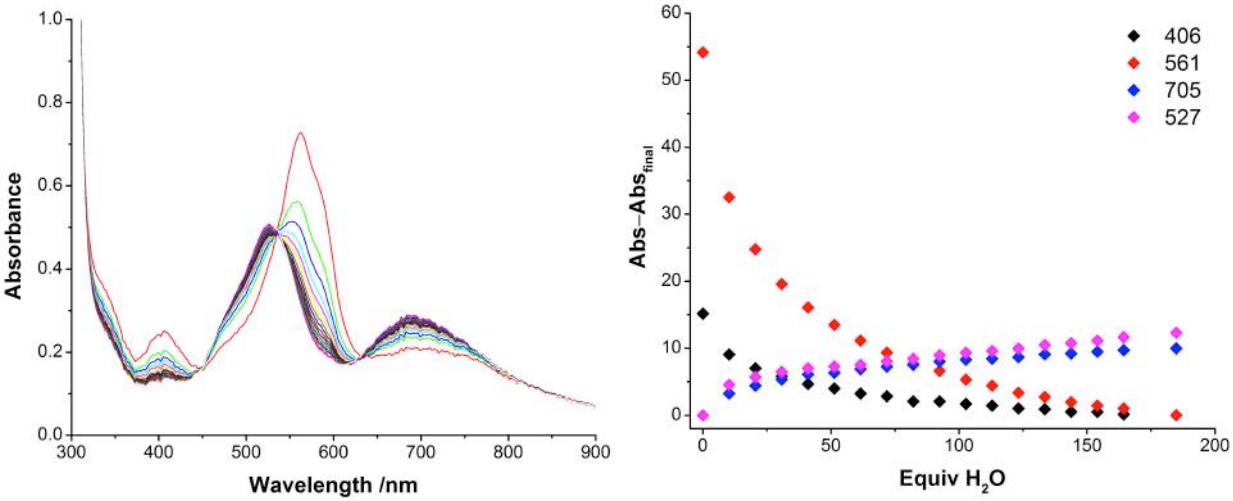


Figure S5. **$Ca1_2$** UV-Vis traces (left) and titration curves (right)

Crystallographic Information

Note for [^{n}Bu$_4$N][**1-OH$_2$**]: These crystals displayed an additional diffraction pattern. The crystals show strong diffraction maxima due to a small sub-cell but additional weak peaks forming distinctive groups of two reflections around each allowed peak. These extra peaks were not commensurate with the lattice vectors ruling out a supercell and were also not due to twinning. Refinement of the crystal structure on the small cell yielded a partial structure, but with some physically unreasonable results. Therefore, crystallographic data for this species are not included in this manuscript.

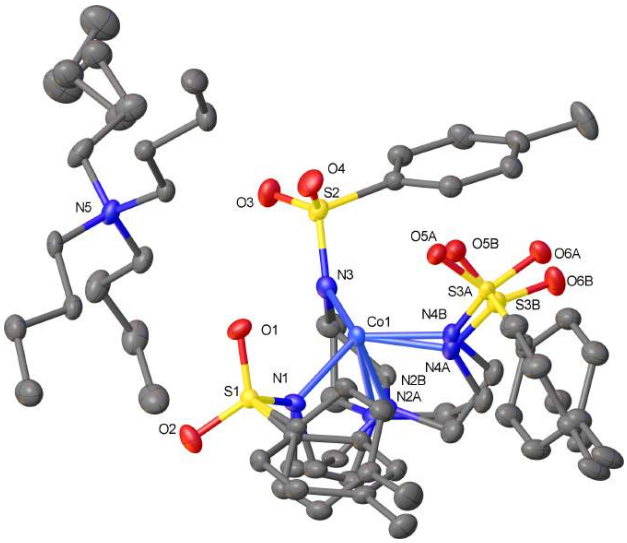
CMW04BuCoTs

EMORY UNIVERSITY | X-ray Crystallography Center

Submitted by: **Christian Wallen**
Emory University
Solved by: **Thomas C. Pickel**

Sample ID: **CMW04BuCoTs**

Crystal Data and Experimental[6]



Experimental. Single violet prism-shaped crystals of (**CMW04BuCoTs**) were recrystallised from a mixture of CH_2Cl_2 and diethyl ether by vapor diffusion. A suitable crystal (0.43×0.43×0.38) was selected and mounted on a loop with paratone oil on a Bruker APEX-II CCD diffractometer. The crystal was kept at T = 100(2) K during data collection. The structure was solved with the **XT** (Sheldrick, 2008) structure solution program, using direct and dual-space solution methods and by using **Olex2** (Dolomanov et al., 2009), as the graphical interface. The model was refined with version 2014/7 of **ShelXL-97** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{43}H_{69}CoN_5O_6S_3$, M_r = 907.17, monoclinic, $P2_1/n$ (No. 14), a = 14.2734(9) Å, b = 14.8425(9) Å, c = 21.9158(14) Å, β = 102.4610(10)°, α = γ = 90°, V = 4533.6(5) Å^3, T = 100(2) K, Z = 4, Z' = 1, μ(MoK$_\alpha$) = 0.568, 104077 reflections measured, 13895 unique (R_{int} = 0.0651) which were used in all calculations. The final wR_2 was 0.1875 (all data) and R_1 was 0.0711 (I > 2(I)).

Compound	**CMW04BuCoTs**
Formula	$C_{43}H_{69}CoN_5O_6S_3$
$D_{calc.}$/ g cm^{-3}	1.329
μ/mm^{-1}	0.568
Formula Weight	907.17
Colour	violet
Shape	prism
Max Size/mm	0.43
Mid Size/mm	0.43
Min Size/mm	0.38
T/K	100(2)
Crystal System	monoclinic
Space Group	$P2_1/n$
a/Å	14.2734(9)
b/Å	14.8425(9)
c/Å	21.9158(14)
α/°	90
β/°	102.4610(10)
γ/°	90
V/Å^3	4533.6(5)
Z	4
Z'	1
Θ_{min}/°	1.562
Θ_{max}/°	30.581
Measured Refl.	104077
Independent Refl.	13895
Reflections Used	10880
R_{int}	0.0651
Parameters	762
Restraints	561
Largest Peak	1.980
Deepest Hole	-1.667
GooF	1.041
wR_2 (all data)	0.1875
wR_2	0.1701
R_1 (all data)	0.0919
R_1	0.0711
CCDC #	1434440

Structure Quality Indicators

Reflections:	d min	0.70	I/σ	17.2	Rint	6.51%	complete 100%
Refinement:	Max Peak	2.0	Min Peak	-1.7	GooF	1.041	

A violet prism-shaped crystal with dimensions 0.43×0.43×0.38 was mounted on a loop with paratone oil. Data were collected using a Bruker APEX-II CCD diffractometer equipped with an Oxford Cryosystems low-temperature apparatus operating at T = 100(2) K.

Data were measured using ϕ and ω scans using MoK$_\alpha$ radiation (fine-focus sealed tube, 45 kV, 35 mA). The total number of runs and images was based on the strategy calculation from the program **APEX2** (Bruker). The actually achieved resolution was Θ = 30.581.

Cell parameters were retrieved using the **SAINT** (Bruker, V8.34A, 2013) software and refined using **SAINT** (Bruker, V8.34A, 2013) on 9735 reflections, 9 of the observed reflections. Data reduction was performed using the **SAINT** (Bruker, V8.34A, 2013) software which corrects for Lorentz polarisation. The final completeness is 99.9% out to 30.581 in Θ. The absorption coefficient (μ) of this material is 0.568 mm^{-1} and the minimum and maximum transmissions are 0.6511 and 0.7461.

The structure was solved with **ShelXT** (Sheldrick, 2015) in the space group P1 using combined Patterson and dual-space recycling methods. **ShelXT** (Sheldrick, 2015) determined that structure belongs to the space group P2$_1$ (# 4). The structure was refined by Least Squares using version of **ShelXL-97** (Sheldrick, 2008). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

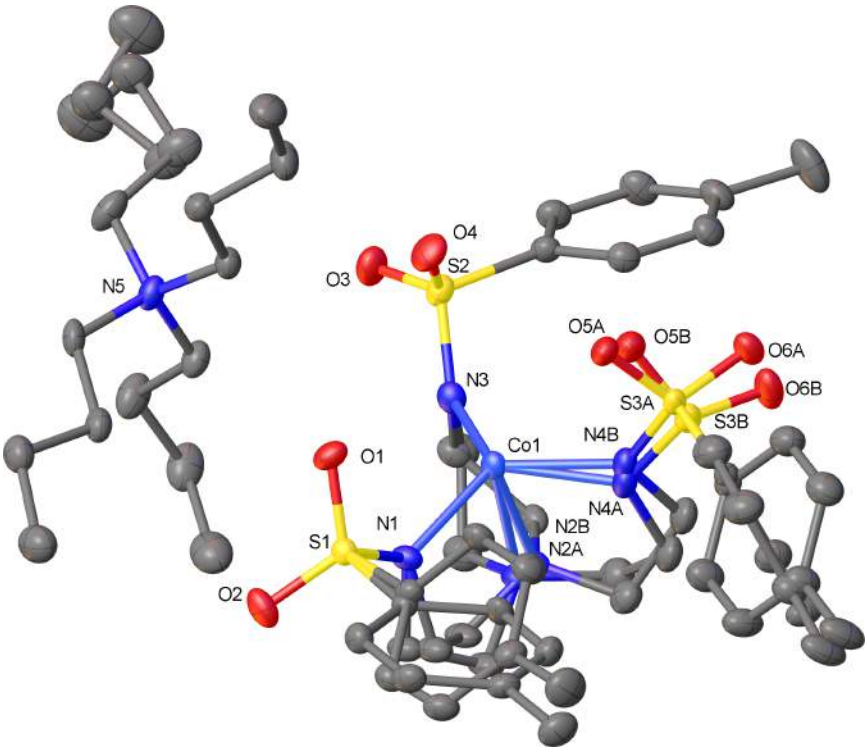


Figure S6:

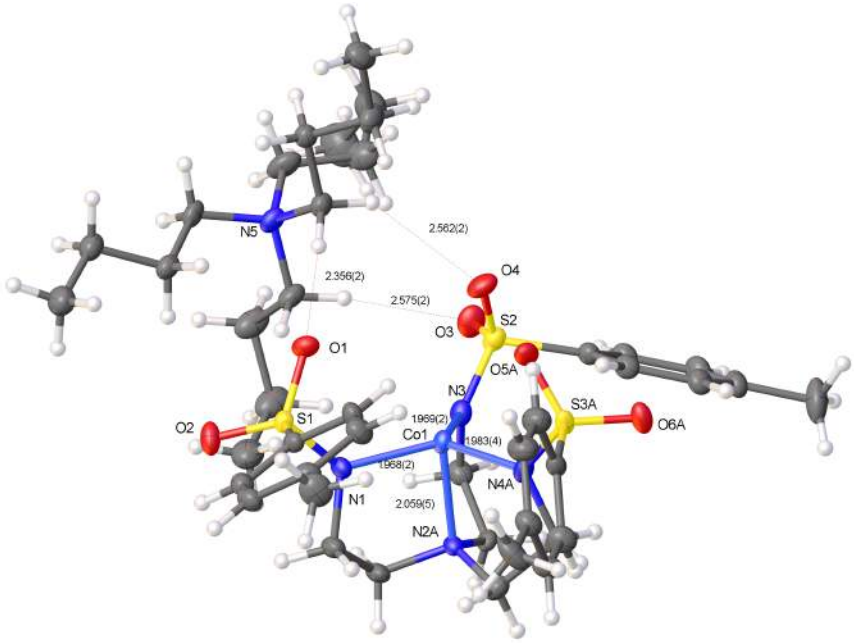


Figure S7: Component 1 and undisordered component.

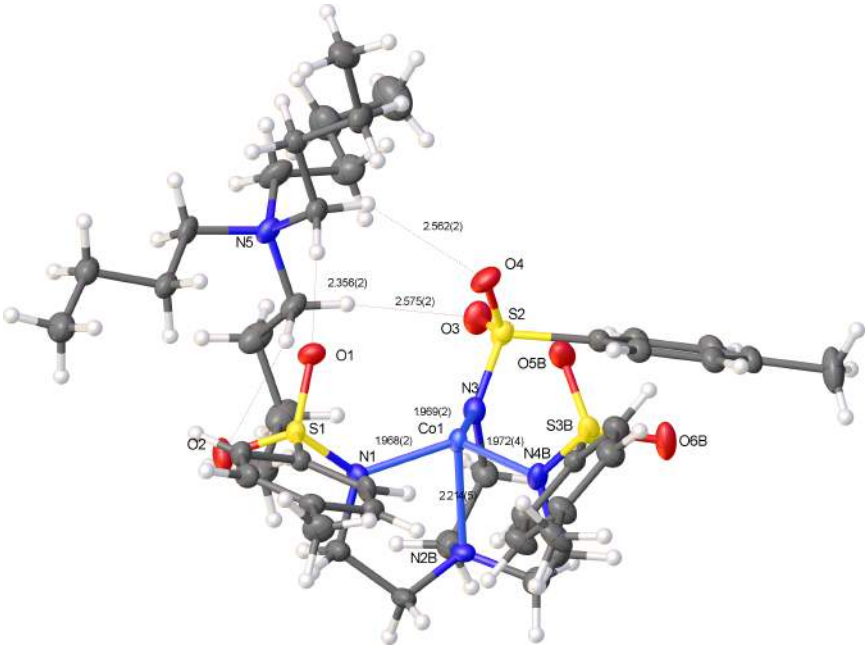
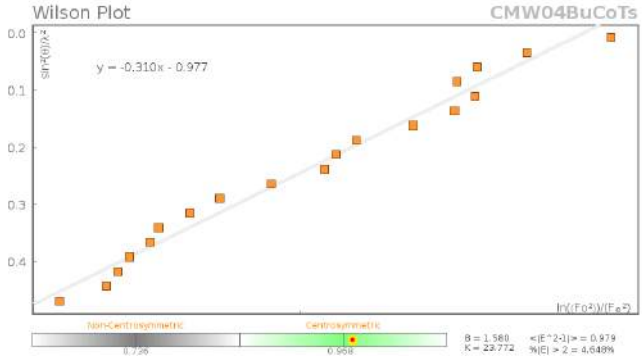
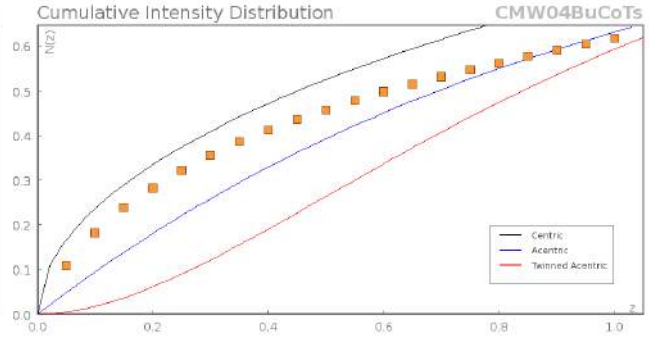
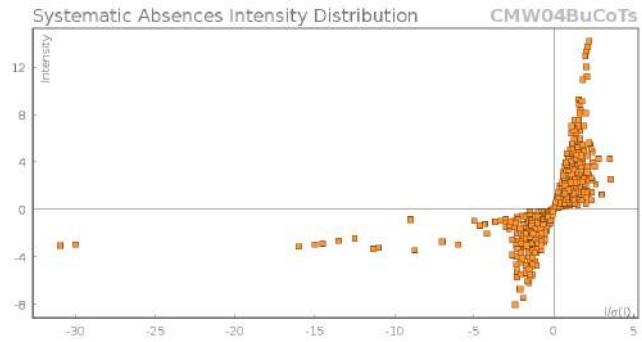


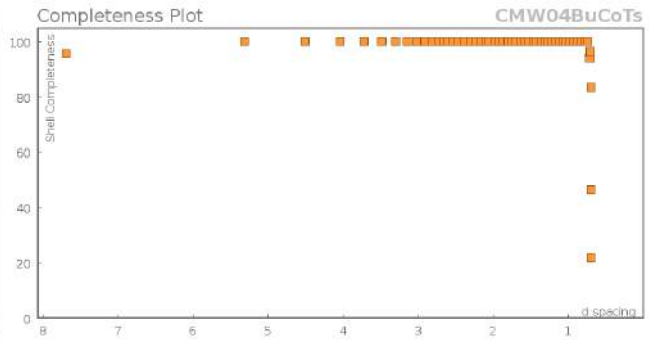
Figure S8: Component 2 and undisordered component.

Data Plots: Diffraction Data

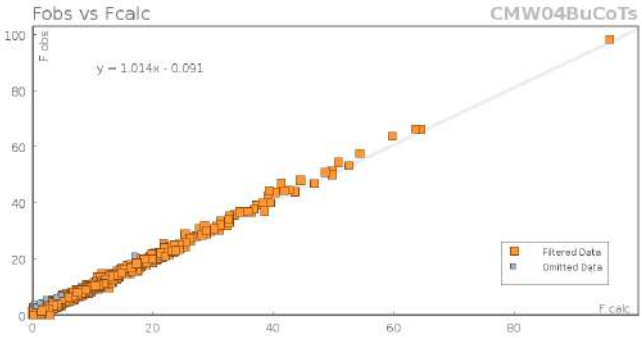


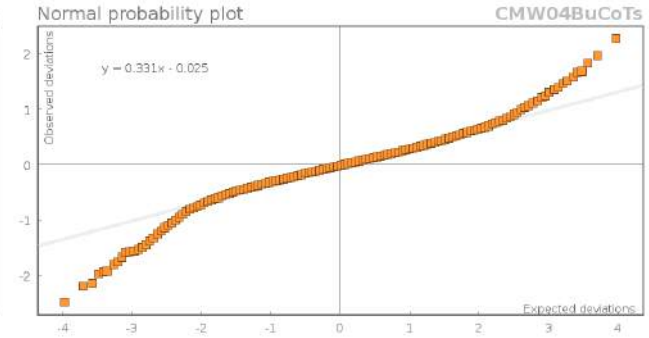






Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	106471	Unique reflections	13895
Completeness	0.997	Mean I/σ	17.17
hklsub>max</sub> collected	(20, 21, 31)	hklsub>min</sub> collected	(-20, -21, -31)
hkl_{max} used	(19, 21, 31)	hkl_{min} used	(-20, 0, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.36
d_{max} used	14.84	d_{min} used	0.7
Friedel pairs	23750	Friedel pairs merged	1
Inconsistent equivalents	0	R_{int}	0.0651
R_{sigma}	0.0365	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	54

Multiplicity	(22470, 12299, 9794, 4957, 1381, 548)	Maximum mulitplicity	18
Removed systematic absences	2340	Filtered off (Shel/OMIT)	0

Images of the Crystal on the Diffractometer

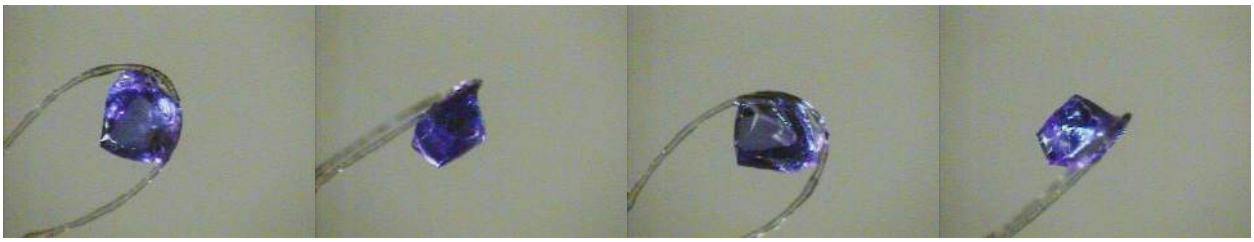


Table S1: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **CMW04BuCoTs**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Co1	6312.8(2)	5578.1(3)	7640.4(2)	17.85(10)
S1	4194.1(4)	5795.1(4)	6820.2(3)	17.69(13)
S2	6685.0(5)	4179.0(5)	8767.8(3)	21.99(14)
O1	4241.4(15)	4822.5(14)	6863.8(10)	25.1(4)
O2	3303.0(14)	6216.0(17)	6883.7(10)	29.2(5)
O3	6342.3(16)	4027.4(17)	9336.4(11)	32.0(5)
O4	6353.8(16)	3567.0(16)	8252.5(11)	31.0(5)
N1	5086.2(16)	6185.6(15)	7300.6(11)	19.0(4)
N3	6480.6(16)	5170.2(17)	8512.9(11)	21.7(4)
C12	7952.5(19)	4076.0(18)	8984.0(12)	19.4(5)
C13	8473(2)	4124.3(19)	8512.8(13)	21.8(5)
C14	9465(2)	4095(2)	8668.3(13)	23.2(5)
C15	9955(2)	4012(2)	9289.3(14)	25.4(6)
C16	9428(2)	3973(2)	9751.0(14)	28.4(6)
C17	8432(2)	4002(2)	9603.0(13)	23.4(5)
C18	11039(2)	3980(3)	9447.1(18)	46.1(10)
N4A	7435(3)	5691(3)	7252.3(16)	22.7(7)
S3A	7828.2(14)	4997.6(13)	6826.0(8)	23.3(4)
O5A	7131(3)	4272(2)	6679(2)	31.9(9)
O6A	8807(3)	4727(4)	7073.2(19)	36.1(10)
C21A	7829(3)	5541(2)	6101.5(15)	21.4(9)
C22A	8129(3)	6423(3)	6037(2)	32.6(10)
C23A	8024(3)	6795(3)	5444(2)	30.6(10)
C24A	7633(3)	6307(3)	4918.7(18)	27.6(10)
C25A	7335(3)	5423(3)	4992(2)	37.1(11)
C26A	7435(3)	5051(3)	5577(2)	37.4(11)
C27A	7509(4)	6701(4)	4269(2)	33.8(11)
N2A	6774(3)	6816(3)	8033.0(17)	19.4(8)
C9A	5892(3)	7370(3)	7970(2)	25.0(8)
C8A	5220(3)	7177(3)	7342(2)	22.9(9)
C10A	7217(3)	6637(3)	8698(2)	21.3(7)
C11A	6669(10)	5890(5)	8952(3)	23.6(13)
C19A	7462(3)	7199(3)	7689(2)	26.0(8)
C20A	8089(3)	6441(3)	7520(2)	26.1(8)
C1A	4368(3)	6025(3)	6054.0(16)	19.8(11)
C2A	3831(3)	6681(3)	5689(2)	27.1(9)
C3A	3967(3)	6845(3)	5089(2)	29.8(10)
C4A	4626(3)	6370(3)	4845.8(18)	26.7(13)
C5A	5172(3)	5697(3)	5219(2)	32.2(10)
C6A	5046(3)	5525(3)	5821(2)	28.5(10)
C7A	4768(4)	6552(5)	4192(2)	42.1(16)

Atom	x	y	z	U_{eq}
N4B	7414(4)	5888(3)	7265.1(19)	22.1(9)
S3B	7985.3(18)	5227.5(18)	6914.2(10)	24.4(6)
O5B	7501(4)	4361(3)	6868(3)	29.0(11)
O6B	9001(3)	5218(4)	7173(2)	27.6(11)
C21B	7839(3)	5629(3)	6132.3(16)	19.9(11)
C22B	7334(3)	6413(3)	5917(2)	25.0(11)
C23B	7314(4)	6720(3)	5318(2)	25.4(11)
C24B	7786(4)	6266(3)	4927.5(18)	25.2(12)
C25B	8288(4)	5482(4)	5148(2)	25.3(11)
C26B	8308(4)	5170(3)	5745(2)	25.0(11)
C27B	7765(6)	6596(5)	4271(2)	33.8(11)
N2B	6605(3)	6923(3)	8084(2)	21.8(11)
C9B	5937(3)	7582(3)	7709(3)	25.0(8)
C8B	4966(4)	7140(3)	7460(3)	22.9(9)
C10B	6439(4)	6849(5)	8728(3)	29.0(9)
C11B	6760(15)	5923(6)	9000(4)	25.9(16)
C19B	7618(4)	7116(5)	8080(2)	28.2(9)
C20B	7840(4)	6784(5)	7466(3)	26.1(8)
C1B	4302(4)	6140(3)	6065.0(17)	15.6(13)
C2B	3515(3)	6177(3)	5571(2)	15(1)
C3B	3633(3)	6446(3)	4984(2)	17.6(10)
C4B	4517(4)	6679(3)	4881(2)	17.9(14)
C5B	5320(3)	6638(3)	5387(2)	16.7(10)
C6B	5214(3)	6370(3)	5978(2)	14.9(10)
C7B	4639(5)	6970(4)	4240(2)	24.6(14)
N5	3444.6(17)	3385.0(17)	8230.0(11)	22.1(5)
C28	2402.8(18)	3541(2)	7909.0(13)	22.9(5)
C29	2229.5(19)	4258(2)	7405.6(14)	23.7(5)
C30	1176(2)	4240(2)	7057.1(15)	28.0(6)
C31	951(2)	4981(2)	6576.4(17)	35.5(7)
C32	3932(2)	4251(2)	8503.4(14)	24.6(6)
C33	3516(3)	4698(3)	9010.2(16)	34.4(7)
C34	4027(3)	5594(3)	9199.9(16)	36.9(8)
C35	3861(3)	6291(3)	8679.5(19)	41.3(8)
C36	4023.2(19)	3056(2)	7769.2(13)	21.8(5)
C37	3600.5(19)	2268.4(19)	7359.2(13)	22.2(5)
C38	4389(2)	1861(2)	7071.5(16)	31.0(6)
C39	4039(3)	1135(2)	6588.5(17)	33.7(7)
C40	3433(2)	2681(2)	8734.1(15)	31.9(7)
C41	4432(4)	2323(5)	9048(3)	36.4(14)
C42	4390(5)	1720(4)	9624(3)	36.9(11)
C43	4120(6)	2267(6)	10141(3)	53.9(15)
C41B	4371(4)	2455(8)	9188(4)	37.1(14)
C42B	3991(5)	1939(7)	9707(4)	38.2(11)
C43B	4806(8)	1508(8)	10169(4)	56.5(17)

Table S2: Anisotropic Displacement Parameters (×10^4) **CMW04BuCoTs**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	12.63(16)	21.38(18)	18.37(17)	3.34(13)	0.76(12)	0.14(12)
S1	14.0(3)	19.3(3)	19.1(3)	2.0(2)	2.0(2)	0.1(2)
S2	18.6(3)	24.3(3)	22.5(3)	4.2(2)	3.5(2)	-3.5(2)
O1	27(1)	18.8(10)	28.3(10)	4.8(8)	3.3(8)	-4.7(8)
O2	17.4(9)	40.7(13)	28.5(11)	-0.8(9)	2.7(8)	7.4(8)
O3	27.5(11)	41.1(13)	29.7(11)	11.3(10)	11.2(9)	-0.8(9)
O4	28.2(11)	28.3(11)	34.3(12)	-2.1(9)	1.8(9)	-11.4(9)
N1	18.3(10)	16.3(9)	20.2(10)	0.5(8)	-0.5(8)	2.7(7)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N3	17.6(10)	26.4(12)	20.1(10)	1.6(9)	2.1(8)	1.1(8)
C12	19.1(11)	18.0(12)	19.8(12)	2.9(9)	1.6(9)	1.6(9)
C13	24.3(12)	22.0(13)	18.4(12)	-0.2(10)	2.8(10)	1(1)
C14	23.4(13)	23.8(13)	23.4(13)	-2.2(10)	7.5(10)	2.9(10)
C15	20.8(12)	25.1(14)	28.0(14)	-1.6(11)	0.5(10)	6.3(10)
C16	28.9(14)	33.5(16)	20.1(13)	3.1(11)	-1.0(11)	6.1(12)
C17	26.8(13)	24.0(13)	18.5(12)	3.4(10)	2.8(10)	3.6(10)
C18	22.0(15)	75(3)	38.1(19)	-4.2(19)	-0.4(13)	16.3(17)
N4A	14.8(12)	27.0(16)	26.3(13)	7.5(11)	4.7(10)	-1.6(11)
S3A	17.5(7)	24.9(8)	30.2(7)	13.8(6)	10.8(5)	5.6(6)
O5A	29(2)	22.8(16)	48(2)	9.1(15)	17.1(17)	0.5(14)
O6A	26.0(16)	47(2)	37(2)	19(2)	11.5(14)	14.1(16)
C21A	17.4(18)	20.6(17)	27.3(16)	5.6(13)	7.0(13)	2.7(14)
C22A	40(2)	31.0(19)	26.7(18)	2.3(15)	7.2(17)	0.0(17)
C23A	42(2)	22.6(19)	28.2(17)	2.1(14)	9.5(16)	-2.1(17)
C24A	29(2)	26.0(18)	28.2(17)	2.0(14)	5.7(15)	4.9(16)
C25A	41(3)	30(2)	37(2)	-1.3(15)	0.6(18)	-3.4(18)
C26A	38(2)	30(2)	41.6(19)	2.4(16)	2.9(17)	-1.7(18)
C27A	41(3)	33.8(17)	29.6(13)	5.7(12)	13.8(13)	20.8(17)
N2A	17.4(15)	16.5(17)	21.9(15)	-1.6(13)	-0.7(12)	-0.3(12)
C9A	23.7(12)	14.7(15)	33.5(18)	-0.2(13)	-0.2(13)	1.5(11)
C8A	20.9(17)	16.3(12)	30.0(19)	1.1(11)	2.3(14)	1.0(11)
C10A	17.1(16)	22.5(18)	22.0(15)	-4.6(13)	-0.8(12)	-1.7(13)
C11A	26(3)	24(2)	20(2)	-4.6(18)	3(2)	1.4(19)
C19A	22.2(15)	24.3(17)	29.2(17)	2.2(15)	0.5(14)	-4.9(13)
C20A	15.4(16)	29(2)	32.6(17)	8.4(16)	1.7(14)	-3.2(13)
C1A	18(2)	20(2)	20(2)	3.3(17)	-0.5(17)	-0.6(17)
C2A	27(2)	27(2)	26(2)	-0.9(18)	3.8(17)	3.9(18)
C3A	32(3)	25(3)	29(2)	4(2)	0(2)	4.9(19)
C4A	28(2)	26(4)	26(2)	2(2)	5.0(17)	-1(2)
C5A	35(2)	30(2)	33(2)	1(2)	11(2)	5(2)
C6A	25(2)	29(2)	30(2)	5.3(19)	2.8(17)	6.4(18)
C7A	46(3)	53(4)	29(3)	11(3)	13(2)	3(3)
N4B	15.2(14)	25.3(18)	26.0(15)	9.0(14)	4.7(12)	-0.6(14)
S3B	17.9(9)	23.7(11)	32.4(10)	12.9(8)	7.2(7)	1.7(8)
O5B	22(2)	24.4(18)	42(3)	11.2(17)	10(2)	1.5(16)
O6B	14.8(17)	36(3)	32(2)	14(2)	5.5(15)	4.5(17)
C21B	16(2)	18(2)	25.9(18)	3.2(15)	4.0(16)	-0.9(17)
C22B	30(2)	24(2)	23(2)	2.2(17)	11.2(18)	6.1(19)
C23B	35(3)	17(2)	26(2)	4.7(16)	11.9(18)	8(2)
C24B	30(3)	24(2)	23.7(19)	2.9(16)	9.6(18)	8(2)
C25B	25(2)	22(2)	29(2)	-2.4(17)	6.3(18)	2.7(18)
C26B	22(2)	19(2)	33(2)	5.5(17)	4.9(17)	1.8(18)
C27B	41(3)	33.8(17)	29.6(13)	5.7(12)	13.8(13)	20.8(17)
N2B	22.4(19)	14(2)	27(2)	-1.9(17)	1.0(15)	-0.6(16)
C9B	23.7(12)	14.7(15)	33.5(18)	-0.2(13)	-0.2(13)	1.5(11)
C8B	20.9(17)	16.3(12)	30.0(19)	1.1(11)	2.3(14)	1.0(11)
C10B	26.5(19)	29.0(19)	29.1(18)	-2.4(15)	0.7(15)	2.0(16)
C11B	27(3)	27(2)	22(2)	-3.7(19)	1(2)	3(2)
C19B	24.1(16)	26.4(18)	31.6(18)	1.1(17)	0.6(15)	-3.5(14)
C20B	15.4(16)	29(2)	32.6(17)	8.4(16)	1.7(14)	-3.2(13)
C1B	15(2)	14(2)	18(2)	0(2)	4(2)	1(2)
C2B	11(2)	16(2)	17(2)	0.0(19)	0.2(18)	-1.7(18)
C3B	17(2)	15(3)	18(2)	4(2)	-3.2(19)	-0.7(19)
C4B	22(2)	12(4)	19(2)	2(2)	4(2)	4(2)
C5B	15(2)	16(2)	20(2)	3.7(19)	7.1(19)	-1.6(18)
C6B	9(2)	19(2)	16(2)	7.7(18)	1.0(17)	5.5(17)
C7B	32(3)	21(3)	21(3)	6(3)	5(2)	0(3)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N5	19.7(10)	26.8(12)	20.4(10)	0.9(9)	5.8(8)	-6.7(9)
C28	14.1(11)	31.6(15)	24.2(13)	-3.4(11)	7.1(9)	-4.7(10)
C29	17.8(12)	26.1(14)	28.3(14)	-2.8(11)	7.3(10)	-3.8(10)
C30	20.5(13)	31.5(16)	31.3(15)	-3.7(12)	4.5(11)	-3.1(11)
C31	28.1(15)	33.8(17)	41.6(18)	-0.4(14)	1.0(13)	-0.2(13)
C32	22.9(13)	27.9(14)	23.2(13)	-3.4(11)	5.4(10)	-9(1)
C33	38.4(17)	41.4(19)	26.7(15)	-9.4(13)	14.0(13)	-14.2(14)
C34	38.6(17)	45(2)	29.5(16)	-15.8(14)	12.1(13)	-12.1(15)
C35	38.8(18)	35.1(19)	49(2)	-12.5(16)	6.3(16)	-3.3(15)
C36	16.6(11)	24.4(13)	24.8(13)	0.8(10)	5.8(9)	-1.7(9)
C37	20.0(12)	20.9(13)	25.7(13)	2.4(10)	5.1(10)	-0.6(9)
C38	21.9(13)	34.5(17)	39.0(17)	-4.7(13)	11.4(12)	-2.2(12)
C39	37.3(17)	27.6(16)	39.7(18)	-1.9(13)	16.0(14)	3.2(13)
C40	36.4(16)	34.9(17)	23.8(14)	5.7(12)	5.4(12)	-15.6(13)
C41	42.4(18)	36(2)	26(2)	2.4(19)	-2.7(15)	-5.4(15)
C42	37(3)	42(3)	31.4(19)	7.6(18)	5.4(18)	7(2)
C43	61(3)	65(4)	33(2)	5(2)	4(2)	15(3)
C41B	43.2(18)	37(2)	26(2)	3(2)	-3.1(15)	-5.7(16)
C42B	38(3)	43(3)	32(2)	8.0(19)	5.1(19)	6(2)
C43B	62(3)	68(4)	36(2)	8(2)	3(2)	17(3)

Table S3: Bond Lengths in Å for **CMW04BuCoTs**.

Atom	Atom	Length/Å
Co1	N1	1.967(2)
Co1	N3	1.970(2)
Co1	N4A	1.976(3)
Co1	N2A	2.075(4)
Co1	N4B	1.979(4)
Co1	N2B	2.220(5)
S1	O1	1.447(2)
S1	O2	1.451(2)
S1	N1	1.577(2)
S1	C1A	1.783(3)
S1	C1B	1.770(3)
S2	O3	1.451(2)
S2	O4	1.447(2)
S2	N3	1.578(3)
S2	C12	1.775(3)
N1	C8A	1.484(4)
N1	C8B	1.478(5)
N3	C11A	1.423(8)
N3	C11B	1.536(13)
C12	C13	1.398(4)
C12	C17	1.386(4)
C13	C14	1.384(4)
C14	C15	1.395(4)
C15	C16	1.387(4)
C15	C18	1.511(4)
C16	C17	1.388(4)
N4A	S3A	1.572(4)
N4A	C20A	1.489(5)
S3A	O5A	1.455(4)
S3A	O6A	1.442(3)
S3A	C21A	1.781(3)
C21A	C22A	1.394(6)
C21A	C26A	1.373(6)
C22A	C23A	1.390(6)
C23A	C24A	1.372(6)
C24A	C25A	1.399(6)
C24A	C27A	1.514(5)
C25A	C26A	1.376(7)
N2A	C9A	1.484(5)
N2A	C10A	1.482(5)
N2A	C19A	1.475(5)
C9A	C8A	1.526(4)
C10A	C11A	1.528(6)
C19A	C20A	1.532(5)
C1A	C2A	1.382(5)
C1A	C6A	1.400(5)
C2A	C3A	1.391(6)
C3A	C4A	1.373(6)
C4A	C5A	1.414(6)
C4A	C7A	1.514(5)
C5A	C6A	1.394(6)
N4B	S3B	1.577(4)
N4B	C20B	1.489(6)
S3B	O5B	1.454(4)
S3B	O6B	1.438(3)
S3B	C21B	1.783(3)
C21B	C22B	1.397(6)
C21B	C26B	1.370(6)
C22B	C23B	1.384(6)
C23B	C24B	1.375(6)
C24B	C25B	1.396(6)
C24B	C27B	1.514(5)
C25B	C26B	1.385(7)
N2B	C9B	1.484(5)
N2B	C10B	1.485(5)
N2B	C19B	1.476(5)
C9B	C8B	1.523(4)
C10B	C11B	1.528(5)

Atom	Atom	Length/Å
C19B	C20B	1.530(5)
C1B	C2B	1.382(5)
C1B	C6B	1.399(6)
C2B	C3B	1.392(6)
C3B	C4B	1.374(6)
C4B	C5B	1.414(6)
C4B	C7B	1.514(5)
C5B	C6B	1.394(6)
N5	C28	1.519(4)
N5	C32	1.522(4)
N5	C36	1.517(4)
N5	C40	1.523(4)
C28	C29	1.515(4)
C29	C30	1.533(4)
C30	C31	1.509(5)
C32	C33	1.520(4)
C33	C34	1.531(5)
C34	C35	1.519(6)
C36	C37	1.518(4)
C37	C38	1.529(4)
C38	C39	1.518(5)
C40	C41	1.537(6)
C40	C41B	1.523(6)
C41	C42	1.560(6)
C42	C43	1.510(7)
C41B	C42B	1.561(6)
C42B	C43B	1.510(7)

Table S4: Bond Angles in ° for **CMW04BuCoTs**.

Atom	Atom	Atom	Angle/°
N1	Co1	N3	114.84(10)
N1	Co1	N4A	122.42(13)
N1	Co1	N2A	85.84(12)
N1	Co1	N4B	117.25(16)
N1	Co1	N2B	79.70(14)
N3	Co1	N4A	120.24(13)
N3	Co1	N2A	84.75(12)
N3	Co1	N4B	122.25(16)
N3	Co1	N2B	83.10(13)
N4A	Co1	N2A	83.67(17)
N4B	Co1	N2B	83.20(18)
O1	S1	O2	116.91(14)
O1	S1	N1	107.64(12)
O1	S1	C1A	103.85(19)
O1	S1	C1B	109.76(18)
O2	S1	N1	112.08(13)
O2	S1	C1A	108.12(17)
O2	S1	C1B	102.70(18)
N1	S1	C1A	107.59(15)
N1	S1	C1B	107.3(2)
O3	S2	N3	112.20(14)
O3	S2	C12	105.69(13)
O4	S2	O3	117.33(14)
O4	S2	N3	107.73(13)
O4	S2	C12	107.26(14)
N3	S2	C12	105.94(13)
S1	N1	Co1	127.48(14)
C8A	N1	Co1	109.8(2)
C8A	N1	S1	118.7(2)
C8B	N1	Co1	119.3(2)
C8B	N1	S1	113.1(2)
S2	N3	Co1	127.19(15)
C11A	N3	Co1	113.0(2)
C11A	N3	S2	117.8(3)
C11B	N3	Co1	114.2(2)
C11B	N3	S2	115.6(3)
C13	C12	S2	118.2(2)
C17	C12	S2	121.9(2)
C17	C12	C13	119.9(3)
C14	C13	C12	119.7(3)
C13	C14	C15	120.9(3)
C14	C15	C18	119.9(3)
C16	C15	C14	118.6(3)
C16	C15	C18	121.5(3)
C17	C16	C15	121.2(3)
C12	C17	C16	119.7(3)
S3A	N4A	Co1	128.8(3)
C20A	N4A	Co1	113.0(3)
C20A	N4A	S3A	116.7(3)
N4A	S3A	C21A	107.60(17)
O5A	S3A	N4A	107.54(18)
O5A	S3A	C21A	105.7(2)
O6A	S3A	N4A	113.6(2)
O6A	S3A	O5A	115.9(3)
O6A	S3A	C21A	105.92(16)
C22A	C21A	S3A	125.1(3)
C26A	C21A	S3A	115.3(3)
C26A	C21A	C22A	119.4(3)
C23A	C22A	C21A	119.6(4)
C24A	C23A	C22A	121.1(4)
C23A	C24A	C25A	118.5(4)
C23A	C24A	C27A	121.9(4)
C25A	C24A	C27A	119.6(4)
C26A	C25A	C24A	120.7(4)
C21A	C26A	C25A	120.6(4)
C9A	N2A	Co1	105.4(2)
C10A	N2A	Co1	106.1(3)
C10A	N2A	C9A	111.4(3)
C19A	N2A	Co1	108.4(3)
C19A	N2A	C9A	112.6(3)
C19A	N2A	C10A	112.4(3)
N2A	C9A	C8A	109.6(3)
N1	C8A	C9A	106.8(3)
N2A	C10A	C11A	110.2(4)
N3	C11A	C10A	109.6(5)
N2A	C19A	C20A	109.2(3)
N4A	C20A	C19A	107.1(3)
C2A	C1A	S1	120.5(3)

Atom	Atom	Atom	Angle/°
C2A	C1A	C6A	120.2(3)
C6A	C1A	S1	119.3(3)
C1A	C2A	C3A	119.8(4)
C4A	C3A	C2A	121.6(4)
C3A	C4A	C5A	118.5(4)
C3A	C4A	C7A	121.3(4)
C5A	C4A	C7A	120.3(4)
C6A	C5A	C4A	120.6(4)
C5A	C6A	C1A	119.3(3)
S3B	N4B	Co1	126.8(3)
C20B	N4B	Co1	113.3(3)
C20B	N4B	S3B	118.5(4)
N4B	S3B	C21B	107.17(18)
O5B	S3B	N4B	107.24(19)
O5B	S3B	C21B	105.8(2)
O6B	S3B	N4B	113.3(3)
O6B	S3B	O5B	116.3(3)
O6B	S3B	C21B	106.38(18)
C22B	C21B	S3B	123.2(3)
C26B	C21B	S3B	117.2(3)
C26B	C21B	C22B	119.4(3)
C23B	C22B	C21B	119.9(4)
C24B	C23B	C22B	121.1(4)
C23B	C24B	C25B	118.5(4)
C23B	C24B	C27B	121.4(4)
C25B	C24B	C27B	120.1(4)
C26B	C25B	C24B	120.7(4)
C21B	C26B	C25B	120.4(4)
C9B	N2B	Co1	108.2(3)
C9B	N2B	C10B	111.1(4)
C10B	N2B	Co1	107.2(3)
C19B	N2B	Co1	105.3(3)
C19B	N2B	C9B	112.5(3)
C19B	N2B	C10B	112.1(3)
N2B	C9B	C8B	110.0(3)
N1	C8B	C9B	110.8(4)
N2B	C10B	C11B	110.0(4)
C10B	C11B	N3	111.8(7)
N2B	C19B	C20B	109.4(3)
N4B	C20B	C19B	113.5(4)
C2B	C1B	S1	121.6(4)
C2B	C1B	C6B	120.4(3)
C6B	C1B	S1	118.0(3)
C1B	C2B	C3B	119.7(4)
C4B	C3B	C2B	121.6(4)
C3B	C4B	C5B	118.6(4)
C3B	C4B	C7B	121.2(4)
C5B	C4B	C7B	120.2(4)
C6B	C5B	C4B	120.6(4)
C5B	C6B	C1B	119.2(3)
C28	N5	C32	111.9(2)
C28	N5	C40	106.1(2)
C32	N5	C40	111.7(2)
C36	N5	C28	111.1(2)
C36	N5	C32	105.4(2)
C36	N5	C40	110.8(2)
C29	C28	N5	115.7(2)
C28	C29	C30	109.8(2)

Atom	Atom	Atom	Angle/°
C31	C30	C29	111.9(3)
C33	C32	N5	116.0(2)
C32	C33	C34	109.8(3)
C35	C34	C33	113.5(3)
N5	C36	C37	116.0(2)
C36	C37	C38	108.4(2)
C39	C38	C37	114.1(3)
N5	C40	C41	114.0(3)
C41B	C40	N5	118.7(4)
C40	C41	C42	111.5(4)
C43	C42	C41	111.1(5)
C40	C41B	C42B	100.9(5)
C43B	C42B	C41B	110.9(5)

Table S5: Hydrogen Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **CMW04BuCoTs**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H13	8148	4177	8088	26
H14	9818	4131	8348	28
H16	9753	3925	10176	34
H17	8081	3971	9925	28
H18A	11259	3450	9250	69
H18B	11267	3942	9901	69
H18C	11294	4527	9292	69
H22A	8402	6768	6396	39
H23A	8228	7396	5401	37
H25A	7060	5076	4634	45
H26A	7230	4450	5620	45
H27A	7222	7302	4261	51
H27B	7089	6310	3969	51
H27C	8137	6747	4158	51
H9AA	6063	8017	7999	30
H9AB	5565	7225	8313	30
H8AA	4596	7482	7316	27
H8AB	5505	7396	6995	27
H10A	7207	7193	8946	26
H10B	7894	6453	8737	26
H11A	7054	5666	9354	28
H11B	6057	6131	9027	28
H19A	7869	7654	7951	31
H19B	7111	7499	7303	31
H20A	8452	6656	7211	31
H20B	8553	6234	7898	31
H2A	3371	7020	5848	33
H3A	3593	7297	4842	36
H5A	5630	5359	5058	39
H6A	5415	5073	6071	34
H7AA	4208	6336	3886	63
H7AB	5344	6237	4130	63
H7AC	4844	7201	4137	63
H22B	7005	6736	6181	30
H23B	6968	7254	5174	30
H25B	8619	5161	4884	30
H26B	8649	4633	5888	30
H27D	7263	6276	3975	51
H27E	8389	6482	4167	51
H27F	7631	7244	4247	51
H9BA	6206	7799	7355	30
H9BB	5857	8106	7972	30
H8BA	4573	7178	7780	27
H8BB	4625	7467	7083	27
H10C	5749	6935	8720	35
H10D	6804	7325	8994	35
H11C	6462	5802	9360	31
H11D	7465	5923	9154	31

Atom	x	y	z	U_{eq}
H19C	8042	6809	8437	34
H19D	7738	7773	8124	34
H20C	7595	7231	7134	31
H20D	8545	6748	7513	31
H2B	2896	6020	5633	18
H3B	3089	6469	4647	21
H5B	5938	6794	5323	20
H6B	5755	6343	6317	18
H7BA	4132	6699	3920	37
H7BB	5267	6770	4179	37
H7BC	4598	7628	4208	37
H28A	2134	2965	7720	27
H28B	2043	3708	8231	27
H29A	2649	4148	7108	28
H29B	2388	4858	7597	28
H30A	1032	3650	6848	34
H30B	760	4307	7362	34
H31A	1370	4923	6278	53
H31B	1057	5567	6785	53
H31C	279	4933	6354	53
H3	4617	4119	8678	29
H2	3904	4689	8159	29
H33A	3597	4296	9378	41
H33B	2821	4805	8853	41
H34A	3801	5843	9562	44
H34B	4724	5481	9335	44
H35A	4200	6107	8356	62
H35B	4103	6877	8850	62
H35C	3172	6337	8497	62
H4	4668	2880	8006	26
H1	4108	3565	7495	26
H37A	3062	2477	7025	27
H37B	3353	1810	7612	27
H38A	4691	2348	6873	37
H38B	4889	1601	7410	37
H39A	3567	1393	6240	51
H39B	3740	647	6780	51
H39C	4583	896	6433	51
H40A	3029	2168	8546	38
H40B	3132	2948	9059	38
H40C	2971	2884	8983	38
H40D	3177	2115	8523	38
H41A	4869	2838	9183	44
H41B	4695	1968	8741	44
H42A	3913	1235	9496	44
H42B	5024	1436	9780	44
H43A	3500	2561	9985	81
H43B	4612	2726	10285	81
H43C	4073	1869	10490	81
H41C	4727	3006	9355	44
H41D	4788	2068	8992	44
H42C	3646	2364	9929	46
H42D	3532	1468	9511	46

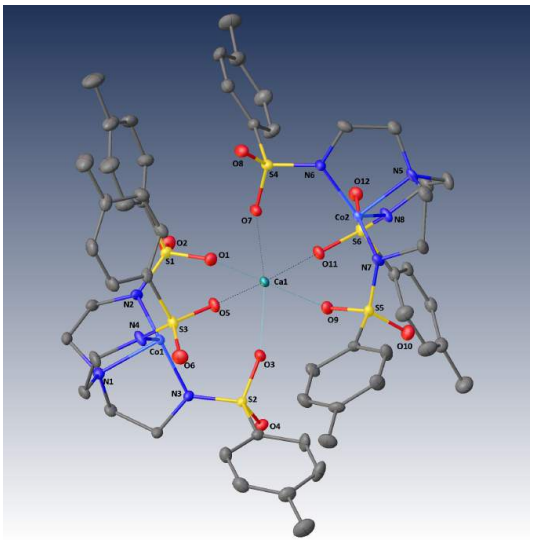
Atom	x	y	z	U_{eq}
H43D	5074	1012	9966	85
H43E	4567	1276	10525	85
H43F	5307	1958	10316	85

MW03045

EMORY UNIVERSITY | X-ray Crystallography Center

Submitted by: **Christian Wallen**
Emory University
Solved by: **Marika Wieliczko**
Sample ID: **MW03045**

Crystal Data and Experimental



Experimental. Single clear bluish violet hexagonal-shaped crystals of (**MW03045**) were recrystallised from toluene by slow evaporation. A suitable crystal (0.33×0.28×0.07) was selected and mounted on a loop with paratone oil on a Bruker APEX-II CCD diffractometer. The crystal was cooled to T = 109.01 K during data collection. The structure was solved with the **Superflip** (L. Palatinus & G. Chapuis, 2007) structure solution program using charge flipping methods and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The crystal structure was refined with version of **XL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{54}H_{66}CaCo_2N_8O_{12}S_6$, M_r = 1369.44, monoclinic, $P2_1$ (No. 4), a = 13.9236(11) Å, b = 13.3642(10) Å, c = 17.2950(13) Å, β = 112.3550(10)°, α = γ = 90°, V = 2976.3(4) Å^3, T = 109.01 K, Z = 2, Z' = 1, μ(MoK$_\alpha$) = 0.921, 22136 reflections measured, 14778 unique (R_{int} = 0.0328) which were used in all calculations. The final wR_2 was 0.1150 (all data) and R_1 was 0.0476 (I > 2(I)).

Compound	**MW03045**
Formula	$C_{54}H_{66}CaCo_2N_8O_{12}S_6$
$D_{calc.}$/ g cm^{-3}	1.528
μ/mm^{-1}	0.921
Formula Weight	1369.44
Colour	clear bluish violet
Shape	hexagonal
Max Size/mm	0.33
Mid Size/mm	0.28
Min Size/mm	0.07
T/K	109.01
Crystal System	monoclinic
Flack Parameter	0.202(8)
Hooft Parameter	0.200(8)
Space Group	$P2_1$
a/Å	13.9236(11)
b/Å	13.3642(10)
c/Å	17.2950(13)
α/°	90
β/°	112.3550(10)
γ/°	90
V/Å^3	2976.3(4)
Z	2
Z'	1
Θ_{min}/°	1.581
Θ_{max}/°	29.216
Measured Refl.	22136
Independent Refl.	14778
$I > 2\sigma(I)$	13032
R_{int}	0.0328
Parameters	754
Restraints	1
Largest Peak	1.052
Deepest Hole	-0.448
GooF	1.009
wR_2 (all data)	0.1150
wR_2	0.1096
R_1 (all data)	0.0561
R_1	0.0476
CCDC #	1434437

Structure Quality Indicators

Reflections:	d min 0.73	I/σ 10.9	Rint 3.28%	complete 91%
Refinement:	Shift -0.001	Max Peak 1.1	Min Peak -0.5	GooF 1.009

A clear bluish violet hexagonal-shaped crystal with dimensions 0.33×0.28×0.07 mm was mounted on a loop with paratone oil.X-ray diffraction data were collected using a Bruker APEX-II CCD diffractometer equipped with an Oxford low-temperature apparatus operating at T = 109.01 K.

Data were measured using ϕ using MoK$_\alpha$ radiation (fine-focus sealed tube, 45 kV, 35 mA). The total number of runs and images was based on the strategy calculation from the program **APEX2** (Bruker, 2014). The maximum resolution achieved was Θ = 29.216°.

Unit cell indexing was performed by using the **APEX2** (Bruker, 2014) software and refined using **SAINT** (Bruker, V8.27A, 2012) on 7388 reflections, 33% of the observed reflections. Data reduction, scaling and absorption corrections were performed using **SAINT** (Bruker, V8.27A, 2012) and **SADABS-2012/1** (Bruker, 2012) was used for absorption correction.wR_2(int) was 0.0641 before and 0.0505 after correction.The Ratio of minimum to maximum transmission is 0.7802.The $\lambda/2$ correction factor is 0.0015. software which corrects for Lorentz polarisation. The final completeness is 100.00% out to 29.216 in Θ. The absorption coefficient (μ) of this material is 0.921 mm^{-1} and the minimum and maximum transmissions are 0.5819 and 0.7458.

The structure was solved in the space group P1 with the **Superflip** (L. Palatinus & G. Chapuis, 2007) structure solution program using using charge flipping methods. The space group P2$_1$ (# 4) was determined by the**Superflip** (L. Palatinus & G. Chapuis, 2007) structure solution program.The crystal structure was refined by Least Squares using version of **XL** (Sheldrick, 2008). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.?

There are two independent molecules in the asymmetric unit.

The Flack parameter was refined to 0.202(8). Determination of absolute structure using Bayesian statistics on Bijvoet differences using the Olex2 results in 0.200(8). Note: The Flack parameter is used to determine chirality of the crystal studied, the value should be near 0, a value of 1 means that the stereochemistry is wrong and the model should be inverted. A value of 0.5 means that the crystal consists of a racemic mixture of the two enantiomers.

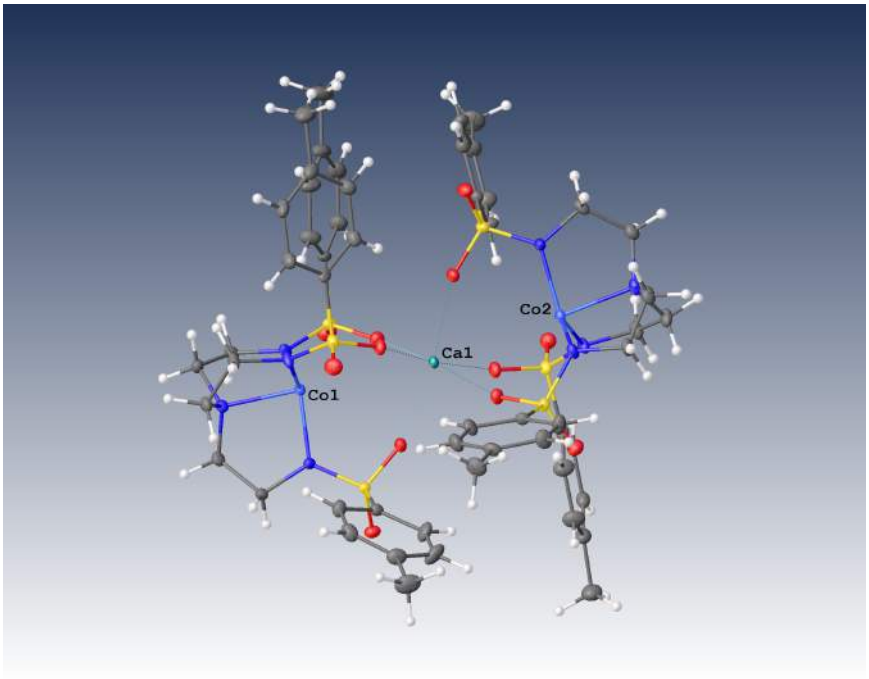


Figure S9:

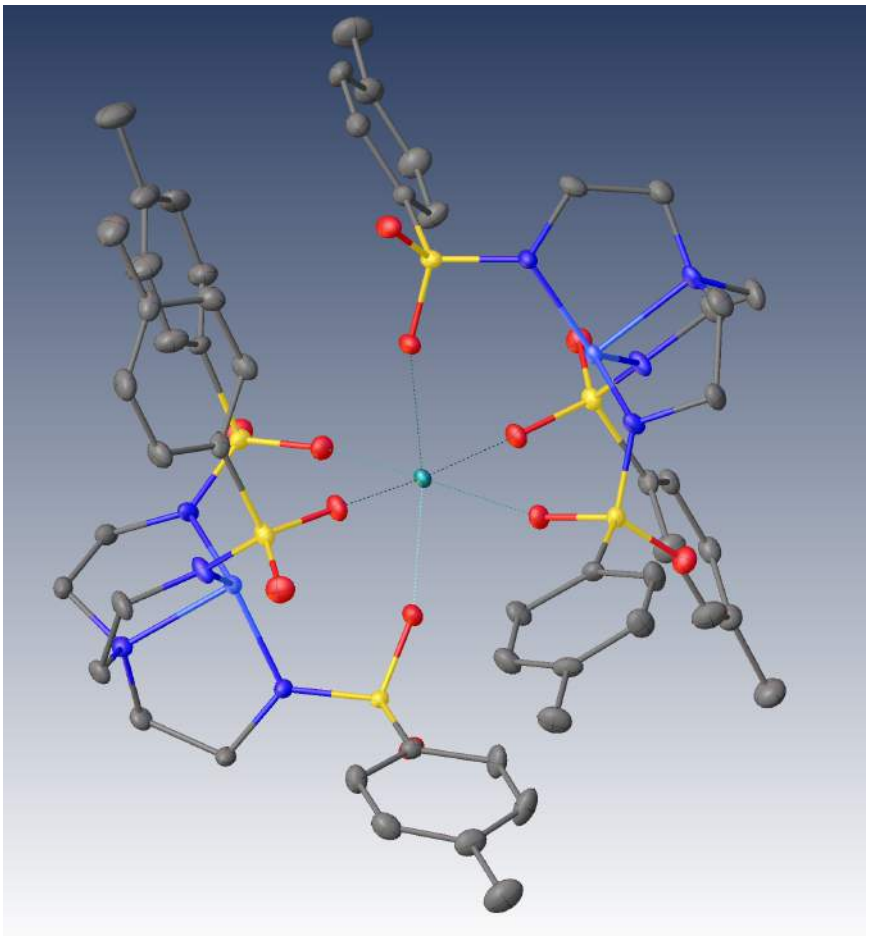


Figure S10:

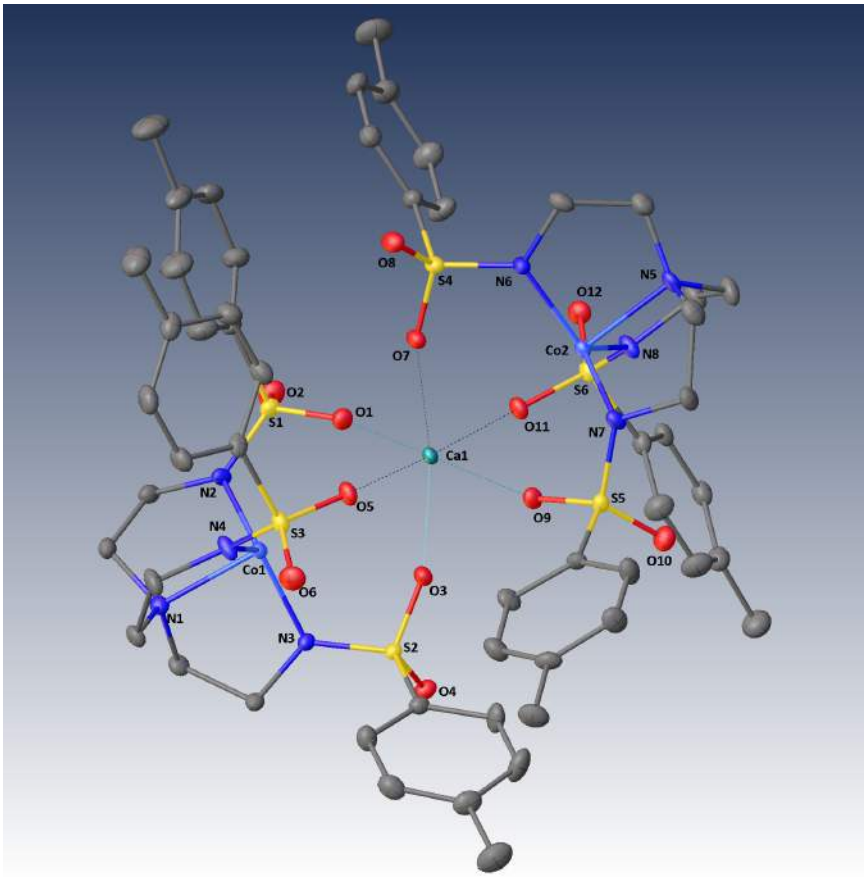
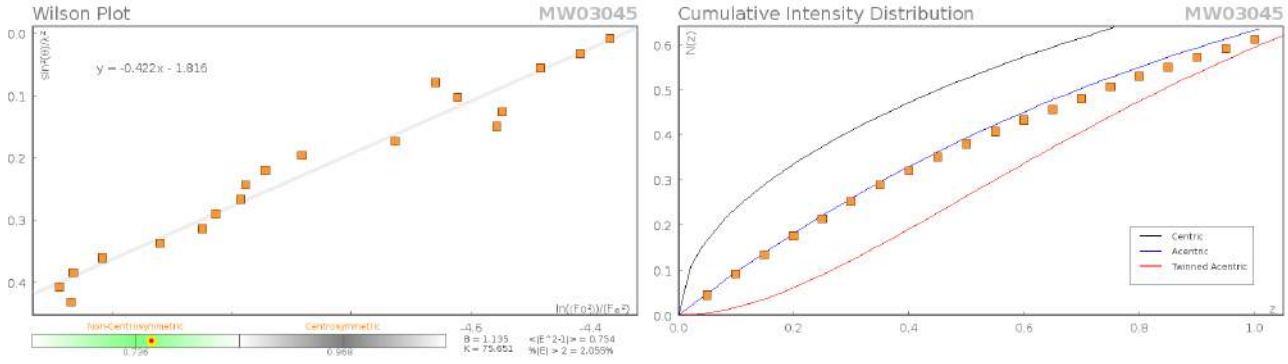
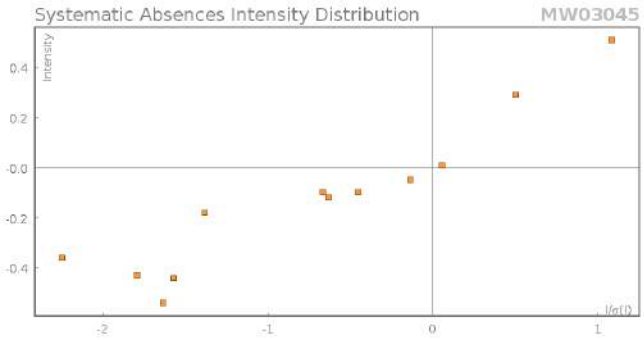
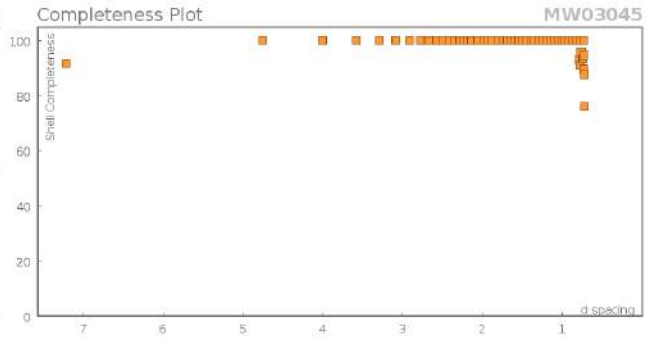


Figure S11:

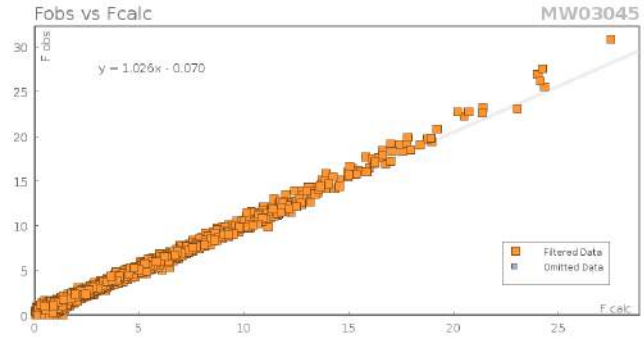
Data Plots: Diffraction Data

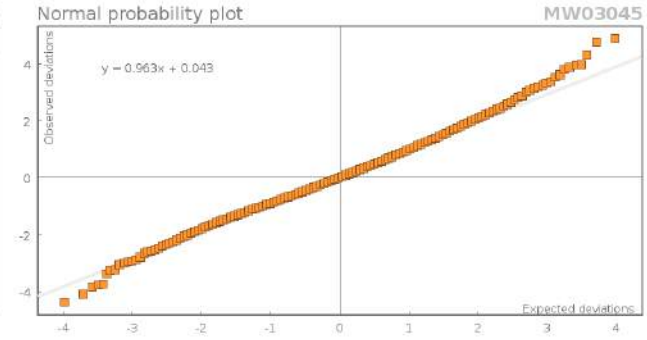






Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	22148	Unique reflections	14778
Completeness	0.914	Mean I/σ	10.93
hklsub>max</sub> collected	(19, 17, 23)	hklsub>min</sub> collected	(-19, -18, -23)
hkl_{max} used	(17, 17, 23)	hkl_{min} used	(-19, -18, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.36
d_{max} used	12.88	d_{min} used	0.73
Friedel pairs	6633	Friedel pairs merged	0
Inconsistent equivalents	2	R_{int}	0.0328
R_{sigma}	0.0676	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	0
Multiplicity	(20902, 620, 2)	Maximum multiplicity	4
Removed systematic absences	12	Filtered off (Shel/OMIT)	0

Images of the Crystal on the Diffractometer

Table S7: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **MW03045**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Co1	9157.2(4)	6608.7(5)	4462.4(4)	12.76(13)
Co2	5726.5(5)	4656.6(4)	649.4(4)	13.25(13)
Ca1	7590.4(7)	5412.6(7)	2585.5(5)	12.63(18)
S2	10457.8(8)	5666.3(8)	3586.5(7)	13.6(2)
S1	7741.0(9)	5054.3(9)	4769.4(7)	16.0(2)
S5	7471.4(9)	5570.9(9)	380.8(7)	14.9(2)
S6	6832.9(9)	2847.4(9)	1739.2(7)	16.1(2)
S4	4695.6(8)	5682.4(9)	1717.3(7)	16.0(2)
S3	7974.4(9)	8163.1(9)	3149.0(7)	16.1(2)
O4	11221(3)	4884(3)	3765(2)	19.6(7)
O11	7267(3)	3732(3)	2257(2)	19.2(7)
O7	5823(3)	5739(3)	2180(2)	19.3(7)
O3	9385(3)	5344(3)	3129(2)	19.2(7)
O10	8025(3)	4859(3)	85(2)	23.6(8)
O9	7701(3)	5552(3)	1281.8(19)	18.4(7)
O12	6338(3)	2127(3)	2090(2)	22.0(7)
O8	4138(3)	6608(3)	1636(2)	22.0(7)
O2	7937(3)	4140(3)	5246(2)	26.3(8)
O6	8415(3)	8874(3)	2754(2)	25.2(8)
O1	7633(3)	4966(3)	3896(2)	20.7(7)
O5	7705(3)	7182(3)	2743(2)	20.2(7)
N3	10447(3)	6226(3)	4374(2)	15.1(8)
N4	8676(3)	7930(3)	4082(3)	19.5(9)
N8	6115(3)	3265(3)	859(3)	18.3(8)
N2	8573(3)	5896(3)	5140(2)	17.6(8)
N7	6251(3)	5477(3)	-45(2)	18.0(8)
N1	10081(3)	7282(3)	5569(2)	16.2(8)
N5	4605(3)	4152(3)	-454(3)	17.3(8)
N6	4564(3)	5164(3)	874(2)	17.7(8)
C48	7910(4)	2223(4)	1646(3)	18.4(10)
C12	10752(3)	6511(4)	2918(3)	16.6(9)
C30	4209(4)	4852(4)	2280(3)	18(1)
C49	8129(4)	1244(4)	1910(3)	18.5(9)
C3	6523(3)	5508(4)	4724(3)	18.8(10)
C21	6802(4)	8713(4)	3120(3)	18.1(10)
C1	9544(4)	7144(4)	6152(3)	19.3(10)
C2	9045(4)	6101(4)	6043(3)	21.1(10)
C11	11392(3)	6535(4)	5076(3)	17.0(9)
C54	8536(4)	2747(4)	1321(4)	28.3(12)
C50	9009(4)	796(4)	1873(3)	20.5(10)
C42	8654(4)	8545(4)	-174(3)	21.5(10)
C45	8448(4)	7396(4)	831(3)	21.3(10)
C24	4973(4)	9625(4)	3063(3)	25.6(11)
C10	11093(4)	6757(4)	5829(3)	19(1)
C33	3375(4)	3511(5)	3081(4)	30.6(13)
C39	7881(3)	6758(3)	185(3)	15.3(9)
C14	11351(4)	8085(4)	2615(3)	25.6(11)
C51	9665(4)	1295(4)	1579(3)	24.6(11)
C46	4930(4)	3142(4)	-595(3)	26.9(12)
C19	10155(4)	8347(4)	5348(3)	19.1(10)
C17	11094(5)	6719(4)	1670(4)	32.5(13)
C38	5740(4)	5224(4)	-934(3)	21.3(10)
C41	8059(4)	7918(4)	-814(3)	27.6(12)
C29	3539(4)	5026(4)	211(3)	22(1)
C47	5416(4)	2568(4)	231(3)	23.5(11)
C43	9082(4)	9509(4)	-371(4)	30.0(12)
C40	7685(4)	7026(4)	-646(3)	27.0(12)

Atom	x	y	z	U_{eq}
C22	6799(4)	9723(4)	3313(3)	23.4(10)
C26	4994(4)	8608(4)	2861(4)	27.5(12)
C18	10772(5)	6128(4)	2172(3)	25.6(11)
C53	9406(5)	2287(5)	1291(4)	31.9(13)
C23	5888(4)	10160(4)	3287(3)	27.2(12)
C27	5898(4)	8154(4)	2900(3)	22.5(10)
C13	11011(4)	7500(4)	3130(3)	22.4(10)
C20	9128(4)	8733(4)	4698(3)	22.8(11)
C28	3605(4)	4157(4)	-336(3)	24.0(11)
C36	3362(4)	5126(4)	2466(3)	24.7(11)
C15	11423(4)	7695(4)	1895(4)	27.3(12)
C31	4653(4)	3905(4)	2500(4)	29.2(12)
C16	11826(5)	8311(5)	1347(4)	40.2(16)
C32	4227(5)	3249(5)	2895(4)	33.8(13)
C35	2963(4)	4457(4)	2866(3)	28.5(12)
C44	8830(4)	8277(4)	642(3)	25.9(11)
C9	5812(4)	4856(5)	4833(4)	29.9(12)
C37	4623(4)	4899(4)	-1090(3)	25.8(11)
C25	3970(5)	10108(5)	3012(4)	38.9(15)
C6	4590(4)	6210(6)	4573(4)	36.5(15)
C4	6266(4)	6496(5)	4531(4)	30.0(12)
C8	4847(4)	5212(5)	4751(4)	35.6(14)
C5	5301(5)	6836(5)	4454(4)	38.8(15)
C7	3536(5)	6583(8)	4487(5)	58(2)
C52	10646(5)	826(5)	1572(4)	33.3(13)
C34	2892(6)	2771(6)	3487(5)	46.8(17)

Table S8: Anisotropic Displacement Parameters (×10^4) **MW03045**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	12.2(3)	12.9(3)	11.7(3)	-0.2(2)	2.9(2)	0.6(2)
Co2	14.5(3)	10.3(3)	13.0(3)	-0.5(2)	3.1(2)	-1.2(2)
Ca1	13.1(4)	11.9(4)	11.5(4)	-1.3(3)	3.1(3)	-1.3(3)
S2	12.3(5)	15.0(5)	13.9(5)	0.3(4)	5.3(4)	0.4(4)
S1	15.9(5)	18.6(6)	14.4(5)	2.6(4)	6.6(4)	0.8(4)
S5	18.0(5)	13.8(6)	13.3(5)	0.1(4)	6.4(4)	-1.0(4)
S6	18.2(5)	10.3(5)	17.7(6)	-0.5(4)	4.3(4)	0.2(4)
S4	12.7(5)	14.6(6)	20.2(5)	-1.6(4)	5.8(4)	0.1(4)
S3	18.6(5)	11.3(5)	15.0(5)	-0.2(4)	2.4(4)	0.3(4)
O4	18.7(16)	20.1(19)	22.2(17)	3.2(14)	10.4(14)	3.3(14)
O11	21.4(17)	14.0(17)	19.5(17)	-2.9(14)	4.9(14)	-2.2(14)
O7	16.2(15)	18.5(17)	21.4(17)	-4.7(14)	5.2(13)	-2.3(14)
O3	17.9(16)	20.3(18)	18.3(16)	-4.8(14)	5.7(13)	-3.3(14)
O10	27.3(18)	20(2)	23.5(18)	1.1(15)	10.1(15)	4.5(15)
O9	22.4(16)	18.7(18)	13.7(15)	1.3(14)	6.2(13)	-2.5(14)
O12	25.1(18)	16.2(18)	24.6(19)	1.4(14)	9.5(15)	-0.9(14)
O8	18.6(16)	17.3(17)	29.3(19)	-2.0(16)	8.3(14)	0.5(14)
O2	32(2)	24(2)	26(2)	8.5(16)	14.7(17)	4.0(16)
O6	28.7(19)	16.0(18)	31(2)	4.0(15)	11.5(17)	-0.8(15)
O1	22.1(17)	23.1(19)	17.8(17)	1.1(14)	8.6(14)	-1.8(14)
O5	23.1(17)	14.7(17)	19.5(18)	-3.3(13)	4.5(14)	-0.7(14)
N3	12.7(17)	20(2)	12.2(18)	0.2(15)	4.2(15)	1.8(15)
N4	21(2)	12(2)	16.3(19)	-1.6(16)	-3.6(16)	2.3(16)
N8	18.3(19)	9.7(19)	19(2)	-0.9(16)	-1.7(16)	1.2(15)
N2	15.0(18)	26(2)	11.3(18)	0.9(16)	4.3(15)	-4.8(16)
N7	17.7(19)	20(2)	13.4(18)	0.5(16)	2.6(15)	-5.5(16)
N1	14.6(18)	17(2)	15.3(19)	0.3(16)	3.4(15)	1.9(15)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N5	21(2)	11.3(19)	15.7(19)	-1.7(15)	2.5(16)	-5.2(16)
N6	12.5(18)	21(2)	18(2)	-5.6(17)	4.2(15)	-1.4(15)
C48	21(2)	14(2)	18(2)	-0.3(18)	4.2(19)	5.0(18)
C12	14(2)	19(2)	16(2)	3.5(19)	5.3(17)	1.1(18)
C30	17(2)	18(3)	19(2)	-0.6(18)	7.0(18)	-1.7(18)
C49	23(2)	15(2)	14(2)	-1.3(18)	3.1(18)	-1.7(19)
C3	13(2)	28(3)	17(2)	-2(2)	6.9(17)	2.2(19)
C21	22(2)	17(2)	11(2)	3.0(18)	2.2(18)	7.4(19)
C1	19(2)	23(3)	16(2)	-3.9(19)	6.0(19)	1.0(19)
C2	16(2)	32(3)	15(2)	1(2)	6.2(19)	-1(2)
C11	13(2)	21(2)	15(2)	-0.2(19)	4.2(17)	2.2(18)
C54	33(3)	21(3)	34(3)	11(2)	17(2)	6(2)
C50	24(2)	14(2)	18(2)	0.5(18)	2.1(19)	3.1(19)
C42	16(2)	17(2)	31(3)	7(2)	10(2)	-0.6(19)
C45	20(2)	23(3)	15(2)	4(2)	0.1(19)	-1(2)
C24	30(3)	26(3)	18(2)	2(2)	6(2)	10(2)
C10	18(2)	21(3)	14(2)	2.0(19)	1.1(17)	1.9(19)
C33	30(3)	35(3)	30(3)	2(2)	15(2)	-6(2)
C39	16(2)	13(2)	19(2)	2.1(17)	8.0(17)	-1.1(17)
C14	26(3)	18(3)	26(3)	5(2)	3(2)	-1(2)
C51	24(3)	23(3)	24(3)	0(2)	6(2)	6(2)
C46	31(3)	19(3)	22(3)	-7(2)	0(2)	4(2)
C19	20(2)	13(2)	20(2)	-3.7(19)	3.0(19)	-2.2(18)
C17	53(4)	26(3)	29(3)	5(2)	29(3)	10(3)
C38	27(2)	23(3)	12(2)	-1.0(19)	4.7(19)	-5(2)
C41	33(3)	29(3)	20(3)	6(2)	10(2)	-5(2)
C29	15(2)	20(2)	24(3)	2(2)	0.8(19)	-2.6(19)
C47	25(3)	16(3)	22(3)	-2(2)	1(2)	-2(2)
C43	29(3)	21(3)	38(3)	7(2)	11(2)	-5(2)
C40	36(3)	26(3)	20(3)	-3(2)	12(2)	-8(2)
C22	24(2)	15(2)	25(3)	-2(2)	3(2)	-1(2)
C26	23(3)	26(3)	31(3)	0(2)	7(2)	-2(2)
C18	41(3)	15(2)	24(3)	-3(2)	16(2)	2(2)
C53	32(3)	30(3)	39(3)	12(3)	20(3)	2(2)
C23	35(3)	19(3)	23(3)	-4(2)	5(2)	5(2)
C27	24(2)	16(2)	23(3)	1(2)	4(2)	0(2)
C13	28(3)	19(3)	18(2)	-0.1(19)	7(2)	1(2)
C20	25(3)	16(2)	19(2)	-5(2)	-1(2)	3(2)
C28	20(2)	25(3)	21(3)	0(2)	2(2)	1(2)
C36	22(2)	28(3)	22(3)	-2(2)	6(2)	1(2)
C15	27(3)	27(3)	29(3)	12(2)	13(2)	5(2)
C31	30(3)	23(3)	43(3)	4(2)	23(3)	4(2)
C16	47(4)	35(4)	49(4)	18(3)	30(3)	7(3)
C32	38(3)	26(3)	43(3)	8(3)	21(3)	5(3)
C35	27(3)	36(3)	27(3)	-6(2)	17(2)	-4(2)
C44	24(3)	23(3)	25(3)	-1(2)	2(2)	-5(2)
C9	24(3)	35(3)	33(3)	-2(2)	13(2)	-3(2)
C37	28(3)	23(3)	19(2)	4(2)	0(2)	0(2)
C25	34(3)	43(4)	39(3)	2(3)	13(3)	14(3)
C6	20(3)	62(4)	26(3)	0(3)	7(2)	9(3)
C4	24(3)	32(3)	38(3)	10(3)	15(2)	3(2)
C8	26(3)	49(4)	36(3)	-6(3)	18(3)	-14(3)
C5	29(3)	44(4)	44(4)	8(3)	15(3)	13(3)
C7	25(3)	99(7)	52(4)	3(5)	17(3)	10(4)
C52	31(3)	32(3)	38(3)	5(3)	14(3)	9(3)
C34	45(4)	52(4)	53(4)	14(4)	30(3)	-7(3)

Table S9: Bond Lengths in Å for **MW03045**.

Atom	Atom	Length/Å
Co1	Ca1	3.5305(11)
Co1	N3	1.928(4)
Co1	N4	1.915(4)
Co1	N2	1.914(4)
Co1	N1	2.063(4)
Co2	Ca1	3.5155(10)
Co2	N8	1.933(4)
Co2	N7	1.961(4)
Co2	N5	2.066(4)
Co2	N6	1.925(4)
Ca1	O11	2.318(3)
Ca1	O7	2.329(3)
Ca1	O3	2.313(3)
Ca1	O9	2.325(3)
Ca1	O1	2.323(3)
Ca1	O5	2.379(4)
S2	O4	1.438(3)
S2	O3	1.464(3)
S2	N3	1.560(4)
S2	C12	1.772(5)
S1	O2	1.441(4)
S1	O1	1.465(4)
S1	N2	1.566(4)
S1	C3	1.774(5)
S5	O10	1.436(4)
S5	O9	1.467(3)
S5	N7	1.579(4)
S5	C39	1.762(5)
S6	O11	1.467(4)
S6	O12	1.445(4)
S6	N8	1.571(4)
S6	C48	1.776(5)
S4	O7	1.468(3)
S4	O8	1.439(4)
S4	N6	1.562(4)
S4	C30	1.771(5)
S3	O6	1.438(4)
S3	O5	1.467(4)
S3	N4	1.567(4)
S3	C21	1.774(5)
N3	C11	1.470(6)
N4	C20	1.475(6)
N8	C47	1.480(6)
N2	C2	1.472(6)
N7	C38	1.467(6)
N1	C1	1.478(6)
N1	C10	1.483(6)
N1	C19	1.487(6)
N5	C46	1.473(7)
N5	C28	1.482(6)
N5	C37	1.493(6)
N6	C29	1.463(6)
C48	C49	1.382(7)
C48	C54	1.393(7)
C12	C18	1.398(7)
C12	C13	1.382(7)
C30	C36	1.384(7)
C30	C31	1.397(7)
C49	C50	1.387(7)
C3	C9	1.385(7)
C3	C4	1.375(8)
C21	C22	1.391(7)
C21	C27	1.386(7)
C1	C2	1.538(7)
C11	C10	1.540(6)
C54	C53	1.376(8)
C50	C51	1.375(7)
C42	C41	1.384(8)
C42	C43	1.512(7)
C42	C44	1.383(7)
C45	C39	1.388(7)
C45	C44	1.381(7)
C24	C26	1.406(8)
C24	C23	1.382(8)
C24	C25	1.510(8)
C33	C32	1.388(8)
C33	C35	1.380(8)
C33	C34	1.509(8)
C39	C40	1.402(7)
C14	C13	1.397(7)
C14	C15	1.389(8)
C51	C53	1.414(8)
C51	C52	1.507(7)
C46	C47	1.534(7)
C19	C20	1.534(7)
C17	C18	1.369(8)
C17	C15	1.389(9)
C38	C37	1.536(7)
C41	C40	1.376(8)
C29	C28	1.522(8)
C22	C23	1.382(7)
C26	C27	1.376(7)
C36	C35	1.372(8)
C15	C16	1.514(8)
C31	C32	1.377(8)
C9	C8	1.381(8)
C6	C8	1.384(10)
C6	C5	1.369(9)
C6	C7	1.504(8)
C4	C5	1.376(8)

Table S10: Bond Angles in ° for **MW03045**.

Atom	Atom	Atom	Angle/°
N3	Co1	Ca1	94.34(12)
N3	Co1	N1	85.30(16)

Atom	Atom	Atom	Angle/°
N4	Co1	Ca1	95.07(12)
N4	Co1	N3	115.59(18)
N4	Co1	N1	85.98(17)
N2	Co1	Ca1	94.57(12)
N2	Co1	N3	122.81(18)
N2	Co1	N4	119.65(19)
N2	Co1	N1	84.81(16)
N1	Co1	Ca1	178.95(12)
N8	Co2	Ca1	92.59(12)
N8	Co2	N7	120.67(18)
N8	Co2	N5	85.32(16)
N7	Co2	Ca1	96.35(11)
N7	Co2	N5	86.78(16)
N5	Co2	Ca1	176.83(11)
N6	Co2	Ca1	94.55(12)
N6	Co2	N8	119.87(18)
N6	Co2	N7	117.65(18)
N6	Co2	N5	84.45(17)
O11	Ca1	O7	91.35(12)
O11	Ca1	O9	85.27(12)
O11	Ca1	O1	85.48(13)
O11	Ca1	O5	171.65(13)
O7	Ca1	O5	82.27(12)
O3	Ca1	O11	98.04(13)
O3	Ca1	O7	169.82(13)
O3	Ca1	O9	86.41(12)
O3	Ca1	O1	88.30(12)
O3	Ca1	O5	88.73(12)
O9	Ca1	O7	98.34(12)
O9	Ca1	O5	90.30(12)
O1	Ca1	O7	88.53(12)
O1	Ca1	O9	168.60(13)
O1	Ca1	O5	99.67(13)
O4	S2	O3	114.9(2)
O4	S2	N3	114.4(2)
O4	S2	C12	105.6(2)
O3	S2	N3	105.5(2)
O3	S2	C12	106.0(2)
N3	S2	C12	110.2(2)
O2	S1	O1	116.4(2)
O2	S1	N2	115.2(2)
O2	S1	C3	106.6(2)
O1	S1	N2	104.4(2)
O1	S1	C3	105.1(2)
N2	S1	C3	108.5(2)
O10	S5	O9	115.9(2)
O10	S5	N7	114.2(2)
O10	S5	C39	105.7(2)
O9	S5	N7	104.8(2)
O9	S5	C39	105.3(2)
N7	S5	C39	110.6(2)
O11	S6	N8	105.5(2)
O11	S6	C48	105.5(2)
O12	S6	O11	115.7(2)
O12	S6	N8	114.4(2)
O12	S6	C48	106.2(2)
N8	S6	C48	109.0(2)
O7	S4	N6	104.6(2)

Atom	Atom	Atom	Angle/°
O7	S4	C30	106.6(2)
O8	S4	O7	115.7(2)
O8	S4	N6	115.0(2)
O8	S4	C30	106.7(2)
N6	S4	C30	107.6(2)
O6	S3	O5	116.2(2)
O6	S3	N4	114.2(2)
O6	S3	C21	105.5(2)
O5	S3	N4	105.1(2)
O5	S3	C21	107.0(2)
N4	S3	C21	108.5(2)
S6	O11	Ca1	157.9(2)
S4	O7	Ca1	160.5(2)
S2	O3	Ca1	158.5(2)
S5	O9	Ca1	164.4(2)
S1	O1	Ca1	160.1(2)
S3	O5	Ca1	159.6(2)
S2	N3	Co1	121.0(2)
C11	N3	Co1	115.4(3)
C11	N3	S2	123.6(3)
S3	N4	Co1	122.5(2)
C20	N4	Co1	115.2(3)
C20	N4	S3	121.8(3)
S6	N8	Co2	123.6(2)
C47	N8	Co2	114.1(3)
C47	N8	S6	119.1(3)
S1	N2	Co1	121.8(2)
C2	N2	Co1	115.8(3)
C2	N2	S1	122.0(3)
S5	N7	Co2	110.1(2)
C38	N7	Co2	111.5(3)
C38	N7	S5	121.0(3)
C1	N1	Co1	106.2(3)
C1	N1	C10	113.8(4)
C1	N1	C19	113.4(4)
C10	N1	Co1	105.1(3)
C10	N1	C19	112.3(4)
C19	N1	Co1	105.0(3)
C46	N5	Co2	106.3(3)
C46	N5	C28	113.0(4)
C46	N5	C37	113.5(4)
C28	N5	Co2	106.9(3)
C28	N5	C37	112.2(4)
C37	N5	Co2	104.1(3)
S4	N6	Co2	122.4(2)
C29	N6	Co2	116.2(3)
C29	N6	S4	121.4(3)
C49	C48	S6	120.2(4)
C49	C48	C54	121.1(5)
C54	C48	S6	118.7(4)
C18	C12	S2	117.4(4)
C13	C12	S2	122.5(4)
C13	C12	C18	120.0(5)
C36	C30	S4	120.0(4)
C36	C30	C31	120.2(5)
C31	C30	S4	119.7(4)
C48	C49	C50	118.8(5)
C9	C3	S1	120.0(4)

Atom	Atom	Atom	Angle/°
C4	C3	S1	119.7(4)
C4	C3	C9	120.2(5)
C22	C21	S3	118.8(4)
C27	C21	S3	120.9(4)
C27	C21	C22	120.3(5)
N1	C1	C2	110.6(4)
N2	C2	C1	107.3(4)
N3	C11	C10	107.9(4)
C53	C54	C48	119.1(5)
C51	C50	C49	122.0(5)
C41	C42	C43	120.1(5)
C44	C42	C41	118.6(5)
C44	C42	C43	121.3(5)
C44	C45	C39	119.0(5)
C26	C24	C25	120.4(5)
C23	C24	C26	117.7(5)
C23	C24	C25	121.9(5)
N1	C10	C11	111.5(4)
C32	C33	C34	120.9(6)
C35	C33	C32	118.2(5)
C35	C33	C34	120.8(5)
C45	C39	S5	121.7(4)
C45	C39	C40	119.8(4)
C40	C39	S5	118.4(4)
C15	C14	C13	121.3(5)
C50	C51	C53	118.0(5)
C50	C51	C52	122.2(5)
C53	C51	C52	119.8(5)
N5	C46	C47	111.0(4)
N1	C19	C20	112.0(4)
C18	C17	C15	121.1(5)

Atom	Atom	Atom	Angle/°
N7	C38	C37	107.8(4)
C40	C41	C42	121.0(5)
N6	C29	C28	108.2(4)
N8	C47	C46	107.6(4)
C41	C40	C39	119.7(5)
C23	C22	C21	119.2(5)
C27	C26	C24	121.3(5)
C17	C18	C12	120.0(5)
C54	C53	C51	121.0(5)
C24	C23	C22	121.9(5)
C26	C27	C21	119.6(5)
C12	C13	C14	118.9(5)
N4	C20	C19	107.9(4)
N5	C28	C29	111.8(4)
C35	C36	C30	119.3(5)
C14	C15	C17	118.3(5)
C14	C15	C16	121.8(6)
C17	C15	C16	119.8(5)
C32	C31	C30	118.9(5)
C31	C32	C33	121.4(6)
C36	C35	C33	121.8(5)
C45	C44	C42	121.8(5)
C8	C9	C3	119.1(6)
N5	C37	C38	111.1(4)
C8	C6	C7	120.1(7)
C5	C6	C8	118.8(5)
C5	C6	C7	121.1(7)
C3	C4	C5	119.7(5)
C9	C8	C6	120.9(5)
C6	C5	C4	121.2(6)

Table S11: Hydrogen Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **MW03045**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H49	7685	884	2114	22
H1A	9000	7663	6045	23
H1B	10047	7224	6734	23
H2A	9578	5590	6327	25
H2B	8509	6085	6289	25
H11A	11691	7140	4924	20
H11B	11918	5994	5217	20
H54	8366	3412	1123	34
H50	9164	123	2057	25
H45	8572	7229	1394	26
H10A	11053	6121	6109	23
H10B	11639	7176	6237	23
H14	11536	8764	2760	31
H46A	5441	3196	-864	32
H46B	4320	2769	-977	32
H19A	10709	8415	5124	23
H19B	10351	8762	5859	23
H17	11092	6456	1159	39
H38A	6117	4674	-1079	26
H38B	5734	5813	-1283	26
H41	7908	8106	-1378	33

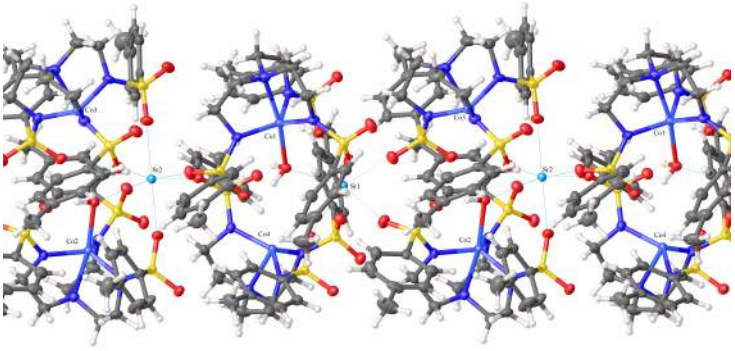
Atom	x	y	z	U_{eq}
H29A	3325	5643	-128	26
H29B	3019	4878	458	26
H47A	4867	2322	416	28
H47B	5813	1985	158	28
H43A	9810	9412	-295	45
H43B	9035	10039	5	45
H43C	8679	9701	-952	45
H40	7295	6593	-1090	32
H22	7417	10108	3461	28
H26	4372	8227	2695	33
H18	10562	5457	2014	31
H53	9839	2642	1073	38
H23	5891	10847	3427	33
H27	5903	7462	2776	27
H13	10958	7777	3618	27
H20A	8646	8914	4973	27
H20B	9254	9336	4417	27
H28A	3527	3519	-75	29
H28B	3026	4207	-889	29
H36	3061	5771	2318	30
H31	5239	3717	2379	35
H16A	11321	8295	769	60
H16B	12488	8034	1371	60
H16C	11929	9005	1546	60
H32	4524	2602	3043	41
H35	2387	4650	2999	34
H44	9224	8711	1084	31
H9	5986	4172	4963	36
H37A	4209	5493	-1067	31
H37B	4303	4603	-1655	31
H25A	3602	10371	2447	58
H25B	4123	10657	3417	58
H25C	3535	9610	3139	58
H4	6752	6941	4452	36
H8	4353	4767	4818	43
H5	5124	7517	4316	47
H7A	3078	6012	4449	87
H7B	3241	6992	3981	87
H7C	3600	6988	4977	87
H52A	11248	1125	2015	50
H52B	10694	944	1029	50
H52C	10633	104	1668	50
H34A	2323	2418	3053	70
H34B	2622	3128	3856	70
H34C	3419	2286	3813	70

CMW-03-086SRTS

EMORY UNIVERSITY | X-ray Crystallography Center

Submitted by: **Christian Wallen**
Emory University
Solved by:
Sample ID: **CMW-030086SRTS**

Crystal Data and Experimental



Experimental. Single violet plate-shaped crystals of (**CMW-03-086SRTS**) were recrystallised from a mixture of CH_2Cl_2 and methanol by vapor diffusion. A suitable crystal (0.92×0.28×0.10 mm) was selected and mounted on a loop with paratone oil on a Bruker APEX-II CCD diffractometer. The crystal was cooled to T = 100(2) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program using combined Patterson and dual-space recycling methods and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The crystal structure was refined with version of **ShelXL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{108}H_{138}Co_4N_{16}O_{27}S_{12}Sr_2$, M_r = 2888.02, monoclinic, $P2_1/c$ (No. 14), a = 29.583(7) Å, b = 16.185(4) Å, c = 25.822(6) Å, β = 95.585(4)°, α = γ = 90°, V = 12305(5) Å^3, T = 100(2) K, Z = 4, Z' = 1, μ(MoK$_\alpha$) = 1.669, 97100 reflections measured, 32412 unique (R_{int} = 0.0842) which were used in all calculations. The final wR_2 was 0.1594 (all data) and R_1 was 0.0630 (I > 2σ(I)).

Compound	**CMW-03-086SRTS**
Formula	$C_{108}H_{138}Co_4N_{16}O_{27}S_{12}Sr_2$
$D_{calc.}$/ g cm^{-3}	1.559
μ/mm^{-1}	1.669
Formula Weight	2888.02
Colour	violet
Shape	plate
Max Size/mm	0.92
Mid Size/mm	0.28
Min Size/mm	0.10
T/K	100(2)
Crystal System	monoclinic
Space Group	$P2_1/c$
a/Å	29.583(7)
b/Å	16.185(4)
c/Å	25.822(6)
α/°	90
β/°	95.585(4)
γ/°	90
V/Å^3	12305(5)
Z	4
Z'	1
Θ_{min}/°	0.692
Θ_{max}/°	29.603
Measured Refl.	97100
Independent Refl.	32412
$I > 2\sigma(I)$	20137
R_{int}	0.0842
Parameters	1537
Restraints	10
Largest Peak	1.516
Deepest Hole	-0.936
GooF	1.033
wR_2 (all data)	0.1594
wR_2	0.1350
R_1 (all data)	0.1207
R_1	0.0630
CCDC #	1434441

Structure Quality Indicators

Reflections:

Refinement:

A violet plate-shaped crystal with dimensions 0.92×0.28×0.10 mm was mounted on a loop with paratone oil. X-ray diffraction data were collected using a Bruker APEX-II CCD diffractometer equipped with an Oxford Cryosystems low-temperature apparatus operating at T = 100(2) K.

Data were measured using ω scans with MoK_α radiation (fine-focus sealed tube, 45 kV, 35 mA). The total number of runs and images was based on the strategy calculation from the program **APEX2** (Bruker, 2014). The maximum resolution achieved was Θ = 29.603°.

Unit cell indexing was performed by using the **APEX2** (Bruker) software and refined using **SAINT** (Bruker, V8.34A, 2013) on 9882 reflections, 10% of the observed reflections. Data reduction, scaling and absorption corrections were performed using **SAINT** (Bruker, V8.34A, 2013) and **SADABS-2014/2** (Bruker, 2014) was used for absorption correction. wR_2(int) was 0.1695 before and 0.0606 after correction. The ratio of minimum to maximum transmission is 0.4684. The $\lambda/2$ correction factor is Not present. software which corrects for Lorentz polarisation. The final completeness is 100.00 out to 29.603 in Θ. The absorption coefficient (μ) of this material is 1.669 mm^{-1} and the minimum and maximum transmissions are 0.3494 and 0.7459.

The structure was solved in the space group P1 with the **ShelXT** (Sheldrick, 2015) structure solution program using combined Patterson and dual-space recycling methods. The space group $P2_1/c$ (# 14) was determined by **ShelXT** (Sheldrick, 2015) structure solution program.The crystal structure was refined by Least Squares using version 2014/7 of **ShelXL** (Sheldrick, 2008). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

There are two independent molecules in the asymmetric unit.

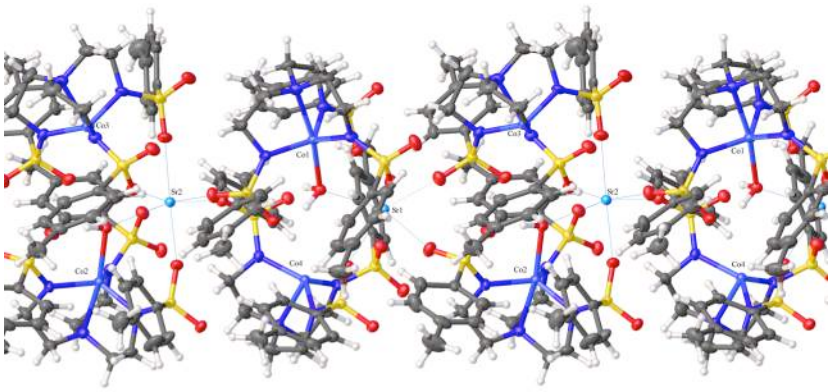


Figure S12:

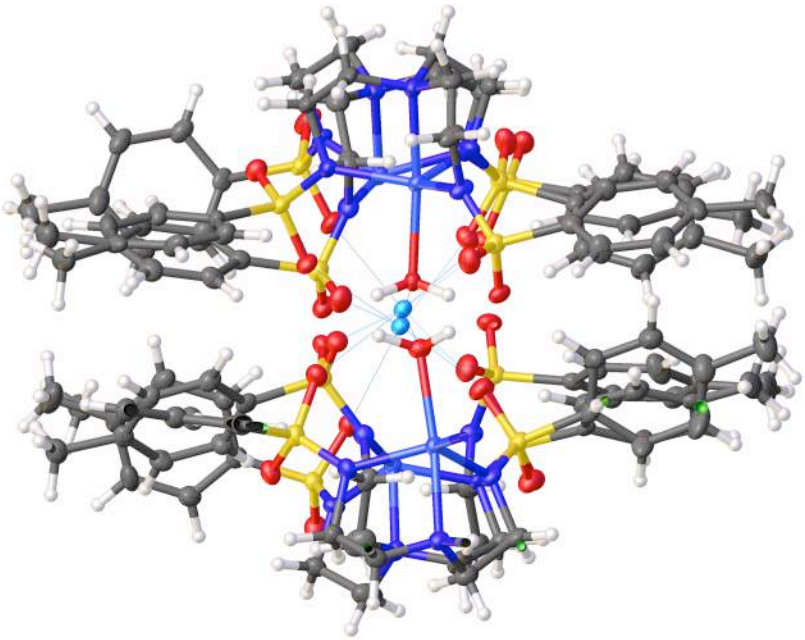


Figure S13:

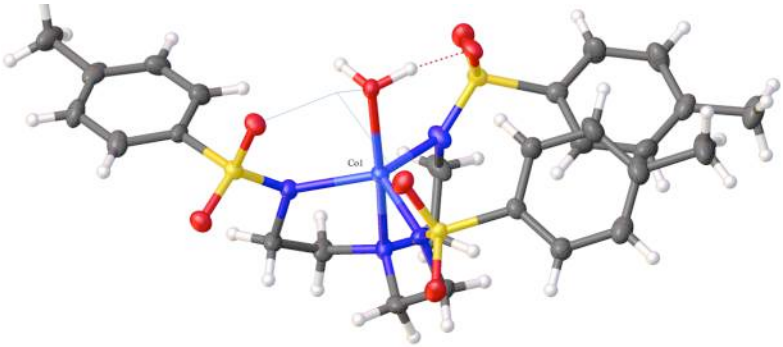


Figure S14:

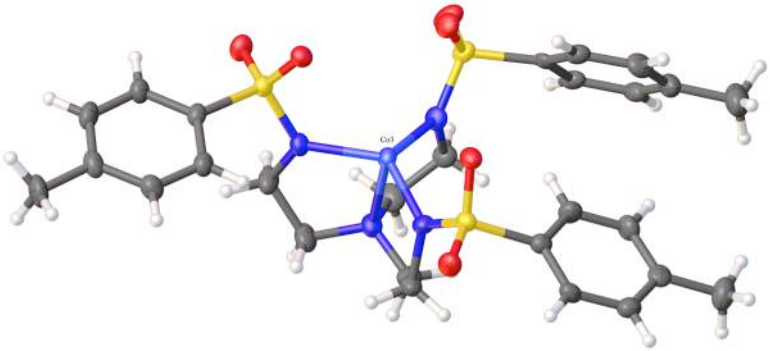
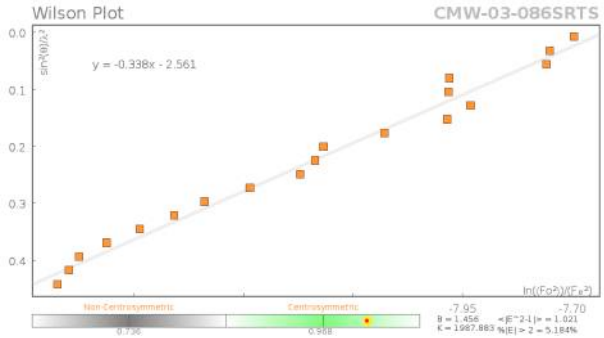
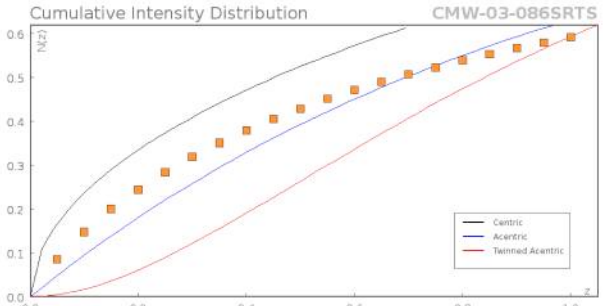
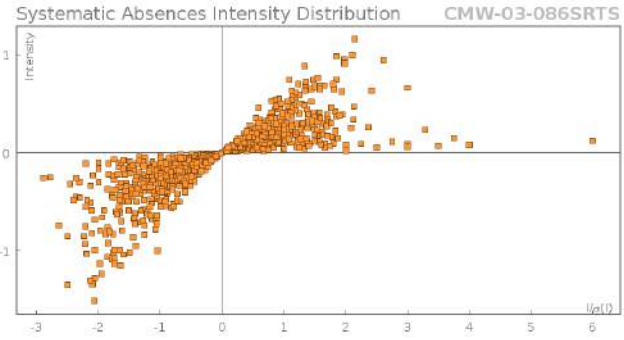


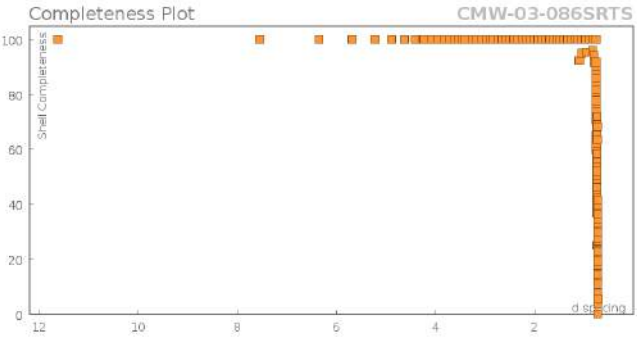
Figure S15:

Data Plots: Diffraction Data

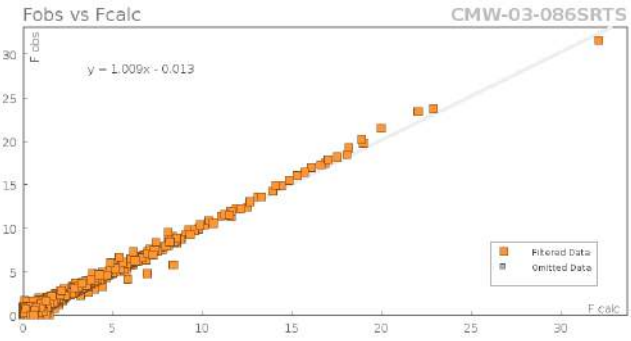


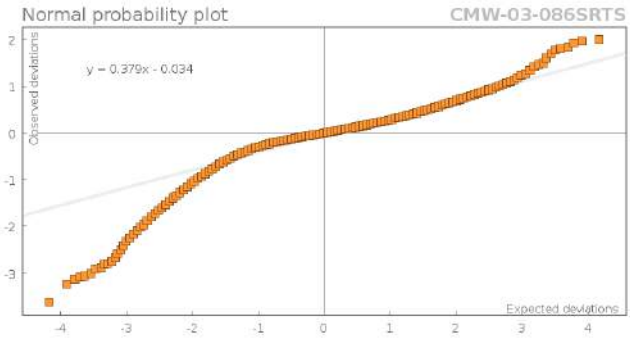






Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	98878	Unique reflections	32412
Completeness	0.936	Mean I/σ	6.7
hklsub>max</sub> collected	(38, 22, 35)	hklsub>min</sub> collected	(-41, -22, -31)
hkl_{max} used	(40, 22, 35)	hkl_{min} used	(-41, 0, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.36
d_{max} used	29.44	d_{min} used	0.72
Friedel pairs	24046	Friedel pairs merged	1
Inconsistent equivalents	0	R_{int}	0.0842
R_{sigma}	0.1104	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	0
Multiplicity	(68410, 15135, 66)	Maximum multiplicity	9
Removed systematic absences	1778	Filtered off (Shel/OMIT)	0

Images of the Crystal on the Diffractometer

Table S12: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **CMW-03-086SRTS**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Co1	3090.1(2)	1499.8(3)	1633.4(2)	18.14(13)
S3	2142.3(4)	747.6(6)	1070.5(4)	19.6(2)
S1	3624.6(4)	-148.1(6)	2053.4(4)	20.9(2)
S2	3347.5(4)	3010.6(6)	2451.5(4)	21.0(2)
O2	3817.9(10)	-860.2(17)	1816.0(12)	30.2(7)
O1	2677.0(8)	1364.1(15)	2276.9(10)	18.9(6)
O4	3178.1(10)	2430.5(17)	2813.2(10)	23.8(7)
O5	3119.3(11)	3801.1(17)	2430.4(12)	29.4(7)
O3	3193.8(10)	-272.1(17)	2266.2(12)	25.5(7)
O6	2076.3(10)	537.8(17)	1607.8(10)	22.8(7)
O7	2125.2(10)	60.0(16)	712.5(11)	24.5(7)
N1	3563.0(12)	616(2)	1678.2(13)	22.7(8)
N2	3439.3(12)	1885(2)	966.9(13)	22.6(8)
N3	3348.2(13)	2594(2)	1907.9(13)	24.8(8)
N4	2584.7(12)	1286(2)	1066.6(13)	21.0(8)
C22	1332.0(15)	1093(3)	499.0(17)	28.4(10)
C23	968.2(16)	1603(3)	329.7(18)	31.9(11)
C8	3931.6(15)	769(3)	1348.4(17)	28.2(10)
C2	3884.4(16)	670(3)	2958.0(17)	27.2(10)
C14	4416.7(17)	3992(3)	3311.2(18)	34.0(12)
C3	4194.9(17)	894(3)	3375.9(18)	35.4(12)
C20	2706.5(15)	1428(3)	529.8(16)	24.8(10)
C13	3995.2(17)	3899(3)	3036.8(18)	32.1(11)
C9	3719.9(16)	1172(3)	847.2(16)	27.5(10)
C1	4016.7(15)	117(2)	2591.1(16)	20.5(9)
C16	4677.1(17)	2779(3)	2923.4(18)	34.4(12)
C12	3908.6(15)	3221(2)	2713.9(16)	22.3(9)
C26	1679.3(16)	2228(3)	981.4(17)	27.6(10)
C10	3715.8(16)	2624(3)	1118.3(17)	29.7(11)
C15	4765.2(16)	3430(3)	3266.4(18)	29.8(11)
C21	1678.8(14)	1397(3)	833.3(16)	22.1(9)
C17	4256.4(16)	2667(3)	2654.5(18)	29.4(11)
C4	4630.1(18)	573(3)	3432.9(18)	36.2(12)
C18	5213.9(16)	3517(3)	3587(2)	41.5(13)
C11	3491.9(18)	3146(3)	1493.3(17)	30.5(11)
C24	953.9(16)	2416(3)	480.9(18)	32.0(11)
C6	4447.0(16)	-216(3)	2644.9(17)	27.6(10)
C5	4751.2(17)	11(3)	3065.7(18)	33.5(11)
C7	4957.1(18)	819(4)	3890.5(19)	52.0(16)
C19	3075.5(15)	2073(3)	548.9(16)	25.9(10)
C25	1317.9(17)	2725(3)	804.0(17)	32.0(11)
C27	552.6(17)	2964(3)	316(2)	42.4(14)
Co2	2166.3(2)	6453.6(3)	3502.6(2)	18.44(13)
S4	2825.4(4)	8051.4(6)	3336.7(4)	21.0(2)
S5	2713.8(4)	4808.7(6)	3913.4(4)	20.7(2)
S6	1328.4(4)	5726.5(6)	2709.2(4)	21.5(2)
O11	2628.5(10)	4110.4(16)	4238.2(11)	25.1(7)

Atom	x	y	z	U_{eq}
O8	2457.5(9)	6280.2(15)	2770.3(11)	22.6(7)
O9	2679.6(11)	8857.5(18)	3147.0(12)	30.4(7)
O13	1024.8(10)	5071.6(16)	2831.0(12)	25.1(7)
O14	1699.1(10)	5476.3(17)	2414.0(11)	25.8(7)
O12	2681.9(11)	4656.3(17)	3357.1(11)	25.9(7)
O10	3000(1)	7509.6(17)	2955.7(11)	27.8(7)
N6	1824.3(12)	6844(2)	4171.1(13)	22.6(8)
N5	2450.8(12)	7592.6(19)	3614.1(13)	21.4(8)
N8	1523.6(12)	6224(2)	3205.4(14)	22.5(8)
N7	2402.8(13)	5570(2)	4003.2(13)	23.5(8)
C47	1177.4(15)	6365(3)	3577.6(17)	27.3(10)
C43	3961.1(16)	5785(3)	3902.1(18)	30.8(11)
C41	3937(2)	5150(3)	4722(2)	49.4(15)
C51	401.5(16)	7478(3)	1703.8(17)	26.6(10)
C28	3298.2(15)	8258(2)	3790.8(16)	21.7(9)
C48	977.1(14)	6421(2)	2312.6(16)	19.6(9)
C42	4176.4(17)	5602(3)	4383(2)	34.7(12)
C36	2054.0(16)	7590(3)	4388.6(16)	26.2(10)
C29	3488.4(16)	7616(3)	4095.0(17)	29.4(11)
C35	2210.2(16)	8133(2)	3960.0(17)	25.7(10)
C50	355.7(16)	6630(3)	1657.1(18)	29.6(11)
C49	640.0(15)	6097(3)	1964.4(17)	25.9(10)
C38	2321.4(16)	5736(3)	4548.4(16)	27.5(10)
C31	4082.3(17)	8528(3)	4461.5(19)	36.1(12)
C53	1031.1(16)	7269(3)	2358.1(17)	25.6(10)
C54	74.1(17)	8051(3)	1400.0(19)	37.4(12)
C40	3495.4(18)	4893(3)	4574.5(19)	40.6(13)
C30	3878.5(17)	7765(3)	4424.7(18)	33.9(12)
C44	3524.5(15)	5544(3)	3748.8(17)	25(1)
C37	1860.3(16)	6148(3)	4547.4(17)	28.9(10)
C32	3888.9(17)	9157(3)	4147(2)	39.0(13)
C46	1354.3(15)	7015(3)	3960.9(17)	26.4(10)
C39	3290.1(16)	5088(2)	4085.3(16)	23.3(10)
C34	4494.5(19)	8695(4)	4840(2)	58.5(17)
C33	3502.4(16)	9037(3)	3811.7(18)	28.8(11)
C52	739.8(15)	7787(3)	2057.3(18)	27.2(10)
C45	4660.7(17)	5875(3)	4540(2)	47.5(15)
Co3	2883.5(2)	-3325.1(3)	1385.9(2)	20.70(13)
S7	3675.2(4)	-4157.3(6)	2100.0(4)	21.2(2)
S8	2431.9(4)	-4966.7(6)	905.3(4)	24.3(2)
S9	2124.7(4)	-2099.6(6)	1715.3(4)	22.1(2)
O15	3282.9(10)	-4362.6(17)	2369.5(11)	24.5(7)
O16	3922.7(11)	-4844.3(18)	1909.9(12)	29.0(7)
O17	2644.2(12)	-5629.0(18)	646.8(11)	35.2(8)
O18	2393.9(11)	-5068.1(18)	1458.1(11)	28.1(7)
O19	2010.9(10)	-2845.9(17)	1986.5(11)	26.6(7)
O20	2151.7(11)	-1348.8(17)	2023.0(12)	30.2(7)
N9	3509.4(12)	-3509(2)	1663.0(13)	22.8(8)
N11	2665.7(13)	-4106(2)	840.8(13)	24.4(8)
N12	2560.9(13)	-2284(2)	1442.1(14)	24.2(8)
N10	3188.3(13)	-2722(2)	786.3(14)	25.9(8)
C62	3861.0(16)	-3230(3)	1332.8(18)	32.5(11)
C78	939.1(16)	-1697(3)	468.0(17)	27.5(10)
C77	1192.2(16)	-2418(3)	492.3(17)	29.1(11)
C76	1550.1(16)	-2533(3)	865.5(18)	28.8(11)
C63	3656.9(16)	-2544(3)	997.3(19)	35.3(12)
C64	3178.7(19)	-3332(3)	350.0(18)	38.4(13)
C65	2756.5(16)	-3851(3)	315.4(16)	28.3(10)

Atom	x	y	z	U_{eq}
C74	2746.0(16)	-1598(3)	1137.1(17)	27.8(10)
C73	2914.7(17)	-1992(3)	655.7(19)	34.4(12)
C55	4070.9(15)	-3617(3)	2539.8(16)	21.6(9)
C56	4483.8(15)	-3957(3)	2712.4(17)	26.1(10)
C57	4788.2(16)	-3508(3)	3042.3(18)	31.1(11)
C58	4688.2(16)	-2720(3)	3204.6(17)	28.9(11)
C59	4267.7(16)	-2389(3)	3023.8(17)	28.7(10)
C60	3960.8(16)	-2820(3)	2684.7(17)	26.8(10)
C61	5017.9(17)	-2228(3)	3563(2)	41.2(13)
C75	1667.0(15)	-1929(2)	1231.0(16)	22.9(10)
C80	1424.4(15)	-1192(2)	1211.6(18)	25(1)
C79	1064.8(16)	-1088(3)	836.5(18)	28.9(11)
C81	547.9(17)	-1558(3)	63(2)	42.6(13)
C66	1873.0(15)	-4873(2)	602.0(17)	22.1(9)
C67	1507.9(16)	-4750(2)	892.7(18)	27.5(10)
C68	1082.4(17)	-4625(3)	642.2(19)	33.9(12)
C69	1009.4(18)	-4592(3)	99.1(19)	34.6(12)
C70	1377.3(17)	-4719(3)	-188.5(17)	29.0(11)
C71	1808.6(17)	-4859(2)	58.4(16)	25.5(10)
C72	546.1(18)	-4424(4)	-176(2)	52.7(16)
Co4	1824.5(2)	1748.2(3)	3422.6(2)	18.01(13)
S10	2694.7(4)	895.8(6)	3932.6(4)	18.9(2)
S11	1721.9(4)	2914.7(6)	2461.3(4)	19.8(2)
S12	1261.5(4)	155.9(6)	3116.3(4)	20.0(2)
O21	2713.0(9)	746.5(16)	3376(1)	20.2(6)
O22	2664.6(10)	171.2(16)	4254.6(11)	23.6(7)
O23	1959.4(10)	3634.8(16)	2290.0(11)	23.7(7)
O24	1856.5(10)	2135.3(17)	2242.4(11)	23.0(7)
O25	1701.8(10)	18.0(17)	2920.9(11)	24.2(7)
O26	1093.5(10)	-477.9(17)	3440.1(11)	27.1(7)
N13	2300.3(11)	1532(2)	3972.2(12)	19.5(8)
N15	1762.3(12)	2809.2(19)	3062.5(13)	20.9(8)
N16	1294.3(12)	1029(2)	3389.8(13)	21.5(8)
N14	1506.7(12)	2365.9(19)	4011.0(13)	20.2(8)
C89	2203.3(15)	1807(2)	4496.8(16)	22.8(9)
C90	1869.3(18)	2520(3)	4425.3(18)	39.0(13)
C91	1314(2)	3131(3)	3770(2)	43.2(14)
C92	1610.8(16)	3489(2)	3388.6(16)	23.7(10)
C101	937.6(15)	1296(3)	3704.6(17)	24.4(10)
C100	1154.8(19)	1800(3)	4163(2)	43.2(14)
C82	3197.3(14)	1417(3)	4175.8(15)	20.1(9)
C83	3276.0(15)	2205(3)	3991.3(16)	23.5(10)
C84	3666.3(17)	2622(3)	4180.8(17)	29.0(11)
C85	3980.4(16)	2265(3)	4552.5(17)	26.4(10)
C86	3890.3(16)	1490(3)	4741.2(17)	28.3(10)
C87	3497.8(15)	1064(3)	4554.7(16)	24.4(10)
C88	4412.8(17)	2721(3)	4742(2)	39.3(13)
C102	867.5(15)	225(2)	2554.3(16)	21.3(9)
C103	418.6(16)	7(3)	2572.6(18)	27.9(10)
C104	113.2(16)	75(3)	2135.2(19)	34.4(12)
C105	255.0(17)	372(3)	1665.8(18)	33.8(12)
C106	705.2(17)	597(3)	1654.6(18)	31.1(11)
C107	1016.9(15)	527(3)	2094.3(17)	24.7(10)
C108	-69.9(19)	441(4)	1186(2)	52.8(16)
C93	1145.1(15)	3052(2)	2237.4(16)	20.7(9)
C94	828.4(15)	2492(2)	2386.9(17)	23.5(10)
C95	380.0(16)	2538(3)	2181.8(17)	26.1(10)
C96	235.8(15)	3146(2)	1821.6(17)	23.4(10)

Atom	x	y	z	U_{eq}
C97	551.4(16)	3719(3)	1691.9(17)	25.4(10)
C98	1001.8(16)	3690(2)	1894.7(16)	23.7(10)
C99	-247.0(16)	3154(3)	1574.5(18)	31.4(11)
O27	3712.2(16)	4788(3)	772.7(17)	71.1(13)
Sr1	2422.7(2)	-87.1(2)	2515.4(2)	17.64(9)
Sr2	2506.3(2)	4814.1(2)	2413.1(2)	17.26(9)

Table S13: Anisotropic Displacement Parameters (×10⁴) **CMW-03-086SRTS**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	18.8(3)	20.8(3)	14.8(3)	-0.7(2)	1.2(2)	0.0(2)
S3	21.7(6)	21.7(5)	15.2(5)	0.7(4)	0.7(4)	0.5(4)
S1	17.6(6)	20.8(5)	23.9(6)	-3.2(4)	0.9(4)	1.5(4)
S2	24.1(6)	18.6(5)	20.5(5)	-2.4(4)	2.7(5)	-0.1(4)
O2	24.2(18)	26.4(16)	39.2(19)	-11.2(14)	-1.0(15)	3.3(14)
O1	15.6(15)	22.4(14)	18.1(14)	-0.6(12)	-1.6(12)	-0.1(12)
O4	28.9(18)	27.7(15)	14.8(15)	-1.8(12)	3.0(13)	-4.3(13)
O5	27.5(18)	24.4(15)	35.1(18)	-3.6(14)	-2.5(15)	5.8(14)
O3	21.2(17)	21.9(15)	33.6(18)	0.9(13)	3.1(14)	-2.0(13)
O6	28.1(18)	23.9(15)	16.2(15)	3.9(12)	1.0(13)	-1.5(13)
O7	28.6(18)	22.3(15)	22.2(16)	-2.5(12)	0.4(14)	0.9(13)
N1	18(2)	30.2(19)	20.2(18)	0.2(15)	5.1(16)	4.6(16)
N2	18(2)	30.8(19)	18.7(18)	0.8(15)	-1.1(15)	-2.9(16)
N3	35(2)	21.8(17)	18.0(18)	1.1(15)	4.1(17)	-8.2(16)
N4	19(2)	28.1(19)	15.8(17)	1.0(15)	-0.5(15)	0.7(15)
C22	26(3)	34(2)	25(2)	9(2)	-1(2)	-6(2)
C23	18(3)	43(3)	33(3)	9(2)	-4(2)	-4(2)
C8	21(2)	40(3)	25(2)	5(2)	5(2)	5(2)
C2	24(3)	29(2)	29(2)	-2(2)	0(2)	2(2)
C14	42(3)	24(2)	34(3)	-3(2)	-7(2)	-5(2)
C3	40(3)	42(3)	24(2)	-7(2)	-1(2)	-6(2)
C20	20(2)	39(2)	16(2)	0.2(19)	1.7(18)	-1(2)
C13	32(3)	22(2)	41(3)	-7(2)	-3(2)	2(2)
C9	24(3)	41(3)	19(2)	-3(2)	5.7(19)	0(2)
C1	24(2)	21(2)	17(2)	3.1(17)	0.6(18)	-1.8(18)
C16	25(3)	47(3)	32(3)	0(2)	4(2)	9(2)
C12	25(3)	19(2)	23(2)	4.3(17)	4.0(19)	0.3(18)
C26	29(3)	33(2)	21(2)	-1.1(19)	0(2)	5(2)
C10	29(3)	39(3)	21(2)	5(2)	5(2)	-10(2)
C15	20(3)	37(3)	32(3)	11(2)	2(2)	-3(2)
C21	17(2)	34(2)	15(2)	1.2(18)	0.2(18)	3.5(19)
C17	30(3)	30(2)	29(3)	-2(2)	4(2)	8(2)
C4	33(3)	49(3)	26(3)	4(2)	-3(2)	-7(2)
C18	24(3)	54(3)	46(3)	12(3)	-3(2)	-8(2)
C11	45(3)	27(2)	20(2)	1.6(19)	3(2)	-14(2)
C24	23(3)	53(3)	21(2)	13(2)	7(2)	10(2)
C6	25(3)	34(2)	24(2)	1(2)	1(2)	0(2)
C5	24(3)	47(3)	30(3)	12(2)	0(2)	-3(2)
C7	35(3)	92(5)	27(3)	-5(3)	-4(2)	-14(3)
C19	25(3)	36(2)	16(2)	7.5(19)	0.3(19)	0(2)
C25	37(3)	36(3)	23(2)	-3(2)	4(2)	12(2)
C27	28(3)	68(4)	31(3)	8(3)	3(2)	18(3)
Co2	19.5(3)	18.8(3)	16.7(3)	0.4(2)	-0.2(2)	-1.5(2)
S4	25.0(6)	20.3(5)	18.0(5)	1.8(4)	3.1(5)	-0.5(4)
S5	25.9(6)	20.1(5)	15.4(5)	2.9(4)	-1.1(4)	-2.2(4)
S6	19.8(6)	20.7(5)	23.5(5)	-1.2(4)	-0.7(5)	0.8(4)
O11	32.4(19)	20.8(14)	21.4(16)	5.1(12)	-0.7(14)	-4.3(13)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O8	26.1(18)	20.9(14)	20.8(16)	0.4(12)	1.9(13)	-1.4(13)
O9	34(2)	25.5(16)	30.7(18)	6.3(14)	-4.8(15)	1.0(14)
O13	20.1(17)	21.4(14)	33.1(18)	0.7(13)	-0.6(14)	-2.6(12)
O14	22.8(17)	26.9(15)	27.6(17)	-3.1(13)	2.4(14)	3.5(13)
O12	35.5(19)	25.3(15)	16.3(15)	1.1(12)	-1.3(14)	1.4(14)
O10	27.8(19)	32.8(17)	24.2(16)	-7.7(14)	10.1(14)	-5.1(14)
N6	24(2)	24.3(18)	20.1(19)	0.4(15)	3.2(16)	-4.0(15)
N5	26(2)	15.6(16)	22.8(19)	-2.2(14)	5.6(16)	-3.2(15)
N8	18(2)	24.4(18)	24.8(19)	1.1(15)	1.1(16)	2.5(15)
N7	29(2)	25.7(18)	15.8(18)	6.0(15)	1.7(16)	-0.2(16)
C47	22(3)	38(3)	22(2)	-3(2)	3(2)	-1(2)
C43	32(3)	35(3)	26(2)	2(2)	5(2)	-1(2)
C41	48(4)	62(4)	34(3)	23(3)	-17(3)	-15(3)
C51	23(3)	32(2)	26(2)	7(2)	7(2)	7(2)
C28	22(2)	22(2)	22(2)	-1.9(17)	7.2(19)	-0.2(18)
C48	16(2)	23(2)	21(2)	-3.3(17)	3.8(18)	0.5(17)
C42	31(3)	31(2)	41(3)	6(2)	-3(2)	-4(2)
C36	30(3)	29(2)	20(2)	-4.1(19)	4(2)	-3(2)
C29	29(3)	32(2)	27(2)	-1(2)	1(2)	2(2)
C35	28(3)	22(2)	28(2)	-6.7(19)	7(2)	-1.1(19)
C50	26(3)	36(3)	26(2)	-3(2)	-1(2)	-2(2)
C49	27(3)	25(2)	26(2)	-3.5(19)	4(2)	0.9(19)
C38	34(3)	33(2)	15(2)	3.4(18)	3(2)	3(2)
C31	25(3)	55(3)	28(3)	-17(2)	2(2)	5(2)
C53	26(3)	27(2)	24(2)	1.5(19)	4(2)	4.6(19)
C54	30(3)	45(3)	37(3)	15(2)	2(2)	9(2)
C40	34(3)	54(3)	33(3)	20(2)	-5(2)	-19(3)
C30	32(3)	47(3)	22(2)	-2(2)	2(2)	10(2)
C44	24(3)	29(2)	23(2)	2.8(19)	5(2)	3.3(19)
C37	32(3)	33(2)	22(2)	2(2)	5(2)	-5(2)
C32	26(3)	34(3)	56(3)	-14(3)	0(3)	-3(2)
C46	24(3)	30(2)	26(2)	-0.9(19)	7(2)	-1(2)
C39	28(3)	20(2)	20(2)	1.5(17)	-1.8(19)	3.1(18)
C34	35(3)	92(5)	46(3)	-25(3)	-11(3)	0(3)
C33	25(3)	24(2)	37(3)	-1(2)	2(2)	-1.7(19)
C52	24(3)	26(2)	32(3)	5(2)	4(2)	1.6(19)
C45	31(3)	46(3)	63(4)	12(3)	-8(3)	-8(3)
Co3	20.4(3)	24.9(3)	16.4(3)	1.5(2)	-0.3(2)	-0.1(2)
S7	19.8(6)	23.9(5)	19.9(5)	-1.0(4)	1.7(4)	0.5(4)
S8	32.2(7)	24.7(5)	15.2(5)	-0.5(4)	-1.6(5)	3.6(5)
S9	25.2(6)	21.1(5)	19.5(5)	-1.5(4)	-0.1(5)	-1.7(4)
O15	23.5(17)	24.8(15)	25.6(16)	0.3(13)	4.6(14)	-1.5(13)
O16	26.6(18)	33.0(17)	27.3(17)	-5.3(14)	2.3(14)	6.6(14)
O17	53(2)	30.7(17)	21.1(16)	-2.6(14)	-1.8(16)	12.8(16)
O18	35(2)	33.8(17)	14.9(15)	-1.0(13)	-2.4(14)	0.0(14)
O19	29.2(19)	28.7(16)	21.4(16)	3.2(13)	0.1(14)	-5.6(14)
O20	34(2)	25.9(16)	30.0(17)	-6.3(14)	-3.6(15)	-0.8(14)
N9	18(2)	28.9(19)	21.5(19)	-0.5(15)	2.3(16)	-0.9(16)
N11	29(2)	30.2(19)	13.1(17)	-3.9(15)	-0.3(16)	-0.7(17)
N12	26(2)	22.3(18)	23.8(19)	5.2(15)	0.2(17)	-0.8(16)
N10	22(2)	33(2)	22.3(19)	2.8(16)	3.1(16)	-3.0(17)
C62	21(3)	49(3)	27(3)	11(2)	3(2)	-1(2)
C78	26(3)	33(2)	24(2)	7(2)	8(2)	-4(2)
C77	30(3)	33(2)	24(2)	-6(2)	-2(2)	-5(2)
C76	32(3)	22(2)	32(3)	-4.1(19)	0(2)	2.9(19)
C63	24(3)	52(3)	30(3)	6(2)	5(2)	-9(2)
C64	49(4)	47(3)	19(2)	-1(2)	4(2)	-7(3)
C65	34(3)	31(2)	19(2)	0.9(19)	1(2)	-2(2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C74	27(3)	27(2)	30(3)	6.2(19)	0(2)	-6(2)
C73	32(3)	36(3)	35(3)	13(2)	3(2)	-4(2)
C55	19(2)	30(2)	17(2)	1.3(18)	2.2(18)	1.6(18)
C56	19(2)	32(2)	27(2)	-1(2)	3(2)	0.9(19)
C57	19(3)	44(3)	30(3)	5(2)	1(2)	5(2)
C58	22(3)	43(3)	21(2)	-2(2)	3(2)	-7(2)
C59	27(3)	32(2)	28(2)	-6(2)	5(2)	-3(2)
C60	20(2)	34(2)	27(2)	2(2)	2(2)	0(2)
C61	25(3)	56(3)	40(3)	-7(3)	-6(2)	-9(2)
C75	24(3)	22(2)	23(2)	0.1(18)	5.5(19)	-0.8(18)
C80	23(3)	20(2)	32(3)	-2.2(19)	6(2)	-3.1(18)
C79	30(3)	25(2)	33(3)	5(2)	5(2)	0(2)
C81	30(3)	59(3)	38(3)	0(3)	-2(2)	7(3)
C66	28(3)	12.8(18)	24(2)	-1.3(17)	-4(2)	-7.2(17)
C67	37(3)	21(2)	24(2)	2.0(18)	1(2)	-1(2)
C68	29(3)	35(3)	40(3)	2(2)	14(2)	-5(2)
C69	34(3)	33(3)	34(3)	5(2)	-9(2)	-8(2)
C70	41(3)	23(2)	22(2)	3.2(18)	-6(2)	-8(2)
C71	38(3)	18(2)	20(2)	-0.4(17)	-1(2)	-1.6(19)
C72	35(3)	68(4)	53(4)	10(3)	-5(3)	-11(3)
Co4	19.4(3)	17.5(3)	17.0(3)	-0.6(2)	0.7(2)	-0.5(2)
S10	19.6(6)	20.5(5)	16.2(5)	0.3(4)	-0.3(4)	-0.8(4)
S11	20.3(6)	19.0(5)	20.3(5)	-0.6(4)	2.5(4)	-1.9(4)
S12	18.4(6)	21.2(5)	20.4(5)	-0.8(4)	1.7(4)	-1.8(4)
O21	19.8(16)	25.4(15)	15.5(14)	-0.7(12)	2.5(12)	-3.1(13)
O22	25.9(18)	23.8(15)	21.0(15)	1.5(12)	1.9(13)	-4.3(13)
O23	25.5(18)	22.0(15)	23.8(16)	1.9(12)	3.4(14)	-2.3(13)
O24	18.5(16)	24.3(15)	26.4(16)	-2.2(13)	3.0(13)	1.3(12)
O25	19.6(17)	27.5(15)	25.2(16)	-3.4(13)	0.6(13)	1.7(13)
O26	28.9(19)	23.2(15)	28.8(17)	3.2(13)	0.6(14)	-5.4(13)
N13	16.5(19)	28.3(18)	13.7(17)	-5.3(14)	1.6(15)	-0.2(15)
N15	22(2)	17.7(17)	23.5(19)	1.6(14)	2.3(16)	0.3(15)
N16	21(2)	23.2(17)	21.8(19)	-2.3(15)	7.1(16)	-2.2(15)
N14	23(2)	17.7(16)	19.4(18)	0.1(14)	0.3(16)	-0.2(15)
C89	29(3)	22(2)	17(2)	-1.8(17)	1.2(19)	3.3(19)
C90	40(3)	53(3)	24(3)	-10(2)	2(2)	4(3)
C91	59(4)	32(3)	39(3)	-1(2)	8(3)	12(3)
C92	31(3)	18(2)	22(2)	-2.8(17)	-1(2)	3.7(18)
C101	21(2)	28(2)	26(2)	-3.0(19)	6.0(19)	1.5(19)
C100	41(3)	50(3)	41(3)	-15(3)	17(3)	-10(3)
C82	21(2)	29(2)	10.4(19)	-1.6(17)	3.3(17)	0.9(18)
C83	25(3)	29(2)	16(2)	-1.4(18)	-0.1(19)	0.5(19)
C84	36(3)	30(2)	22(2)	-1.3(19)	5(2)	-9(2)
C85	24(3)	36(3)	20(2)	-9.7(19)	8(2)	-5(2)
C86	22(3)	40(3)	22(2)	-7(2)	-2(2)	3(2)
C87	25(3)	27(2)	21(2)	0.3(18)	3.1(19)	-2.1(19)
C88	25(3)	51(3)	41(3)	-15(3)	1(2)	-10(2)
C102	26(2)	16.6(19)	21(2)	-4.8(17)	0.7(19)	2.2(18)
C103	26(3)	33(2)	25(2)	-3(2)	6(2)	-3(2)
C104	19(3)	46(3)	37(3)	-12(2)	-4(2)	5(2)
C105	29(3)	42(3)	29(3)	-10(2)	-5(2)	13(2)
C106	39(3)	32(2)	22(2)	-2(2)	1(2)	9(2)
C107	21(2)	26(2)	27(2)	1.0(19)	3(2)	0.6(19)
C108	45(4)	78(4)	33(3)	-10(3)	-10(3)	22(3)
C93	27(3)	17.3(19)	17(2)	-5.0(16)	1.9(18)	0.4(18)
C94	24(3)	22(2)	26(2)	4.0(18)	4(2)	-1.1(18)
C95	26(3)	23(2)	30(3)	1.3(19)	7(2)	-4.5(19)
C96	23(2)	22(2)	25(2)	-7.3(18)	1.2(19)	5.3(18)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C97	32(3)	20(2)	23(2)	0.2(18)	-2(2)	4.8(19)
C98	31(3)	18(2)	22(2)	-0.7(17)	1(2)	-1.7(18)
C99	26(3)	34(3)	33(3)	-4(2)	0(2)	4(2)
O27	86(4)	67(3)	61(3)	0(2)	14(3)	3(3)
Sr1	19.6(2)	17.79(18)	15.40(19)	0.46(15)	1.16(16)	-0.66(15)
Sr2	19.9(2)	16.80(18)	14.92(19)	-0.37(15)	0.71(16)	0.08(15)

Table S14: Bond Lengths in Å for **CMW-03-086SRTS**.

Atom	Atom	Length/Å
Co1	O1	2.167(3)
Co1	N1	1.996(3)
Co1	N2	2.183(3)
Co1	N3	2.029(3)
Co1	N4	2.018(3)
S3	O6	1.460(3)
S3	O7	1.444(3)
S3	N4	1.573(4)
S3	C21	1.788(4)
S1	O2	1.449(3)
S1	O3	1.450(3)
S1	N1	1.571(4)
S1	C1	1.773(4)
S2	O4	1.448(3)
S2	O5	1.445(3)
S2	N3	1.557(4)
S2	C12	1.764(5)
O1	Sr1	2.560(3)
O5	Sr2	2.442(3)
O3	Sr1	2.448(3)
O6	Sr1	2.664(3)
N1	C8	1.468(5)
N2	C9	1.472(5)
N2	C10	1.480(5)
N2	C19	1.480(5)
N3	C11	1.487(5)
N4	C20	1.484(5)
C22	C23	1.392(6)
C22	C21	1.367(6)
C23	C24	1.374(7)
C8	C9	1.528(6)
C2	C3	1.395(6)
C2	C1	1.387(6)
C14	C13	1.381(6)
C14	C15	1.387(7)
C3	C4	1.383(7)
C20	C19	1.508(6)
C13	C12	1.387(6)
C1	C6	1.377(6)
C16	C15	1.385(7)
C16	C17	1.377(7)
C12	C17	1.384(6)
C26	C21	1.398(6)
C26	C25	1.379(6)
C10	C11	1.488(6)
C15	C18	1.501(6)
C4	C5	1.386(7)
C4	C7	1.506(6)
C24	C25	1.389(7)
C24	C27	1.509(6)
C6	C5	1.391(6)
Co2	O8	2.171(3)
Co2	N6	2.178(3)
Co2	N5	2.035(3)
Co2	N8	2.014(4)
Co2	N7	2.008(3)
S4	O9	1.445(3)
S4	O10	1.450(3)
S4	N5	1.564(4)
S4	C28	1.767(4)
S5	O11	1.444(3)
S5	O12	1.452(3)
S5	N7	1.568(4)
S5	C39	1.778(5)
S6	O13	1.444(3)
S6	O14	1.453(3)
S6	N8	1.575(4)
S6	C48	1.784(4)
O8	Sr2	2.555(3)
O14	Sr2	2.618(3)
O12	Sr2	2.456(3)
N6	C36	1.469(5)
N6	C37	1.485(5)
N6	C46	1.469(6)
N5	C35	1.481(5)
N8	C47	1.488(5)
N7	C38	1.476(5)
C47	C46	1.503(6)
C43	C42	1.372(6)
C43	C44	1.370(6)
C41	C42	1.387(7)
C41	C40	1.389(7)
C51	C50	1.383(6)
C51	C54	1.506(6)
C51	C52	1.381(6)
C28	C29	1.387(6)
C28	C33	1.398(6)
C48	C49	1.380(6)
C48	C53	1.387(6)
C42	C45	1.516(7)
C36	C35	1.521(6)
C29	C30	1.387(7)
C50	C49	1.397(6)
C38	C37	1.518(6)
C31	C30	1.374(7)
C31	C32	1.390(7)

Atom	Atom	Length/Å
C31	C34	1.511(7)
C53	C52	1.385(6)
C40	C39	1.384(6)
C44	C39	1.378(6)
C32	C33	1.379(6)
Co3	N9	1.942(4)
Co3	N11	1.954(3)
Co3	N12	1.948(4)
Co3	N10	2.106(4)
S7	O15	1.449(3)
S7	O16	1.443(3)
S7	N9	1.584(4)
S7	C55	1.780(4)
S8	O17	1.439(3)
S8	O18	1.452(3)
S8	N11	1.571(4)
S8	C66	1.766(5)
S9	O19	1.452(3)
S9	O20	1.450(3)
S9	N12	1.558(4)
S9	C75	1.773(5)
O15	Sr2[1]	2.668(3)
O20	Sr1	2.496(3)
N9	C62	1.478(5)
N11	C65	1.468(5)
N12	C74	1.496(5)
N10	C63	1.468(6)
N10	C64	1.496(6)
N10	C73	1.454(6)
C62	C63	1.499(6)
C78	C77	1.385(6)
C78	C79	1.394(6)
C78	C81	1.499(6)
C77	C76	1.373(6)
C76	C75	1.379(6)
C64	C65	1.501(6)
C74	C73	1.524(6)
C55	C56	1.374(6)
C55	C60	1.391(6)
C56	C57	1.384(6)
C57	C58	1.384(6)
C58	C59	1.393(6)
C58	C61	1.505(6)
C59	C60	1.386(6)
C75	C80	1.391(6)
C80	C79	1.377(6)
C66	C67	1.388(6)
C66	C71	1.398(6)
C67	C68	1.373(7)
C68	C69	1.399(7)
C69	C70	1.391(7)
C69	C72	1.506(7)
C70	C71	1.389(6)
Co4	N13	1.931(3)
Co4	N15	1.953(3)
Co4	N16	1.948(3)
Co4	N14	2.114(3)
S10	O21	1.464(3)
S10	O22	1.445(3)
S10	N13	1.567(3)
S10	C82	1.771(4)
S11	O23	1.452(3)
S11	O24	1.454(3)
S11	N15	1.555(4)
S11	C93	1.762(5)
S12	O25	1.459(3)
S12	O26	1.442(3)
S12	N16	1.579(3)
S12	C102	1.774(4)
O21	Sr1	2.669(3)
O23	Sr2	2.502(3)
O25	Sr1	2.471(3)
N13	C89	1.480(5)
N15	C92	1.481(5)
N16	C101	1.458(5)
N14	C90	1.461(6)
N14	C91	1.475(6)
N14	C100	1.468(6)
C89	C90	1.519(6)
C91	C92	1.498(7)
C101	C100	1.526(6)
C82	C83	1.389(6)
C82	C87	1.380(6)
C83	C84	1.385(6)
C84	C85	1.394(6)
C85	C86	1.381(6)
C85	C88	1.517(6)
C86	C87	1.395(6)
C102	C103	1.379(6)
C102	C107	1.396(6)
C103	C104	1.380(6)
C104	C105	1.405(7)
C105	C106	1.383(7)
C105	C108	1.498(6)
C106	C107	1.396(6)
C93	C94	1.385(6)
C93	C98	1.398(5)
C94	C95	1.382(6)
C95	C96	1.392(6)
C96	C97	1.381(6)
C96	C99	1.507(6)
C97	C98	1.384(6)

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

Table S15: Bond Angles in ° for **CMW-03-086SRTS**.

Atom	Atom	Atom	Angle/°

Atom	Atom	Atom	Angle/°
O1	Co1	N2	168.20(12)
N1	Co1	O1	109.10(12)
N1	Co1	N2	82.39(14)
N1	Co1	N3	111.56(15)
N1	Co1	N4	112.62(14)
N3	Co1	O1	92.39(12)
N3	Co1	N2	80.51(13)
N4	Co1	O1	96.05(12)
N4	Co1	N2	81.45(13)
N4	Co1	N3	129.07(14)
O6	S3	N4	108.86(18)
O6	S3	C21	107.05(19)
O7	S3	O6	115.43(17)
O7	S3	N4	113.58(18)
O7	S3	C21	104.83(19)
N4	S3	C21	106.43(19)
O2	S1	O3	116.61(18)
O2	S1	N1	113.08(19)
O2	S1	C1	105.59(19)
O3	S1	N1	106.81(18)
O3	S1	C1	105.60(19)
N1	S1	C1	108.68(19)
O4	S2	N3	109.38(17)
O4	S2	C12	104.44(19)
O5	S2	O4	114.13(19)
O5	S2	N3	112.99(19)
O5	S2	C12	105.19(19)
N3	S2	C12	110.2(2)
Co1	O1	Sr1	118.58(10)
S2	O5	Sr2	159.8(2)
S1	O3	Sr1	163.43(18)
S3	O6	Sr1	148.08(18)
S1	N1	Co1	129.7(2)
C8	N1	Co1	113.7(3)
C8	N1	S1	116.2(3)
C9	N2	Co1	105.2(3)
C9	N2	C10	112.4(4)
C9	N2	C19	113.1(3)
C10	N2	Co1	108.3(2)
C10	N2	C19	111.7(3)
C19	N2	Co1	105.5(3)
S2	N3	Co1	131.2(2)
C11	N3	Co1	113.4(3)
C11	N3	S2	114.5(3)
S3	N4	Co1	130.4(2)
C20	N4	Co1	114.9(3)
C20	N4	S3	111.7(3)
C21	C22	C23	119.6(4)
C24	C23	C22	121.5(5)
N1	C8	C9	107.3(4)
C1	C2	C3	119.2(4)
C13	C14	C15	121.8(4)
C4	C3	C2	121.4(5)
N4	C20	C19	108.5(3)
C14	C13	C12	119.9(4)
N2	C9	C8	110.5(3)
C2	C1	S1	119.0(3)
C6	C1	S1	120.8(3)

Atom	Atom	Atom	Angle/°
C6	C1	C2	120.2(4)
C17	C16	C15	121.8(4)
C13	C12	S2	119.7(3)
C17	C12	S2	120.9(3)
C17	C12	C13	118.9(4)
C25	C26	C21	119.3(4)
N2	C10	C11	111.2(4)
C14	C15	C18	121.2(5)
C16	C15	C14	117.2(4)
C16	C15	C18	121.7(4)
C22	C21	S3	120.5(3)
C22	C21	C26	120.0(4)
C26	C21	S3	119.5(3)
C16	C17	C12	120.2(4)
C3	C4	C5	118.3(4)
C3	C4	C7	120.3(5)
C5	C4	C7	121.4(5)
N3	C11	C10	107.7(3)
C23	C24	C25	118.1(4)
C23	C24	C27	121.9(5)
C25	C24	C27	120.0(5)
C1	C6	C5	119.8(4)
C4	C5	C6	121.1(5)
N2	C19	C20	110.7(3)
C26	C25	C24	121.4(4)
O8	Co2	N6	169.17(12)
N5	Co2	O8	92.68(12)
N5	Co2	N6	80.94(13)
N8	Co2	O8	94.83(12)
N8	Co2	N6	82.03(14)
N8	Co2	N5	125.64(14)
N7	Co2	O8	109.01(13)
N7	Co2	N6	81.73(14)
N7	Co2	N5	116.16(15)
N7	Co2	N8	111.76(14)
O9	S4	O10	115.48(18)
O9	S4	N5	112.48(19)
O9	S4	C28	104.22(19)
O10	S4	N5	109.78(18)
O10	S4	C28	104.68(19)
N5	S4	C28	109.6(2)
O11	S5	O12	116.33(17)
O11	S5	N7	112.99(18)
O11	S5	C39	105.74(19)
O12	S5	N7	107.30(18)
O12	S5	C39	105.0(2)
N7	S5	C39	109.01(19)
O13	S6	O14	115.29(18)
O13	S6	N8	112.63(19)
O13	S6	C48	104.33(19)
O14	S6	N8	109.49(19)
O14	S6	C48	107.57(19)
N8	S6	C48	106.96(18)
Co2	O8	Sr2	118.40(11)
S6	O14	Sr2	148.21(18)
S5	O12	Sr2	162.13(18)
C36	N6	Co2	107.9(3)
C36	N6	C37	111.8(3)

Atom	Atom	Atom	Angle/°
C37	N6	Co2	106.8(3)
C46	N6	Co2	104.9(3)
C46	N6	C36	111.9(3)
C46	N6	C37	112.9(3)
S4	N5	Co2	131.8(2)
C35	N5	Co2	113.8(3)
C35	N5	S4	113.5(3)
S6	N8	Co2	131.4(2)
C47	N8	Co2	114.2(3)
C47	N8	S6	112.5(3)
S5	N7	Co2	129.6(2)
C38	N7	Co2	113.9(3)
C38	N7	S5	115.9(3)
N8	C47	C46	108.3(4)
C44	C43	C42	122.8(4)
C42	C41	C40	120.6(5)
C50	C51	C54	120.9(4)
C52	C51	C50	118.4(4)
C52	C51	C54	120.6(4)
C29	C28	S4	119.1(3)
C29	C28	C33	120.2(4)
C33	C28	S4	120.5(3)
C49	C48	S6	118.6(3)
C49	C48	C53	120.1(4)
C53	C48	S6	121.3(3)
C43	C42	C41	117.7(5)
C43	C42	C45	121.5(5)
C41	C42	C45	120.8(5)
N6	C36	C35	111.0(3)
C30	C29	C28	119.0(4)
N5	C35	C36	107.1(3)
C51	C50	C49	121.0(4)
C48	C49	C50	119.5(4)
N7	C38	C37	108.0(3)
C30	C31	C32	117.7(5)
C30	C31	C34	121.8(5)
C32	C31	C34	120.5(5)
C52	C53	C48	119.4(4)
C39	C40	C41	120.0(5)
C31	C30	C29	122.1(5)
C43	C44	C39	119.2(4)
N6	C37	C38	110.0(4)
C33	C32	C31	122.2(5)
N6	C46	C47	111.6(4)
C40	C39	S5	119.7(4)
C44	C39	S5	120.5(3)
C44	C39	C40	119.7(4)
C32	C33	C28	118.7(4)
C51	C52	C53	121.5(4)
N9	Co3	N11	113.71(15)
N9	Co3	N12	124.13(15)
N9	Co3	N10	83.14(15)
N11	Co3	N10	84.54(14)
N12	Co3	N11	118.92(15)
N12	Co3	N10	84.39(14)
O15	S7	N9	106.70(18)
O15	S7	C55	108.31(19)
O16	S7	O15	116.30(18)
O16	S7	N9	113.60(19)
O16	S7	C55	105.8(2)
N9	S7	C55	105.52(19)
O17	S8	O18	116.80(18)
O17	S8	N11	113.3(2)
O17	S8	C66	106.9(2)
O18	S8	N11	106.34(18)
O18	S8	C66	106.7(2)
N11	S8	C66	106.26(19)
O19	S9	N12	107.45(18)
O19	S9	C75	105.82(19)
O20	S9	O19	115.83(18)
O20	S9	N12	113.89(19)
O20	S9	C75	104.69(19)
N12	S9	C75	108.6(2)
S7	O15	$Sr2^{1}$	150.26(17)
S9	O20	Sr1	164.3(2)
S7	N9	Co3	125.6(2)
C62	N9	Co3	116.1(3)
C62	N9	S7	115.3(3)
S8	N11	Co3	128.0(2)
C65	N11	Co3	114.0(3)
C65	N11	S8	118.0(3)
S9	N12	Co3	129.2(2)
C74	N12	Co3	113.3(3)
C74	N12	S9	117.2(3)
C63	N10	Co3	106.0(3)
C63	N10	C64	110.9(4)
C64	N10	Co3	105.7(3)
C73	N10	Co3	106.2(3)
C73	N10	C63	114.2(4)
C73	N10	C64	113.1(4)
N9	C62	C63	107.0(4)
C77	C78	C79	117.2(4)
C77	C78	C81	122.4(4)
C79	C78	C81	120.4(4)
C76	C77	C78	121.5(4)
C77	C76	C75	120.6(4)
N10	C63	C62	112.4(4)
N10	C64	C65	111.6(4)
N11	C65	C64	109.2(4)
N12	C74	C73	106.5(3)
N10	C73	C74	111.7(4)
C56	C55	S7	121.2(3)
C56	C55	C60	120.6(4)
C60	C55	S7	118.1(3)
C55	C56	C57	119.6(4)
C56	C57	C58	121.6(4)
C57	C58	C59	117.6(4)
C57	C58	C61	121.9(5)
C59	C58	C61	120.5(4)
C60	C59	C58	121.8(4)
C59	C60	C55	118.7(4)
C76	C75	S9	119.7(3)
C76	C75	C80	119.3(4)
C80	C75	S9	121.0(3)
C79	C80	C75	119.3(4)
C80	C79	C78	122.0(4)

Atom	Atom	Atom	Angle/°
C67	C66	S8	121.1(3)
C67	C66	C71	120.2(4)
C71	C66	S8	118.5(4)
C68	C67	C66	119.5(4)
C67	C68	C69	121.5(5)
C68	C69	C72	121.6(5)
C70	C69	C68	118.5(5)
C70	C69	C72	119.9(5)
C71	C70	C69	120.7(4)
C70	C71	C66	119.5(4)
N13	Co4	N15	122.49(15)
N13	Co4	N16	116.75(15)
N13	Co4	N14	84.30(14)
N15	Co4	N14	84.18(13)
N16	Co4	N15	117.80(15)
N16	Co4	N14	84.33(14)
O21	S10	N13	105.75(17)
O21	S10	C82	108.48(18)
O22	S10	O21	116.18(17)
O22	S10	N13	114.07(18)
O22	S10	C82	106.20(18)
N13	S10	C82	105.57(19)
O23	S11	O24	114.78(17)
O23	S11	N15	113.56(18)
O23	S11	C93	106.30(18)
O24	S11	N15	107.19(18)
O24	S11	C93	105.99(18)
N15	S11	C93	108.63(19)
O25	S12	N16	105.87(18)
O25	S12	C102	105.32(19)
O26	S12	O25	117.47(18)
O26	S12	N16	112.78(18)
O26	S12	C102	106.44(19)
N16	S12	C102	108.45(18)
S10	O21	Sr1	149.47(16)
S11	O23	Sr2	154.12(18)
S12	O25	Sr1	173.32(19)
S10	N13	Co4	124.40(19)
C89	N13	Co4	115.2(3)
C89	N13	S10	118.0(3)
S11	N15	Co4	124.51(19)
C92	N15	Co4	113.7(3)
C92	N15	S11	119.2(3)
S12	N16	Co4	124.6(2)
C101	N16	Co4	115.0(3)
C101	N16	S12	119.9(3)
C90	N14	Co4	105.1(3)
C90	N14	C91	113.1(4)
C90	N14	C100	113.6(4)
C91	N14	Co4	105.9(3)
C100	N14	Co4	105.8(3)
C100	N14	C91	112.4(4)
N13	C89	C90	107.4(3)
N14	C90	C89	112.4(4)
N14	C91	C92	112.0(4)
N15	C92	C91	108.4(3)
N16	C101	C100	108.5(4)
N14	C100	C101	112.5(4)
C83	C82	S10	118.6(3)
C87	C82	S10	121.0(3)
C87	C82	C83	120.3(4)
C84	C83	C82	119.2(4)
C83	C84	C85	121.2(4)
C84	C85	C88	120.3(4)
C86	C85	C84	118.7(4)
C86	C85	C88	120.9(4)
C85	C86	C87	120.6(4)
C82	C87	C86	119.9(4)
C103	C102	S12	120.9(3)
C103	C102	C107	120.3(4)
C107	C102	S12	118.7(3)
C102	C103	C104	120.5(4)
C103	C104	C105	120.4(5)
C104	C105	C108	121.2(5)
C106	C105	C104	118.5(4)
C106	C105	C108	120.3(5)
C105	C106	C107	121.5(4)
C106	C107	C102	118.8(4)
C94	C93	S11	119.1(3)
C94	C93	C98	119.2(4)
C98	C93	S11	121.7(3)
C95	C94	C93	120.5(4)
C94	C95	C96	121.0(4)
C95	C96	C99	120.4(4)
C97	C96	C95	117.8(4)
C97	C96	C99	121.8(4)
C96	C97	C98	122.3(4)
C97	C98	C93	119.1(4)

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

Table S16: Hydrogen Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **CMW-03-086SRTS**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H22	1339	537	383	34
H23	724	1384	105	38
H8A	4081	242	1269	34
H8B	4162	1139	1529	34
H2	3586	893	2925	33
H14	4469	4453	3537	41

Atom	x	y	z	U_{eq}
H3	4106	1275	3626	43
H20A	2437	1620	305	30
H20B	2815	908	383	30
H13	3765	4299	3069	38
H9A	3963	1356	636	33
H9B	3530	763	641	33
H16	4914	2400	2872	41
H26	1926	2448	1202	33
H10A	3761	2952	804	36
H10B	4018	2448	1279	36
H17	4205	2208	2427	35
H18A	5242	4078	3730	62
H18B	5460	3415	3367	62
H18C	5232	3116	3872	62
H11A	3706	3569	1647	37
H11B	3225	3430	1314	37
H6	4536	-599	2395	33
H5	5047	-223	3102	40
H7A	5033	1406	3863	78
H7B	5235	488	3893	78
H7C	4817	724	4214	78
H19A	3205	2091	210	31
H19B	2945	2623	612	31
H25	1318	3289	905	38
H27A	393	2751	-7	64
H27B	659	3527	259	64
H27C	345	2969	590	64
H47A	1120	5845	3762	33
H47B	888	6550	3388	33
H43	4121	6092	3665	37
H41	4077	5014	5058	59
H36A	2320	7427	4630	31
H36B	1843	7905	4589	31
H29	3353	7083	4078	35
H35A	1946	8399	3762	31
H35B	2416	8571	4111	31
H50	128	6407	1412	36
H49	602	5515	1934	31
H38A	2561	6102	4714	33
H38B	2326	5212	4747	33
H53	1266	7494	2594	31
H54A	-49	7780	1077	56
H54B	233	8558	1316	56
H54C	-175	8190	1609	56
H40	3334	4583	4809	49
H30	4009	7324	4632	41
H44	3385	5689	3414	30
H37A	1618	5739	4450	35
H37B	1820	6356	4900	35
H32	4027	9687	4164	47
H46A	1341	7561	3787	32
H46B	1158	7037	4250	32
H34A	4406	9030	5129	88
H34B	4723	8992	4662	88
H34C	4622	8169	4974	88
H33	3378	9476	3599	35
H52	773	8368	2095	33
H45A	4871	5486	4399	71

Atom	x	y	z	U_{eq}
H45B	4716	5886	4920	71
H45C	4708	6428	4401	71
H62A	3953	-3691	1114	39
H62B	4132	-3031	1552	39
H77	1117	-2843	245	35
H76	1719	-3033	872	35
H63A	3661	-2029	1205	42
H63B	3845	-2451	706	42
H64A	3448	-3695	404	46
H64B	3194	-3032	18	46
H65A	2496	-3530	151	34
H65B	2797	-4345	98	34
H74A	2999	-1316	1347	33
H74B	2506	-1186	1035	33
H73A	2651	-2146	409	41
H73B	3098	-1584	481	41
H56	4560	-4497	2606	31
H57	5073	-3748	3160	37
H59	4189	-1853	3136	34
H60	3681	-2575	2554	32
H61A	5165	-2593	3832	62
H61B	4855	-1788	3727	62
H61C	5249	-1983	3363	62
H80	1506	-764	1455	30
H79	897	-587	829	35
H81A	636	-1158	-194	64
H81B	288	-1343	229	64
H81C	464	-2082	-111	64
H67	1552	-4753	1262	33
H68	832	-4558	842	41
H70	1333	-4709	-558	35
H71	2058	-4945	-141	31
H72A	413	-4942	-316	79
H72B	573	-4034	-462	79
H72C	350	-4187	70	79
H89A	2487	1989	4700	27
H89B	2071	1348	4685	27
H90A	1734	2615	4756	47
H90B	2035	3028	4343	47
H91A	1275	3543	4046	52
H91B	1010	3010	3589	52
H92A	1439	3904	3167	28
H92B	1877	3764	3576	28
H10C	780	809	3833	29
H10D	712	1637	3492	29
H10E	916	2123	4315	52
H10F	1291	1418	4434	52
H83	3065	2455	3738	28
H84	3721	3160	4055	35
H86	4098	1244	5000	34
H87	3437	533	4688	29
H88A	4655	2570	4526	59
H88B	4504	2571	5105	59
H88C	4359	3318	4718	59
H103	319	-192	2888	33
H104	-195	-79	2152	41
H106	804	803	1340	37
H107	1325	684	2081	30

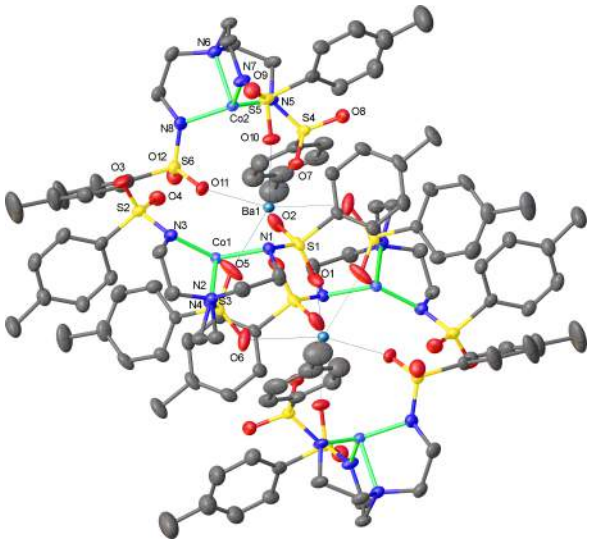
Atom	x	y	z	U_{eq}
H10G	-352	152	1240	79
H10H	66	192	891	79
H10I	-136	1025	1111	79
H94	920	2073	2632	28
H95	167	2149	2288	31
H97	456	4149	1455	30
H98	1211	4098	1802	28
H99A	-285	2727	1305	47
H99B	-316	3696	1418	47
H99C	-454	3043	1840	47
H1A	2847	1671	2555	26
H1B	2400	1677	2189	26
H8C	2684	6723	2842	26
H8D	2248(8)	6512(13)	2490(11)	26

CMW-03-052

EMORY UNIVERSITY | X-ray Crystallography Center

Submitted by: **Christian Wallen**
Emory University
Solved by: **John Bacsa**
Sample ID: **CMW-03-052**

Crystal Data and Experimental



Experimental. Single violet prism-shaped crystals of (**CMW-03-052**) were recrystallised from a mixture of CH_2Cl_2 and diethyl ether by vapor diffusion. A suitable crystal (0.48×0.35×0.27) was selected and mounted on a loop with paratone oil on a Bruker APEX-II CCD diffractometer. The crystal was cooled to T = 100(2) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program using combined Patterson and dual-space recycling methods and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The crystal structure was refined with version of **ShelXL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{112}H_{138}Ba_2Co_4N_{18}O_{24}S_{12}$, M_r = 3015.52, triclinic, P-1 (No. 2), a = 15.199(3) Å, b = 15.322(3) Å, c = 16.472(4) Å, α = 116.330(3)°, β = 93.430(3)°, γ = 102.116(3)°, V = 3309.8(12) Å^3, T = 100(2) K, Z = 1, Z' = 0.5, μ(MoK$_\alpha$) = 1.336, 60531 reflections measured, 20361 unique (R_{int} = 0.0387) which were used in all calculations. The final wR_2 was 0.1429 (all data) and R_1 was 0.0502 (I > 2σ(I)).

Compound	**CMW-03-052**
Formula	$C_{112}H_{138}Ba_2Co_4N_{18}O_{24}S_{12}$
$D_{calc.}$/ g cm^{-3}	1.513
μ/mm^{-1}	1.336
Formula Weight	3015.52
Colour	violet
Shape	prism
Max Size/mm	0.48
Mid Size/mm	0.35
Min Size/mm	0.27
T/K	100(2)
Crystal System	triclinic
Space Group	P-1
a/Å	15.199(3)
b/Å	15.322(3)
c/Å	16.472(4)
α/°	116.330(3)
β/°	93.430(3)
γ/°	102.116(3)
V/Å^3	3309.8(12)
Z	1
Z'	0.5
Θ_{min}/°	1.794
Θ_{max}/°	30.783
Measured Refl.	60531
Independent Refl.	20361
$I > 2\sigma(I)$	16303
R_{int}	0.0387
Parameters	846
Restraints	164
Largest Peak	2.478
Deepest Hole	-0.896
GooF	1.071
wR_2 (all data)	0.1429
wR_2	0.1293
R_1 (all data)	0.0680
R_1	0.0502
CCDC #	1434432

Structure Quality Indicators

Reflections:	d min 0.69	I/σ 15.4	Rint 3.87%	complete 98%
Refinement:	Shift -0.030	Max Peak 2.5	Min Peak -0.9	GooF 1.071

A violet prism-shaped crystal with dimensions 0.48×0.35×0.27 mm was mounted on a loop with paratone oil.X-ray diffraction data were collected using a Bruker APEX-II CCD diffractometer equipped with an Oxford Cryosystems low-temperature apparatus operating at T = 100(2) K.

Data were measured using ω scans with MoK$_\alpha$ radiation (fine-focus sealed tube, 45 kV, 35 mA). The total number of runs and images was based on the strategy calculation from the program **APEX2** (Bruker, 2014). The maximum resolution achieved was Θ = 30.783°.

Unit cell indexing was performed by using the **APEX2** (Bruker) software and refined using **SAINT** (Bruker, V8.34A, 2013) on 9976 reflections, 16% of the observed reflections. Data reduction, scaling and absorption corrections were performed using **SAINT** (Bruker, V8.34A, 2013) and **SADABS-2014/2** (Bruker, 2014) was used for absorption correction. wR_2(int) was 0.0844 before and 0.0456 after correction. The ratio of minimum to maximum transmission is 0.8376. The $\lambda/2$ correction factor is Not present. The software corrects for Lorentz polarisation. The final completeness is 99.6% out to 30.783° in Θ. The absorption coefficient (μ) of this material is 1.336 mm^{-1} and the minimum and maximum transmissions are 0.6249 and 0.7461.

The structure was solved in the space group P1 with the **ShelXT** (Sheldrick, 2015) structure solution program using combined Patterson and dual-space recycling methods. The space group P-1 (# 2) was determined by the **ShelXT** (Sheldrick, 2015) structure solution program. The crystal structure was refined by Least Squares using version of **ShelXL** (Sheldrick, 2008). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

The value of Z' is 0.5. This means that only half of the formula unit is present in the asymmetric unit, with the other half consisting of symmetry equivalent atoms.

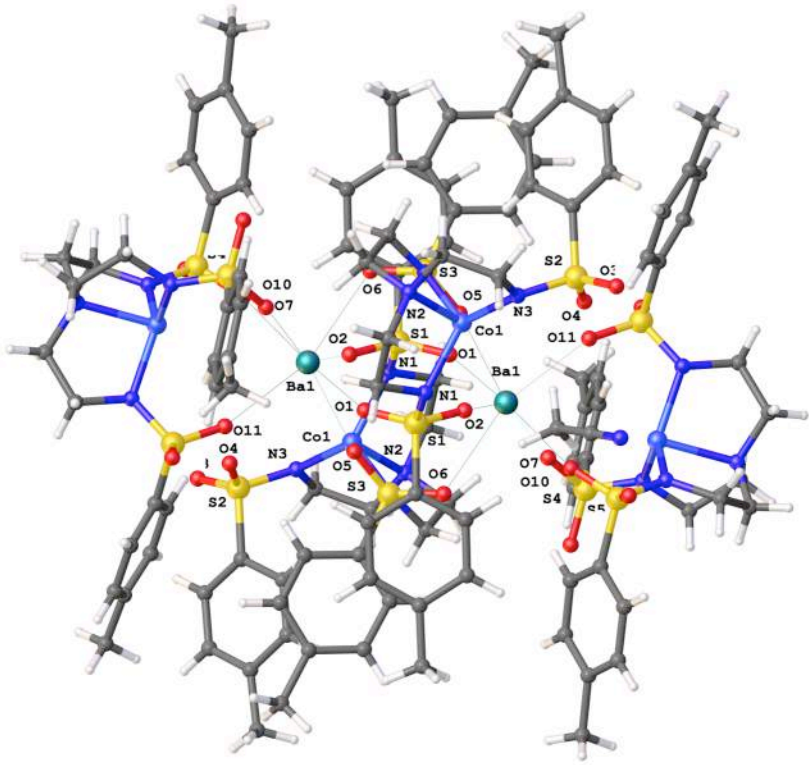

O10
O7
S3
O6
O5
N2
S1
Co1
N3
S2
O4
O11
O2
N1
O1
Ba1
Ba1
N1
O1
O2
Co1
S1
O11
O4
N3
N2
O5
O6
S3
S2
O7
O10
S4

Figure S16:

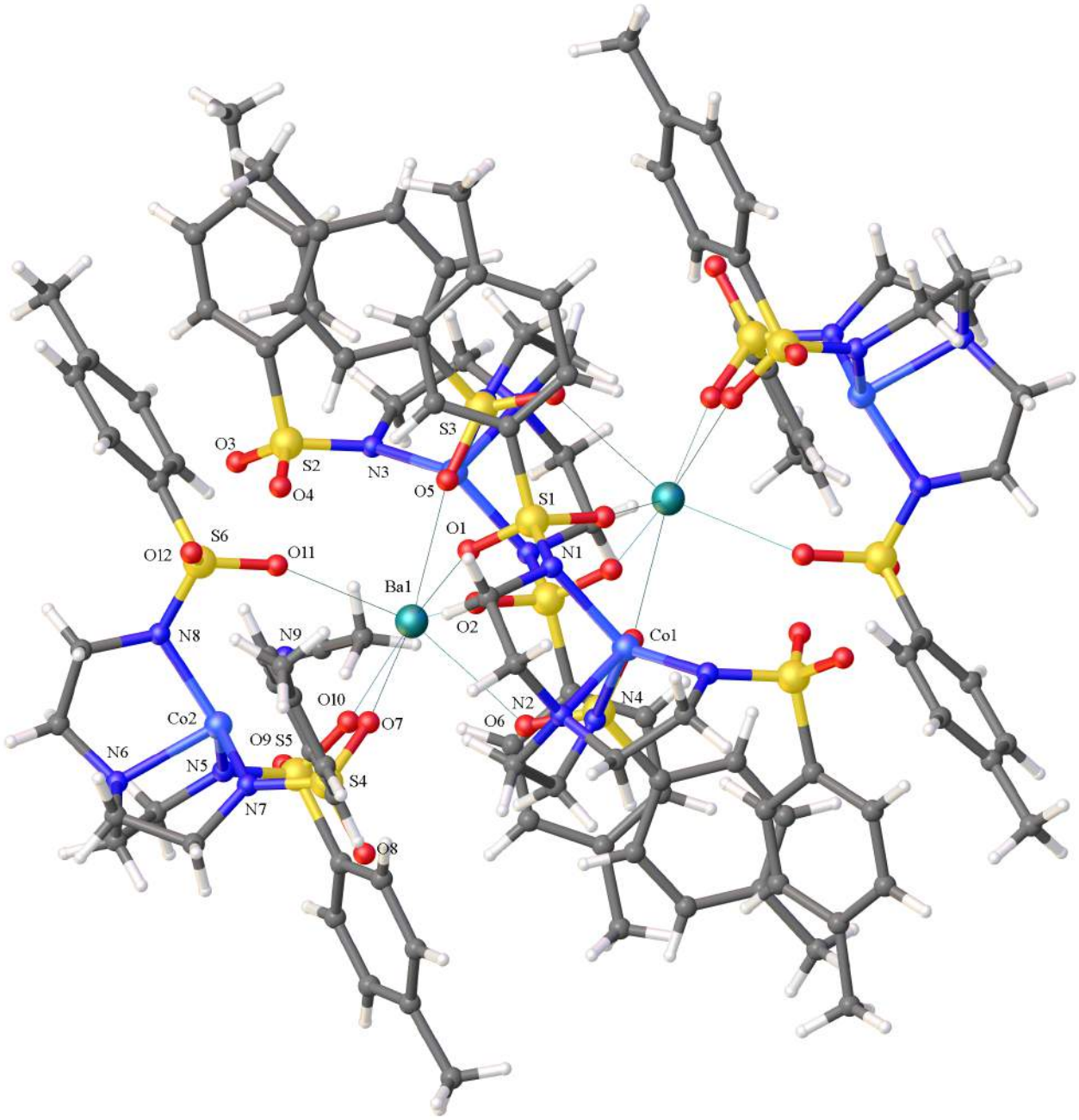
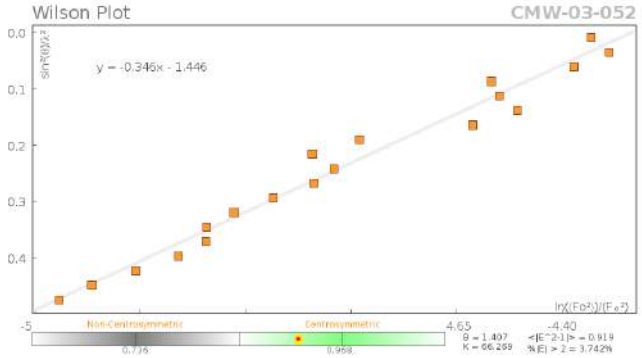
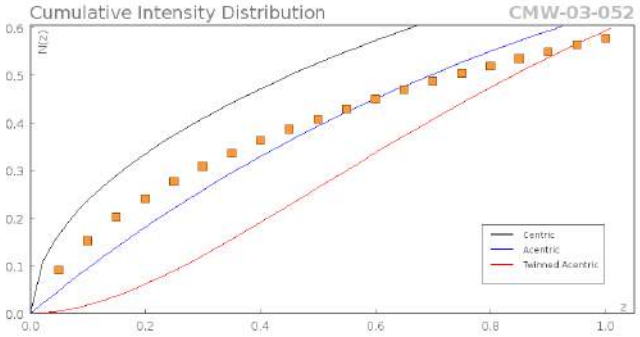
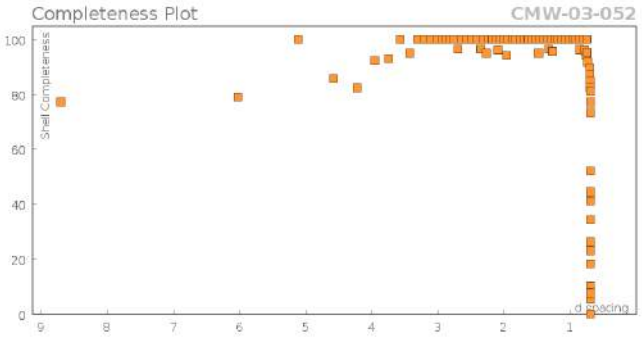

O3
S2
O4
N3
S3
O5
S1
O1
N1
S6
O12
O11
Ba1
O2
Co1
N8
N9
O10
O7
N2
N4
O6
Co2
N6
O9
S5
N5
S4
N7
O8

Figure S17:

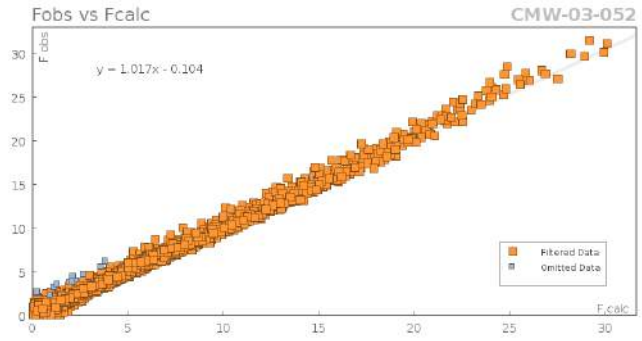
Data Plots: Diffraction Data

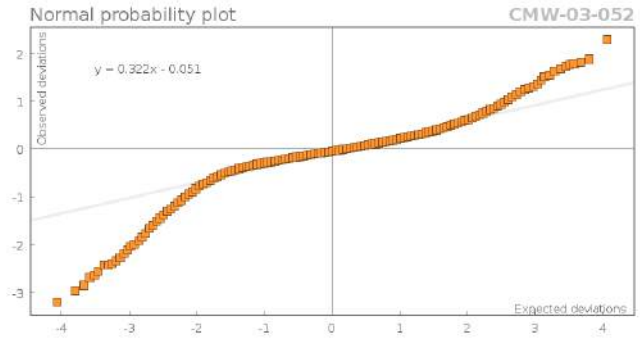






Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	60588	Unique reflections	20361
Completeness	0.984	Mean I/σ	15.43
hklsub>max</sub> collected	(21, 21, 22)	hklsub>min</sub> collected	(-21, -22, -23)
hkl_{max} used	(21, 19, 23)	hkl_{min} used	(-21, -22, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.36
d_{max} used	11.44	d_{min} used	0.69
Friedel pairs	18091	Friedel pairs merged	1
Inconsistent equivalents	0	R_{int}	0.0387
R_{sigma}	0.0452	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	57
Multiplicity	(20254, 14798, 2918, 496)	Maximum multiplicity	8
Removed systematic absences	0	Filtered off (Shel/OMIT)	0

Images of the Crystal on the Diffractometer

Table S17: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **CMW-03-052**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Ba1	-562.3(2)	1178.1(2)	6383.4(2)	17.06(5)
Co1	2631.4(3)	2175.4(3)	6388.8(3)	17.94(9)
Co2	-1568.7(3)	2952.8(3)	8438.1(3)	17.82(9)
S1	1212.2(5)	1829.1(6)	4931.2(6)	22.28(16)
S2	3279.5(6)	3621.6(7)	8498.1(6)	24.98(17)
S3	1635.9(5)	-22.7(7)	6101.6(6)	23.87(17)
S4	-3168.2(5)	1294.4(6)	6911.5(6)	22.77(16)
S5	-631.8(6)	4139.0(6)	7484.2(6)	23.02(16)
S6	-677.6(6)	1674.4(7)	9019.0(6)	24.28(16)
O1	1085.9(19)	817(2)	4211(2)	37.5(7)
O2	816.4(19)	1957(2)	5753(2)	35.9(6)
O3	3685(2)	4685(2)	9090.5(19)	36.5(6)
O4	2302.8(18)	3246(2)	8419.9(19)	33.6(6)
O5	912.1(18)	471(3)	6323(3)	47.1(9)
O6	1427(2)	-960(2)	5239.6(19)	40.3(7)
O7	-2339.5(16)	1026.8(19)	6581.9(17)	26.6(5)
O8	-3792.0(18)	1393(2)	6283.6(18)	31.0(6)
O9	165.9(19)	4962(2)	7717(2)	32.0(6)
O10	-524.1(19)	3123.7(19)	6964.4(18)	28.8(5)
O11	-451.5(19)	1429(2)	8107.3(17)	29.2(5)
O12	-1332(2)	884(2)	9086(2)	35.9(6)
N1	2241.4(18)	2408(2)	5326.3(19)	20.5(5)
N2	3847.5(18)	2056(2)	5829.9(19)	21.2(5)
N3	3458.5(18)	3265(2)	7479.3(19)	22.0(5)
N4	2502.8(18)	772(2)	6136(2)	20.2(5)
N5	-2835.3(19)	2249(2)	7879(2)	24.0(6)
N6	-2112.2(19)	3903(2)	9507.0(19)	22.8(5)
N7	-1046(2)	4153(2)	8335(2)	26.3(6)
N8	-953(2)	2702(2)	9354(2)	25.7(6)
C1	2891(2)	2224(3)	4667(3)	30.8(8)
C2	3847(3)	2490(3)	5196(3)	32.0(8)
C3	4620(2)	2636(3)	6624(3)	31.9(8)
C4	4409(2)	3552(3)	7359(2)	27.2(7)
C5	3844(2)	2976(3)	8947(2)	24.2(6)
C6	3676(2)	1933(3)	8435(2)	27.4(7)
C7	4109(3)	1408(3)	8750(3)	30.9(8)
C8	4719(3)	1916(3)	9589(3)	33.6(8)
C9	4879(3)	2960(3)	10093(3)	32.2(8)
C10	4448(3)	3493(3)	9777(3)	30.7(8)
C11	5213(4)	1330(4)	9907(4)	50.4(12)
C12	3809(3)	964(3)	5362(3)	29.3(7)
C13	3321(2)	418(3)	5844(3)	26.2(7)
C14	1854(2)	-357(2)	6975(2)	20.7(6)
C15	2307(2)	-1094(3)	6832(3)	26.8(7)
C16	2535(3)	-1281(3)	7567(3)	33.4(8)
C17	2301(3)	-752(4)	8420(3)	37.5(9)
C18	1825(3)	-36(3)	8530(3)	36.4(9)

Atom	x	y	z	U_{eq}
C19	1608(3)	169(3)	7823(3)	29.7(7)
C20	2589(4)	-921(5)	9219(4)	60.2(16)
C21	635(2)	2411(3)	4437(2)	21.4(6)
C22	278(3)	3185(3)	5019(3)	27.8(7)
C23	-249(3)	3596(3)	4647(3)	31.4(8)
C24	-427(2)	3252(3)	3698(3)	31.4(8)
C25	-54(3)	2486(3)	3134(3)	32.3(8)
C26	471(3)	2058(3)	3494(3)	28.8(7)
C27	-1027(3)	3687(4)	3306(4)	43.9(11)
C28	-3768(2)	291(3)	7093(3)	28.4(7)
C29	-4663(2)	-213(3)	6670(3)	34.9(9)
C30	-5106(3)	-1027(4)	6812(4)	47.7(11)
C31	-4661(4)	-1310(4)	7375(4)	50.9(12)
C32	-3773(4)	-783(4)	7799(4)	53.7(12)
C33	-3320(3)	23(3)	7669(3)	40.6(9)
C34	-5129(5)	-2208(5)	7498(6)	77(2)
C35	-3502(2)	2756(3)	8370(3)	30.1(8)
C36	-3078(2)	3357(3)	9388(3)	29.1(7)
C37	-2037(3)	4842(3)	9420(3)	27.9(7)
C38	-1161(3)	5099(3)	9062(3)	28.0(7)
C46	-1545(3)	4084(3)	10358(2)	29.2(7)
C47	-1296(3)	3112(3)	10233(2)	28.9(7)
C48	346(3)	1905(3)	9741(2)	26.7(7)
C49	1167(3)	2421(3)	9646(3)	27.4(7)
C50	1970(3)	2641(4)	10229(3)	39.0(9)
C51	1956(3)	2358(5)	10918(4)	56.3(14)
C52	1141(4)	1820(6)	10997(4)	70(2)
C53	323(3)	1578(5)	10405(4)	51.7(13)
C54	2844(4)	2650(8)	11573(6)	96(3)
C39A	-1523(6)	4263(8)	6832(6)	23.3(14)
C40A	-2277(6)	3465(7)	6274(5)	35.2(16)
C41A	-2926(6)	3630(9)	5765(5)	49(2)
C42A	-2839(7)	4568(10)	5800(7)	54(3)
C43A	-2080(9)	5349(9)	6361(9)	46(2)
C44A	-1428(7)	5211(8)	6873(9)	30.8(18)
C45A	-3557(11)	4742(15)	5235(11)	85(5)
C39B	-1414(4)	4269(5)	6729(5)	23.1(12)
C40B	-2132(5)	3431(5)	6160(5)	34.4(14)
C41B	-2764(5)	3524(7)	5578(5)	49(2)
C42B	-2696(6)	4430(7)	5552(6)	53(2)
C43B	-1973(6)	5253(6)	6127(6)	45(2)
C44B	-1337(5)	5186(5)	6710(6)	29.7(15)
C45B	-3366(9)	4510(11)	4871(10)	84(5)
N9	3155(4)	6612(4)	8121(4)	72.5(15)
C55	2742(3)	5777(4)	7677(3)	45.6(10)
C57	2197(4)	4746(4)	7159(3)	46.1(11)

Table S18: Anisotropic Displacement Parameters ($\times 10^4$) **CMW-03-052**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ba1	18.10(9)	17.12(9)	16.30(9)	7.01(7)	4.07(6)	6.87(6)
Co1	17.02(18)	17.7(2)	19.5(2)	9.20(16)	2.58(15)	4.47(15)
Co2	19.67(19)	16.49(19)	16.80(19)	6.71(16)	4.96(15)	5.74(15)
S1	18.4(3)	23.6(4)	32.0(4)	19.0(3)	3.6(3)	6.1(3)
S2	27.0(4)	23.2(4)	21.1(4)	5.5(3)	6.1(3)	10.1(3)
S3	17.4(3)	27.6(4)	31.5(4)	20.7(4)	-2.0(3)	1.5(3)
S4	17.5(3)	21.3(4)	22.6(4)	3.5(3)	3.6(3)	7.0(3)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S5	31.3(4)	16.5(3)	22.9(4)	9.4(3)	10.5(3)	7.6(3)
S6	29.8(4)	26.3(4)	20.1(4)	13.1(3)	5.3(3)	8.3(3)
O1	33.6(14)	18.5(12)	49.8(17)	9.6(12)	-11.6(12)	5.7(10)
O2	29.0(13)	55.4(18)	46.4(17)	40.2(15)	14.1(12)	17.3(12)
O3	47.4(16)	22.4(13)	29.2(14)	1.7(11)	4.5(12)	13.2(12)
O4	25.9(12)	42.9(16)	33.2(14)	15.1(12)	11.4(11)	15.8(11)
O5	19.2(12)	59(2)	99(3)	65(2)	17.7(14)	17.0(13)
O6	46.1(16)	39.3(16)	26.0(13)	19.4(12)	-10.2(12)	-12.4(13)
O7	19.7(11)	26.6(12)	26.3(12)	4.8(10)	6.5(9)	8.4(9)
O8	26.6(12)	31.8(14)	27.9(13)	7.8(11)	0(1)	10(1)
O9	33.6(13)	27.7(13)	35.9(14)	18.2(12)	7.8(11)	2.2(11)
O10	42.9(15)	20.4(12)	29.8(13)	12.9(10)	18.5(11)	15.5(11)
O11	41.7(14)	31.4(13)	16.9(11)	11.3(10)	5.8(10)	14.2(11)
O12	38.2(15)	35.6(15)	36.4(15)	21.5(13)	5.2(12)	4.6(12)
N1	21.2(12)	20.6(13)	20.9(13)	10.5(11)	3.2(10)	6(1)
N2	20.2(12)	19.6(13)	22.0(13)	8.0(11)	4(1)	5.4(10)
N3	19.8(12)	20.6(13)	22.4(13)	7.5(11)	3.9(10)	4.5(10)
N4	17.7(11)	19.4(12)	27.1(14)	13.6(11)	3.6(10)	6(1)
N5	20.6(12)	21.0(13)	23.4(13)	2.3(11)	6.4(10)	9.1(10)
N6	23.5(13)	21.2(13)	20.8(13)	7.1(11)	7.4(10)	5.4(10)
N7	38.8(16)	16.8(13)	23.7(14)	8.7(11)	15.1(12)	7.6(11)
N8	30.8(14)	29.6(15)	21.4(13)	13.7(12)	7.5(11)	12.6(12)
C1	23.4(16)	45(2)	30.2(18)	24.4(17)	6.7(13)	6.5(15)
C2	27.1(17)	40(2)	36(2)	21.6(17)	12.3(15)	10.8(15)
C3	23.1(16)	32.6(19)	31.8(19)	8.7(15)	2.9(14)	5.9(14)
C4	22.7(15)	23.5(16)	25.7(16)	5.1(13)	3.0(12)	1.7(12)
C5	24.1(15)	26.4(16)	18.3(14)	7.6(13)	5.9(12)	5.0(12)
C6	27.6(16)	26.3(17)	23.1(16)	9.6(14)	-0.4(13)	3.1(13)
C7	31.8(18)	28.6(18)	30.5(18)	14.7(15)	-0.3(14)	4.0(14)
C8	30.1(18)	39(2)	35(2)	22.3(17)	0.9(15)	5.9(15)
C9	25.3(16)	38(2)	25.8(17)	13.5(16)	-0.8(13)	-1.7(14)
C10	28.4(17)	31.4(19)	23.9(17)	8.4(14)	3.9(13)	2.1(14)
C11	52(3)	49(3)	54(3)	31(2)	-10(2)	10(2)
C12	28.1(17)	27.6(18)	32.6(18)	12.9(15)	10.1(14)	9.3(14)
C13	28.0(16)	21.4(16)	29.0(17)	9.8(13)	10.2(13)	9.5(13)
C14	20.1(13)	22.3(15)	23.3(15)	14.1(12)	3.8(11)	4.7(11)
C15	25.3(15)	30.4(18)	33.7(18)	21.0(15)	10.2(13)	10.2(13)
C16	27.3(17)	41(2)	51(2)	36(2)	9.1(16)	14.3(15)
C17	32.0(19)	51(3)	38(2)	33(2)	5.3(16)	1.7(17)
C18	38(2)	43(2)	28.6(19)	17.4(17)	11.8(16)	7.9(17)
C19	33.7(18)	27.2(18)	30.7(18)	13.5(15)	11.3(14)	11.2(14)
C20	52(3)	95(5)	56(3)	61(3)	4(2)	7(3)
C21	19.7(13)	22.4(15)	27.9(16)	16.7(13)	4.0(12)	5.9(11)
C22	33.7(18)	29.2(18)	27.6(17)	17.3(15)	7.6(14)	12.4(14)
C23	33.8(18)	31.0(19)	40(2)	22.2(17)	12.0(16)	16.0(15)
C24	25.0(16)	36(2)	48(2)	32.6(18)	3.7(15)	6.4(14)
C25	38.0(19)	37(2)	28.0(18)	21.4(16)	2.1(15)	8.2(16)
C26	31.3(17)	30.3(18)	30.5(18)	18.9(15)	7.0(14)	8.8(14)
C27	38(2)	52(3)	62(3)	44(2)	1(2)	13.9(19)
C28	27.1(16)	18.4(15)	31.7(18)	4.6(13)	10.0(13)	5.0(12)
C29	20.6(15)	31.4(19)	45(2)	10.1(17)	11.2(15)	9.1(14)
C30	28.3(19)	37(2)	65(3)	13(2)	22.0(19)	4.1(16)
C31	53(3)	35(2)	64(3)	21(2)	31(2)	10.0(19)
C32	62(3)	40(2)	62(3)	28(2)	15(2)	8(2)
C33	40(2)	32(2)	45(2)	16.8(18)	3.2(18)	4.2(17)
C34	81(4)	56(4)	98(5)	42(4)	35(4)	4(3)
C35	23.7(16)	25.6(17)	32.5(18)	4.7(14)	8.7(13)	9.0(13)
C36	27.1(16)	25.2(17)	28.2(17)	5.8(14)	13.6(13)	6.4(13)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C37	33.3(18)	21.5(16)	25.8(17)	6.5(13)	10.3(14)	10.0(13)
C38	37.0(18)	16.5(15)	27.1(17)	6.3(13)	13.2(14)	7.0(13)
C46	33.8(18)	29.9(18)	18.6(15)	7.3(13)	6.5(13)	7.1(14)
C47	36.0(18)	32.5(19)	20.6(16)	14.2(14)	10.4(13)	8.4(15)
C48	31.6(17)	35.3(19)	19.8(15)	15.2(14)	7.5(13)	15.6(14)
C49	32.6(17)	24.6(16)	25.5(16)	10.3(14)	8.7(14)	11.1(14)
C50	35(2)	43(2)	38(2)	14.9(19)	6.8(17)	17.3(18)
C51	37(2)	101(5)	47(3)	43(3)	8(2)	32(3)
C52	51(3)	142(6)	67(4)	82(4)	19(3)	43(4)
C53	43(2)	94(4)	49(3)	56(3)	16(2)	24(3)
C54	47(3)	174(9)	89(5)	81(6)	-5(3)	35(4)
C39A	29(2)	24.6(18)	21(2)	12.8(17)	13(2)	8.9(17)
C40A	35(3)	34(2)	33(3)	14(2)	6(2)	4(2)
C41A	45(3)	54(3)	42(4)	20(3)	-2(3)	11(3)
C42A	55(4)	61(3)	51(5)	29(3)	5(4)	19(3)
C43A	55(3)	49(3)	47(5)	28(3)	10(3)	23(2)
C44A	38(3)	29(2)	34(4)	19(2)	15(3)	13.1(18)
C45A	82(7)	91(8)	87(10)	47(8)	-16(7)	26(5)
C39B	30(2)	23.8(17)	21(2)	13.3(16)	12.8(18)	8.2(16)
C40B	36(3)	33(2)	33(3)	15(2)	5(2)	5.6(19)
C41B	45(3)	54(3)	42(4)	19(3)	-2(3)	10(3)
C42B	54(4)	62(3)	49(5)	30(4)	3(4)	21(3)
C43B	55(3)	49(3)	47(5)	30(3)	11(3)	22(2)
C44B	38(2)	28(2)	33(3)	20(2)	15(2)	12.7(18)
C45B	81(7)	93(8)	85(9)	48(8)	-17(7)	29(5)
N9	72(3)	67(3)	68(3)	36(2)	-11(2)	-8(2)
C55	41(2)	60(2)	41(2)	28.9(18)	4.5(17)	12.6(17)
C57	54(2)	43(2)	41(2)	13.5(18)	0.4(19)	28.9(18)

Table S19: Bond Lengths in Å for **CMW-03-052**.

Atom	Atom	Length/Å
Ba1	O1[1]	2.677(3)
Ba1	O2	2.684(3)
Ba1	O5	2.675(3)
Ba1	O6[1]	2.755(3)
Ba1	O7	2.714(2)
Ba1	O10	2.683(3)
Ba1	O11	2.681(3)
Co1	N1	2.015(3)
Co1	N2	2.120(3)
Co1	N3	1.945(3)
Co1	N4	1.963(3)
Co2	N5	1.937(3)
Co2	N6	2.075(3)
Co2	N7	1.929(3)
Co2	N8	1.948(3)
S1	O1	1.437(3)
S1	O2	1.465(3)
S1	N1	1.562(3)
S1	C21	1.764(3)
S2	O3	1.443(3)
S2	O4	1.451(3)
S2	N3	1.579(3)
S2	C5	1.786(4)
S3	O5	1.438(3)
S3	O6	1.458(3)
S3	N4	1.575(3)
S3	C14	1.764(3)
S4	O7	1.466(2)
S4	O8	1.440(3)
S4	N5	1.568(3)
S4	C28	1.772(4)
S5	O9	1.443(3)
S5	O10	1.457(3)
S5	N7	1.564(3)
S5	C39A	1.772(4)
S5	C39B	1.772(4)
S6	O11	1.459(3)
S6	O12	1.447(3)
S6	N8	1.579(3)
S6	C48	1.770(4)
O1	Ba1[1]	2.677(3)
O6	Ba1[1]	2.755(3)
N1	C1	1.486(5)
N2	C2	1.467(5)
N2	C3	1.493(5)
N2	C12	1.485(5)
N3	C4	1.471(4)
N4	C13	1.482(4)
N5	C35	1.468(4)
N6	C36	1.482(4)
N6	C37	1.490(5)
N6	C46	1.482(5)

Atom	Atom	Length/Å
N7	C38	1.468(4)
N8	C47	1.479(5)
C1	C2	1.524(5)
C3	C4	1.506(5)
C5	C6	1.393(5)
C5	C10	1.386(5)
C6	C7	1.379(5)
C7	C8	1.403(5)
C8	C9	1.393(6)
C8	C11	1.516(6)
C9	C10	1.390(6)
C12	C13	1.510(5)
C14	C15	1.383(5)
C14	C19	1.390(5)
C15	C16	1.403(5)
C16	C17	1.389(6)
C17	C18	1.389(7)
C17	C20	1.507(6)
C18	C19	1.372(6)
C21	C22	1.394(5)
C21	C26	1.386(5)
C22	C23	1.382(5)
C23	C24	1.396(6)
C24	C25	1.392(6)
C24	C27	1.505(5)
C25	C26	1.388(5)
C28	C29	1.378(5)
C28	C33	1.386(6)
C29	C30	1.410(6)
C30	C31	1.383(8)
C31	C32	1.375(8)
C31	C34	1.515(7)
C32	C33	1.392(7)
C35	C36	1.525(5)
C37	C38	1.534(5)
C46	C47	1.542(6)
C48	C49	1.388(5)
C48	C53	1.391(5)
C49	C50	1.387(6)
C50	C51	1.384(7)
C51	C52	1.384(8)
C51	C54	1.527(7)
C52	C53	1.405(7)
C39A	C40A	1.393(6)
C39A	C44A	1.400(6)
C40A	C41A	1.391(7)
C41A	C42A	1.390(9)
C42A	C43A	1.388(8)
C42A	C45A	1.532(9)
C43A	C44A	1.373(7)
C39B	C40B	1.393(5)
C39B	C44B	1.400(6)
C40B	C41B	1.390(7)
C41B	C42B	1.390(9)
C42B	C43B	1.389(8)
C42B	C45B	1.532(9)
C43B	C44B	1.373(7)
N9	C55	1.159(7)
C55	C57	1.442(7)

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

Table S20: Bond Angles in ° for **CMW-03-052**.

Atom	Atom	Atom	Angle/°
O1[1]	Ba1	O2	119.79(10)
O1[1]	Ba1	O6[1]	91.45(9)
O1[1]	Ba1	O7	82.36(9)
O1[1]	Ba1	O10	164.48(9)
O1[1]	Ba1	O11	88.07(9)
O2	Ba1	O6[1]	77.40(9)
O2	Ba1	O7	145.27(8)
O5	Ba1	O1[1]	70.39(9)
O5	Ba1	O2	64.18(9)
O5	Ba1	O6[1]	117.55(11)
O5	Ba1	O7	149.45(8)
O5	Ba1	O10	125.05(9)
O5	Ba1	O11	85.71(10)
O7	Ba1	O6[1]	75.53(9)
O10	Ba1	O2	72.96(9)
O10	Ba1	O6[1]	82.56(9)
O10	Ba1	O7	82.28(8)
O11	Ba1	O2	123.96(9)
O11	Ba1	O6[1]	155.04(10)
O11	Ba1	O7	79.69(8)
O11	Ba1	O10	91.38(8)
N1	Co1	N2	83.91(11)
N3	Co1	N1	120.23(12)
N3	Co1	N2	83.56(11)
N3	Co1	N4	119.42(12)
N4	Co1	N1	117.25(12)
N4	Co1	N2	84.93(11)
N5	Co2	N6	84.37(11)
N5	Co2	N8	120.72(14)
N7	Co2	N5	117.77(14)
N7	Co2	N6	84.55(12)
N7	Co2	N8	119.28(14)
N8	Co2	N6	86.13(12)
O1	S1	O2	117.56(19)
O1	S1	N1	112.79(16)
O1	S1	C21	105.16(17)
O2	S1	N1	103.41(16)
O2	S1	C21	105.11(16)
N1	S1	C21	112.79(15)
O3	S2	O4	117.41(18)
O3	S2	N3	112.90(17)
O3	S2	C5	105.97(17)
O4	S2	N3	105.63(16)
O4	S2	C5	108.00(17)

Atom	Atom	Atom	Angle/°
N3	S2	C5	106.36(16)
O5	S3	O6	115.9(2)
O5	S3	N4	107.39(16)
O5	S3	C14	106.31(18)
O6	S3	N4	111.80(17)
O6	S3	C14	105.71(17)
N4	S3	C14	109.52(15)
O7	S4	N5	105.95(15)
O7	S4	C28	106.12(17)
O8	S4	O7	115.85(16)
O8	S4	N5	114.80(16)
O8	S4	C28	106.37(18)
N5	S4	C28	107.13(17)
O9	S5	O10	116.50(17)
O9	S5	N7	113.85(17)
O9	S5	C39A	108.9(4)
O9	S5	C39B	104.1(3)
O10	S5	N7	105.64(15)
O10	S5	C39A	107.4(4)
O10	S5	C39B	105.0(3)
N7	S5	C39A	103.6(4)
N7	S5	C39B	111.5(3)
O11	S6	N8	105.56(16)
O11	S6	C48	106.59(16)
O12	S6	O11	115.94(17)
O12	S6	N8	114.62(18)
O12	S6	C48	105.72(18)
N8	S6	C48	107.94(17)
S1	O1	Ba1[1]	149.8(2)
S1	O2	Ba1	144.54(19)
S3	O5	Ba1	168.8(3)
S3	O6	Ba1[1]	123.17(18)
S4	O7	Ba1	161.06(15)
S5	O10	Ba1	163.40(15)
S6	O11	Ba1	160.14(17)
S1	N1	Co1	108.25(15)
C1	N1	Co1	112.1(2)
C1	N1	S1	117.4(2)
C2	N2	Co1	106.5(2)
C2	N2	C3	112.5(3)
C2	N2	C12	113.0(3)
C3	N2	Co1	106.4(2)
C12	N2	Co1	106.5(2)
C12	N2	C3	111.4(3)
S2	N3	Co1	124.99(16)
C4	N3	Co1	115.4(2)
C4	N3	S2	117.0(2)
S3	N4	Co1	128.94(16)
C13	N4	Co1	112.9(2)
C13	N4	S3	117.8(2)
S4	N5	Co2	124.99(16)
C35	N5	Co2	114.8(2)
C35	N5	S4	119.7(2)
C36	N6	Co2	106.6(2)
C36	N6	C37	111.8(3)
C36	N6	C46	113.0(3)
C37	N6	Co2	107.1(2)
C46	N6	Co2	105.1(2)
C46	N6	C37	112.6(3)
S5	N7	Co2	123.66(17)
C38	N7	Co2	115.6(2)
C38	N7	S5	120.3(2)
S6	N8	Co2	118.37(17)
C47	N8	Co2	112.1(2)
C47	N8	S6	118.7(2)
N1	C1	C2	108.6(3)
N2	C2	C1	111.5(3)
N2	C3	C4	111.3(3)
N3	C4	C3	108.5(3)
C6	C5	S2	118.4(3)
C10	C5	S2	121.4(3)
C10	C5	C6	120.2(4)
C7	C6	C5	120.2(3)
C6	C7	C8	120.5(4)
C7	C8	C11	119.6(4)
C9	C8	C7	118.6(4)
C9	C8	C11	121.8(4)
C10	C9	C8	121.2(3)
C5	C10	C9	119.4(4)
N2	C12	C13	111.8(3)
N4	C13	C12	110.5(3)
C15	C14	S3	120.4(3)
C15	C14	C19	120.7(3)
C19	C14	S3	118.8(3)
C14	C15	C16	118.7(4)
C17	C16	C15	121.0(4)
C16	C17	C18	118.6(4)
C16	C17	C20	120.6(5)
C18	C17	C20	120.8(5)
C19	C18	C17	121.3(4)
C18	C19	C14	119.7(4)
C22	C21	S1	117.8(3)
C26	C21	S1	121.4(3)
C26	C21	C22	120.6(3)
C23	C22	C21	119.4(3)
C22	C23	C24	121.1(4)
C23	C24	C27	120.2(4)
C25	C24	C23	118.3(3)
C25	C24	C27	121.5(4)
C26	C25	C24	121.4(4)
C21	C26	C25	119.1(4)
C29	C28	S4	120.7(3)
C29	C28	C33	120.7(4)
C33	C28	S4	118.6(3)
C28	C29	C30	118.8(4)
C31	C30	C29	121.0(4)
C30	C31	C34	120.8(5)
C32	C31	C30	118.8(5)
C32	C31	C34	120.3(6)
C31	C32	C33	121.3(5)
C28	C33	C32	119.3(4)
N5	C35	C36	107.4(3)
N6	C36	C35	110.5(3)
N6	C37	C38	110.7(3)
N7	C38	C37	107.8(3)
N6	C46	C47	110.5(3)

Atom	Atom	Atom	Angle/°
N8	C47	C46	107.1(3)
C49	C48	S6	119.7(3)
C49	C48	C53	120.3(4)
C53	C48	S6	120.0(3)
C50	C49	C48	120.4(4)
C51	C50	C49	120.2(4)
C50	C51	C52	119.4(4)
C50	C51	C54	118.8(5)
C52	C51	C54	121.8(5)
C51	C52	C53	121.2(5)
C48	C53	C52	118.4(5)
C40A	C39A	S5	123.2(6)
C40A	C39A	C44A	120.1(4)
C44A	C39A	S5	116.7(6)
C41A	C40A	C39A	118.9(5)
C42A	C41A	C40A	121.6(5)
C41A	C42A	C45A	121.2(6)
C43A	C42A	C41A	118.3(5)
C43A	C42A	C45A	120.5(6)
C44A	C43A	C42A	121.6(5)
C43A	C44A	C39A	119.6(4)
C40B	C39B	S5	118.0(4)
C40B	C39B	C44B	120.1(4)
C44B	C39B	S5	121.9(4)
C41B	C40B	C39B	118.9(5)
C42B	C41B	C40B	121.6(5)
C41B	C42B	C45B	121.2(6)
C43B	C42B	C41B	118.3(5)
C43B	C42B	C45B	120.5(6)
C44B	C43B	C42B	121.5(5)
C43B	C44B	C39B	119.6(4)
N9	C55	C57	177.0(6)

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

Table S21: Hydrogen Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **CMW-03-052**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H1A	2881	2637	4361	37
H1B	2717	1521	4203	37
H2A	4252	2240	4764	38
H2B	4078	3219	5541	38
H3A	5167	2847	6411	38
H3B	4739	2204	6882	38
H4A	4821	3801	7933	33
H4B	4488	4084	7180	33
H6	3270	1589	7879	33
H7	3995	711	8403	37
H9	5281	3306	10652	39
H10	4564	4190	10118	37
H11A	4793	941	10113	76
H11B	5705	1792	10404	76
H11C	5453	885	9406	76
H12A	4426	886	5346	35
H12B	3495	661	4732	35
H13A	3139	-303	5432	31
H13B	3732	538	6379	31
H15	2457	-1458	6260	32
H16	2848	-1767	7482	40
H18	1650	311	9093	44
H19	1298	658	7912	36
H20A	2723	-1565	8992	90
H20B	2103	-908	9567	90
H20C	3124	-398	9606	90
H22	392	3422	5652	33
H23	-489	4111	5034	38
H25	-159	2256	2501	39
H26	710	1542	3108	35
H27A	-1573	3703	3570	66
H27B	-1186	3276	2651	66
H27C	-705	4361	3446	66
H29	-4970	-19	6299	42
H30	-5707	-1378	6523	57

Atom	x	y	z	U_{eq}
H32	-3470	-968	8180	64
H33	-2722	377	7967	49
H34A	-5775	-2274	7446	115
H34B	-4891	-2110	8094	115
H34C	-5018	-2811	7032	115
H35A	-4065	2263	8281	36
H35B	-3639	3205	8140	36
H36A	-3421	3836	9708	35
H36B	-3107	2901	9654	35
H37A	-2032	5397	10015	34
H37B	-2564	4750	8999	34
H38A	-1209	5562	8818	34
H38B	-639	5417	9558	34
H46A	-1878	4307	10865	35
H46B	-990	4614	10507	35
H47A	-829	3263	10739	35
H47B	-1829	2626	10218	35
H49	1179	2621	9188	33
H50	2519	2980	10156	47
H52	1135	1614	11450	85
H53	-220	1209	10457	62
H54A	3301	2401	11224	144
H54B	2740	2361	11981	144
H54C	3050	3372	11924	144
H40A	-2346	2832	6243	42
H41A	-3430	3099	5391	58
H43A	-2013	5981	6391	56
H44A	-925	5744	7245	37
H45A	-3951	4103	4788	128
H45B	-3257	5093	4928	128
H45C	-3912	5138	5637	128
H40B	-2187	2819	6169	41
H41B	-3245	2967	5196	59
H43B	-1919	5865	6118	54
H44B	-859	5746	7090	36
H45D	-3322	4057	4253	126
H45E	-3218	5189	4957	126
H45F	-3978	4333	4975	126
H57A	2197	4522	6515	69
H57B	1581	4706	7273	69
H57C	2449	4325	7344	69

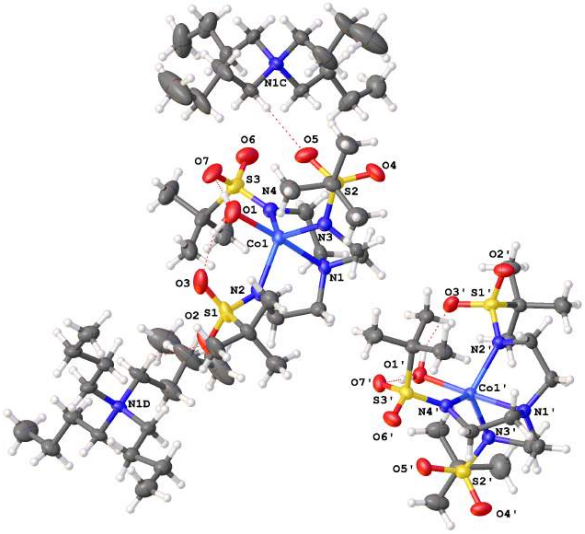
CMW-02-139aq

EMORY UNIVERSITY | X-ray Crystallography Center

Submitted by: **Christian Wallen**
Emory University
Solved by: **John Bacsa**

Sample ID: **CMW-02-139aq**

Crystal Data and Experimental



Experimental. Single violet needle-shaped crystals of (**CMW-02-139aq**) were recrystallised from --•by vapor diffusion. A suitable crystal (1.43×0.33×0.32 mm) was selected and mounted on a loop on a Bruker APEX-II CCD diffractometer. The crystal was cooled to T = 100(2) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program using combined Patterson and dual-space recycling methods and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The crystal structure was refined with version 2013-4 of **ShelXL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{68}H_{154}Co_2N_{10}O_{14}S_6$, M_r = 1646.22, monoclinic, $P2_1/c$ (No. 14), a = 16.5036(15) Å, b = 25.928(2) Å, c = 22.811(2) Å, β = 106.650(2)°, $\alpha = \gamma = 90°$, V = 9351.7(14) Å^3, T = 100(2) K, Z = 4, Z' = 1, μ(MoK$_\alpha$) = 0.545, 52521 reflections measured, 21341 unique (R_{int} = 0.0607) which were used in all calculations. The final wR_2 was 0.1613 (all data) and R_1 was 0.0600 (I > 2σ(I)).

Compound	**CMW-02-139aq**
Formula	$C_{68}H_{154}Co_2N_{10}O_{14}S_6$
$D_{calc.}$/ g cm^{-3}	1.169
μ/mm^{-1}	0.545
Formula Weight	1645.22
Colour	violet
Shape	needle
Max Size/mm	1.43
Mid Size/mm	0.33
Min Size/mm	0.32
T/K	100(2)
Crystal System	monoclinic
Space Group	$P2_1/c$
a/Å	16.5036(15)
b/Å	25.928(2)
c/Å	22.811(2)
α/°	90
β/°	106.650(2)
γ/°	90
V/Å^3	9351.7(14)
Z	4
Z'	1
Θ_{min}/°	1.826
Θ_{max}/°	27.484
Measured Refl.	52521
Independent Refl.	21341
$I > 2\sigma(I)$	12581
R_{int}	0.0607
Parameters	952
Restraints	140
Largest Peak	1.171
Deepest Hole	-0.669
GooF	1.027
wR_2 (all data)	0.1613
wR_2	0.1361
R_1 (all data)	0.1153
R_1	0.0600
CCDC #	1344433

Structure Quality Indicators

Reflections:	d min 0.77	I/σ 7.8	Rint 6.07%	complete 100%
Refinement:	Shift 0.002	Max Peak 1.2	Min Peak -0.7	GooF 1.027

A violet needle-shaped crystal with dimensions 1.43×0.33×0.32 mm was mounted on a loop with paratone oil. X-ray diffraction data were collected using a Bruker APEX-II CCD diffractometer equipped with an Oxford Cryosystems low-temperature apparatus operating at T = 100(2) K.

Data were measured using ϕ and ω scans using MoK$_\alpha$ radiation (fine-focus sealed tube, 45 kV, 35 mA). The total number of runs and images was based on the strategy calculation from the program **APEX2** (Bruker, 2013). The maximum resolution achieved was Θ = 27.484.

Unit cell indexing was performed by using the **APEX2** (Bruker, 2013) software and refined using **SAINT** (Bruker, V8.34A, 2013) on 6548 reflections, 12% of the observed reflections. Data reduction, scaling and absorption corrections were performed using **SAINT** (Bruker, V8.34A, 2013) and **SADABS-2012/1** (Bruker, 2012) was used for absorption correction.wR_2(int) was 0.0753 before and 0.0483 after correction.The Ratio of minimum to maximum transmission is 0.8728.The $\lambda/2$ correction factor is 0.0015. The software corrects for Lorentz polarisation. The final completeness is 99.7% out to 27.484° in Θ. The absorption coefficient (μ) of this material is 0.545 mm-1 and the minimum and maximum transmissions are 0.6509 and 0.7458.

The structure was solved in the space group P1 with the **ShelXT** (Sheldrick, 2015) structure solution program using combined Patterson and dual-space recycling methods. The space group $P2_1/c$ (# 14) was determined by the**ShelXT** (Sheldrick, 2015) structure solution program.The crystal structure was refined by Least Squares using version 2013-4 of **ShelXL** (Sheldrick, 2008). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

There are two independent molecules in the asymmetric unit.

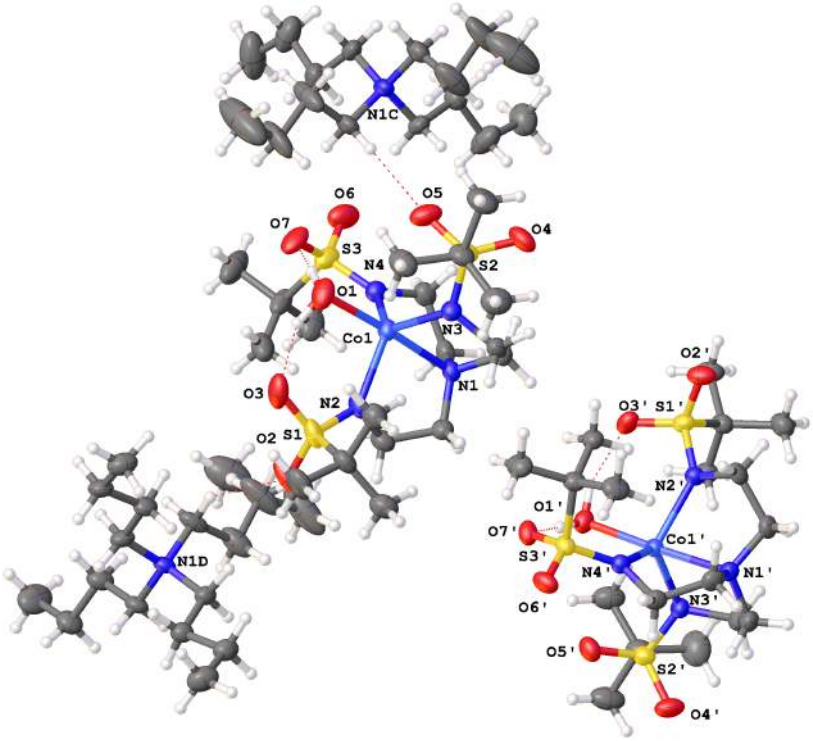
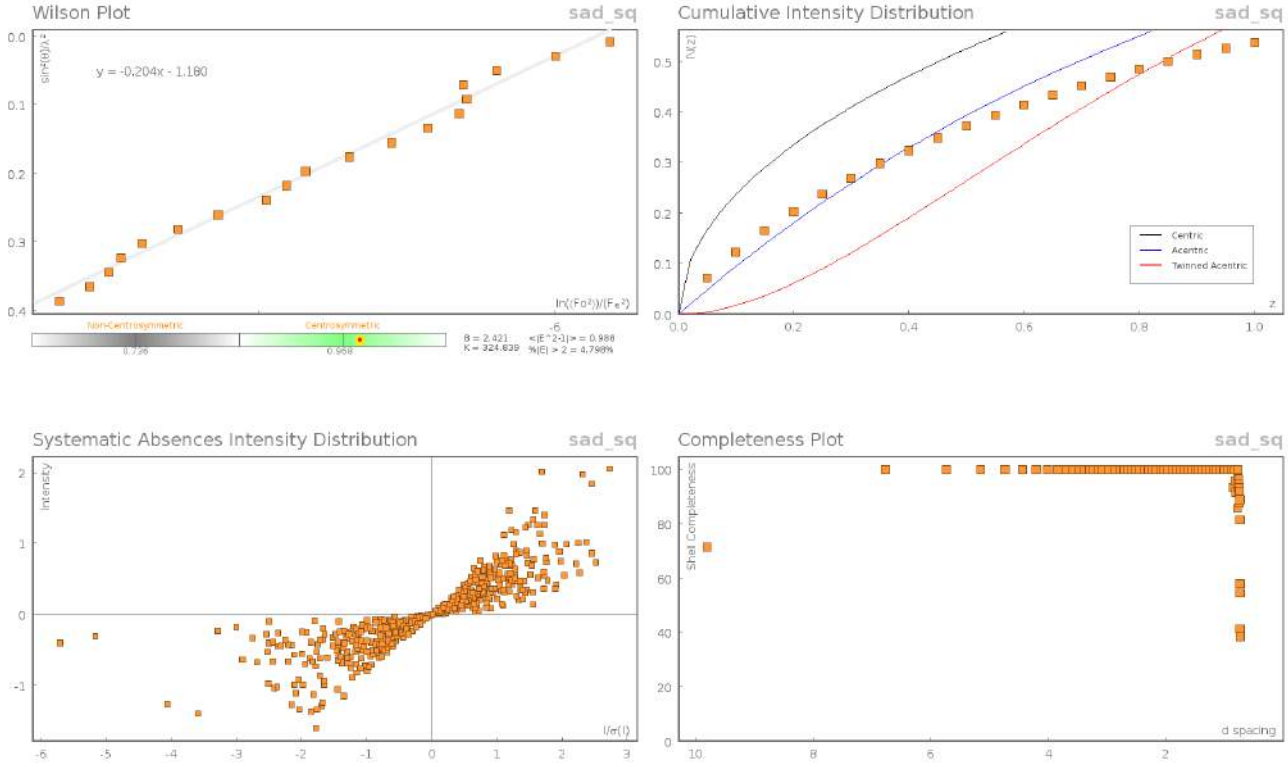
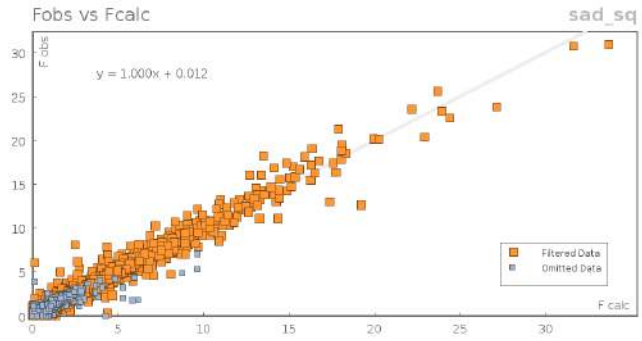


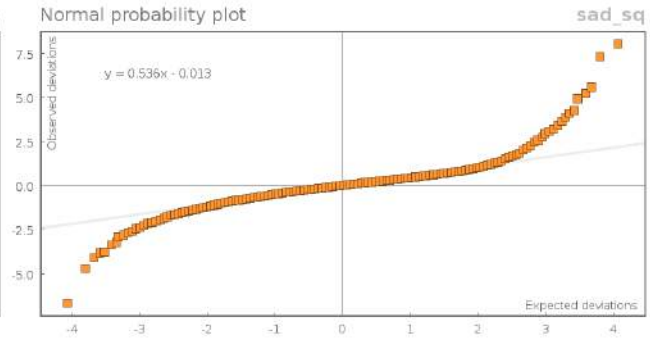
Figure S18:

Data Plots: Diffraction Data



Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	53423	Unique reflections	21341
Completeness	0.995	Mean I/σ	7.76
hklsub>max</sub> collected	(22, 34, 30)	hklsub>min</sub> collected	(-22, -28, -15)
hkl_{max} used	(20, 33, 29)	hkl_{min} used	(-21, 0, 0)
Lim d_{max} collected	20.0	Lim d_{min} collected	0.77
d_{max} used	11.15	d_{min} used	0.77
Friedel pairs	6036	Friedel pairs merged	1
Inconsistent equivalents	0	R_{int}	0.0607
R_{sigma}	0.09	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	158
Multiplicity	(41686, 8320)	Maximum multiplicity	6
Removed systematic absences	744	Filtered off (Shel/OMIT)	4903

Images of the Crystal on the Diffractometer

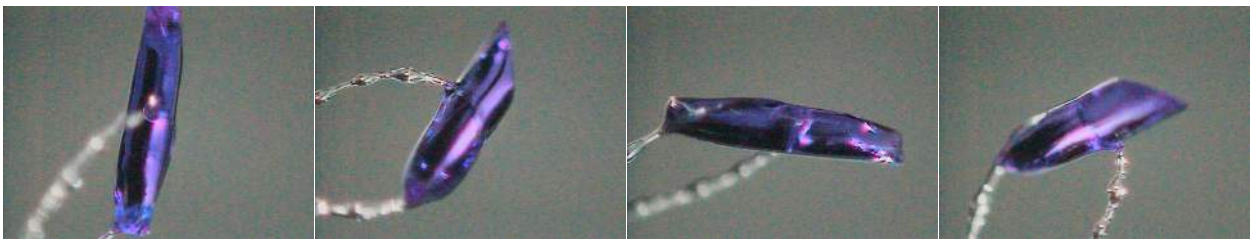


Table S17: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **sad_sq**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
C1	5661(2)	5141.0(13)	3051.1(17)	34.4(8)
C2	4900(2)	5472.9(14)	3030.7(17)	39.1(9)
C3	5952(2)	4246.2(13)	2849.7(15)	31.2(8)
C4	5517(2)	4196.8(14)	2167.5(16)	33.2(8)
C5	5532(2)	4466.5(14)	3766.2(15)	33.9(8)
C6	4905(2)	4042.8(14)	3796.9(17)	37.5(9)
C7	3826(2)	5774.2(14)	1454.8(17)	39.6(9)
C8	3164(3)	6138.9(17)	1046(2)	59.2(12)
C9	4707(3)	6015.8(15)	1614.3(19)	49.1(10)
C10	3818(2)	5257.1(14)	1137.5(17)	42.4(9)
C11	3960(2)	3502.1(14)	1007.6(16)	37.8(9)
C12	4606(3)	3763.0(16)	745.1(18)	52.4(11)

Atom	x	y	z	U_{eq}
C13	3813(3)	2941.5(15)	779(2)	56.8(12)
C14	3129(3)	3797.8(16)	835.0(18)	49.7(10)
C15	3118(2)	4681.6(16)	4110.9(19)	47.8(11)
C16	2356(3)	4566(2)	4347(3)	77.5(17)
C17	2952(3)	5139.2(16)	3677(2)	58.4(12)
C18	3907(3)	4765.5(18)	4651.8(19)	58.4(12)
N1	5454.9(16)	4597.7(10)	3126.2(12)	28.1(6)
N2	4155.2(18)	5261.8(11)	2567.0(13)	35.3(7)
N3	4627.6(17)	4050.1(11)	2079.4(12)	30.5(6)
N4	4057.7(18)	4203.4(11)	3430.0(13)	34.2(7)
O1	2779.9(16)	4405.6(12)	2126.3(13)	50.7(7)
O2	3572(2)	6166.3(11)	2438.0(13)	65.9(9)
O3	2689.4(17)	5429.4(12)	1947.5(13)	56.7(8)
O4	5106.5(17)	3143.4(10)	1962.5(12)	50.9(7)
O5	3674.9(17)	3312.3(10)	2059.3(12)	51.3(7)
O6	3447.9(19)	3689.4(11)	4126.8(13)	58.4(8)
O7	2519.8(16)	4069.7(11)	3186.3(13)	54.0(8)
S1	3526.9(6)	5664.1(4)	2150.4(4)	43.3(3)
S2	4371.8(6)	3482.0(3)	1838.8(4)	35.1(2)
S3	3289.4(6)	4108.4(4)	3693.3(5)	42.7(2)
Co1	4090.9(3)	4478.1(2)	2604.0(2)	30.88(13)
C1'	281(2)	4694.3(13)	2010.8(18)	36.3(8)
C2'	-440(2)	4345.8(13)	2039.8(16)	33.9(8)
C3'	695(2)	5596.1(14)	2203.9(17)	36.9(9)
C4'	823(2)	5636.2(15)	2885.1(17)	37.6(9)
C5'	-455(2)	5361.9(14)	1293.1(16)	35.9(8)
C6'	-1138(2)	5759.8(13)	1261.6(16)	33.9(8)
C7'	-289(2)	3999.7(13)	3601.2(15)	31.7(8)
C8'	-628(2)	3605.6(14)	3972.4(17)	42.4(9)
C9'	469(2)	3773.4(14)	3428.7(18)	42.4(9)
C10'	-50(2)	4501.5(13)	3961.0(16)	35.4(8)
C11'	160(2)	6314.8(14)	4056.0(16)	37.5(9)
C12'	1045(3)	6085.0(19)	4313.1(19)	62.9(13)
C13'	123(3)	6869.2(15)	4276.4(19)	55.0(12)
C14'	-502(3)	5981.9(15)	4226.0(18)	49.5(11)
C15'	-3096(2)	5038.6(13)	1003.1(14)	29.5(8)
C16'	-4053(2)	5111.1(15)	748.5(17)	41.8(9)
C17'	-2894(2)	4607.1(13)	1476.4(16)	33.2(8)
C18'	-2705(3)	4927.0(14)	489.6(16)	41.4(9)
N1'	-6.5(17)	5235.1(10)	1938.3(13)	31.1(7)
N2'	-814.5(17)	4547.2(10)	2514.7(12)	28.3(6)
N3'	3.0(16)	5768.7(10)	2989.9(13)	30.7(6)
N4'	-1671.2(16)	5591.2(10)	1645.1(12)	27.4(6)
O1'	-1872.0(15)	5388.1(10)	2951.1(11)	33.5(6)
O2'	-1318.8(16)	3641.4(9)	2585.9(11)	40.8(6)
O3'	-1810.2(14)	4354.1(9)	3111.0(11)	38.5(6)
O4'	520.2(17)	6684.2(10)	3096.1(12)	46.0(7)
O5'	-973.6(15)	6482.9(9)	3006.5(11)	39.9(6)
O6'	-2908.6(15)	6033.9(9)	907.4(11)	39.7(6)
O7'	-3030.5(14)	5688.0(9)	1884.4(10)	34.4(6)
S1'	-1132.0(5)	4133.1(3)	2902.2(4)	30.5(2)
S2'	-91.8(5)	6331.0(3)	3225.0(4)	32.2(2)
S3'	-2662.0(5)	5640.5(3)	1377.0(4)	29.11(19)
Co1'	-947.9(3)	5330.9(2)	2469.4(2)	25.66(11)
C1D	2639(2)	7880.9(12)	3283.2(15)	31.4(8)
C2D	2200(3)	7814.5(14)	3771.4(17)	42.0(9)
C3D	2188(3)	8314.4(14)	4116.3(17)	43.3(9)
C4D	1797(3)	8257.0(19)	4640(2)	69.8(14)

Atom	x	y	z	U_{eq}
C5D	3173(2)	7513.4(13)	2461.9(16)	32.5(8)
C6D	2866(2)	7920.6(13)	1968.0(16)	34.1(8)
C7D	3375(2)	7891.3(15)	1505.3(16)	39.7(9)
C8D	2993(3)	8224.6(16)	941.9(18)	51.3(11)
C9D	1688(2)	7341.9(13)	2475.2(16)	34.6(8)
C10D	1572(2)	6961.0(14)	1948.5(17)	37.5(9)
C11D	669(2)	6970.5(14)	1530.0(16)	37.3(9)
C12D	564(3)	6662.3(16)	951.3(18)	49(1)
C13D	2896(3)	6933.5(13)	3240.8(17)	42.3(9)
C14D	3794(3)	6946.3(16)	3659.7(18)	57.2(12)
C15D	3997(4)	6460.4(18)	4033(2)	82.8(17)
C16D	3642(8)	6402(4)	4569(4)	98(4)
C16E	4881(5)	6424(4)	4469(4)	104(4)
N1D	2600.0(18)	7416.3(10)	2866.2(12)	29.5(6)
C1C	2825(2)	1923.3(14)	2668.9(18)	44.3(9)
C2C	3243(4)	2026.1(18)	2172(2)	80.0(17)
C3C	3229(4)	1509.7(18)	1811(3)	87.7(18)
C4C	3530(6)	1540(2)	1293(3)	138(3)
C5C	3617(2)	2575.9(14)	3431.1(18)	37.9(9)
C6C	4162(2)	2207.8(15)	3894.3(18)	43.0(9)
C7C	4977(3)	2457.3(19)	4236(2)	63.2(13)
C8C	5577(3)	2145.6(17)	4718.7(19)	57.4(12)
C9C	2257(2)	2187.4(15)	3486(2)	45.2(10)
C10C	2134(3)	2569.1(16)	3957(2)	56.7(11)
C11C	1663(3)	2315(2)	4365(2)	71.9(14)
C12C	1523(4)	2651(2)	4855(3)	99(2)
C13C	2315(2)	2839.6(14)	2692.5(19)	42.6(9)
C14C	1430(3)	2740.9(17)	2273(2)	76.6(16)
C15C	1109(3)	3228.1(18)	1894(2)	78.9(16)
C16C	313(5)	3197(3)	1432(3)	156(4)
N1C	2752.2(18)	2381.7(11)	3074.1(14)	36.7(7)

Table S18: Anisotropic Displacement Parameters (×10^4) **sad_sq**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	30.5(18)	30(2)	41(2)	-3.5(16)	7.5(16)	-2.8(16)
C2	43(2)	28(2)	44(2)	-3.8(16)	8.0(18)	1.9(17)
C3	23.3(17)	32(2)	40(2)	0.5(16)	10.5(15)	3.8(15)
C4	33.5(19)	28(2)	43(2)	1.1(16)	18.2(17)	1.1(15)
C5	29.0(18)	37(2)	33.2(19)	-3.2(16)	4.3(15)	10.0(16)
C6	41(2)	36(2)	38(2)	4.2(16)	14.5(17)	6.3(17)
C7	48(2)	27(2)	44(2)	3.5(17)	13.3(18)	10.3(17)
C8	72(3)	46(3)	60(3)	18(2)	19(2)	28(2)
C9	60(3)	36(2)	49(2)	1.4(19)	13(2)	1(2)
C10	44(2)	42(2)	39(2)	1.4(17)	8.2(18)	5.2(18)
C11	45(2)	30(2)	36(2)	-7.0(16)	7.2(17)	-1.6(17)
C12	67(3)	52(3)	39(2)	-8(2)	18(2)	-8(2)
C13	70(3)	38(2)	58(3)	-16(2)	13(2)	-3(2)
C14	53(3)	44(2)	43(2)	-6.5(19)	0(2)	3(2)
C15	33(2)	55(3)	62(3)	-31(2)	24(2)	-14.4(19)
C16	54(3)	94(4)	101(4)	-52(3)	48(3)	-25(3)
C17	40(2)	48(3)	82(3)	-23(2)	10(2)	5(2)
C18	48(3)	72(3)	56(3)	-31(2)	16(2)	-1(2)
N1	26.3(14)	27.3(16)	30.7(15)	-1.5(12)	8.1(12)	4.1(12)
N2	34.8(17)	29.9(17)	38.7(17)	0.4(13)	6.7(14)	10.8(13)
N3	28.8(15)	28.2(16)	34.4(15)	-4.0(13)	9.0(13)	-1.5(12)
N4	32.8(16)	30.9(17)	41.3(17)	-2.8(13)	14.6(14)	-0.7(13)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	30.4(14)	69(2)	50.0(17)	-16.8(16)	6.7(13)	-0.6(14)
O2	98(3)	48.3(19)	51.1(18)	-1.9(14)	21.8(17)	42.1(18)
O3	39.2(16)	76(2)	57.1(18)	20.7(15)	18.1(14)	25.6(15)
O4	56.9(18)	28.6(15)	60.3(18)	0.9(13)	5.9(15)	12.7(13)
O5	59.3(18)	46.4(17)	51.8(17)	-5.4(13)	21.6(15)	-22.2(14)
O6	76(2)	49.6(18)	65.5(19)	-10.1(15)	45.3(17)	-15.8(16)
O7	37.7(15)	66(2)	62.2(18)	-31.1(15)	19.9(14)	-24.6(14)
S1	46.0(6)	41.9(6)	43.3(5)	4.2(4)	14.6(5)	22.3(5)
S2	39.6(5)	26.3(5)	38.6(5)	-0.1(4)	9.7(4)	-1.9(4)
S3	41.2(5)	41.3(6)	52.4(6)	-15.5(5)	24.3(5)	-13.5(5)
Co1	24.9(2)	31.4(3)	35.7(3)	-4.6(2)	7.5(2)	1.4(2)
C1'	32.6(19)	34(2)	48(2)	-1.6(17)	21.6(17)	5.1(16)
C2'	38(2)	26.2(19)	40(2)	-2.5(16)	15.9(17)	8.0(16)
C3'	28.3(18)	33(2)	53(2)	1.6(17)	18.7(17)	-0.2(16)
C4'	24.2(18)	35(2)	52(2)	-4.7(17)	9.3(17)	-0.8(16)
C5'	37(2)	37(2)	39(2)	2.5(17)	20.0(17)	-4.3(17)
C6'	36(2)	30(2)	37(2)	5.5(15)	12.9(16)	-3.0(16)
C7'	30.8(18)	24.6(19)	36.2(19)	1.1(15)	4.1(15)	0.7(15)
C8'	53(2)	32(2)	39(2)	9.1(17)	7.5(18)	-8.1(18)
C9'	40(2)	34(2)	50(2)	2.1(18)	7.1(18)	6.2(17)
C10'	35(2)	32(2)	38(2)	-0.1(16)	8.4(16)	-2.9(16)
C11'	43(2)	33(2)	33.6(19)	-2.0(16)	7.0(17)	-6.7(17)
C12'	55(3)	81(4)	42(2)	-8(2)	-4(2)	7(2)
C13'	85(3)	38(2)	45(2)	-7.2(19)	24(2)	-13(2)
C14'	67(3)	42(2)	40(2)	-1.5(18)	17(2)	-14(2)
C15'	33.6(18)	26.5(19)	26.6(17)	-2.6(14)	5.8(15)	-3.5(15)
C16'	35(2)	38(2)	44(2)	-4.0(18)	-1.2(17)	-3.9(17)
C17'	28.6(18)	28(2)	41(2)	-2.2(16)	6.7(16)	-2.6(15)
C18'	57(2)	36(2)	34(2)	-10.4(17)	17.8(19)	-4.8(19)
N1'	27.9(15)	27.7(17)	40.1(16)	1.5(13)	13.6(13)	-1.0(12)
N2'	29.7(15)	22.4(15)	34.4(15)	1.3(12)	12.0(13)	-0.7(12)
N3'	23.8(14)	27.8(16)	40.4(16)	-2.1(13)	9.0(13)	0.1(12)
N4'	26.7(14)	25.2(15)	31.9(15)	1.3(12)	10.7(12)	0.5(12)
O1'	29.0(13)	38.6(16)	35.1(14)	-3.7(12)	12.5(11)	-0.2(11)
O2'	47.4(15)	29.6(14)	40.8(14)	-0.1(11)	5.3(12)	-11.5(12)
O3'	30.3(13)	41.5(15)	46.5(15)	13.8(12)	15.4(12)	-0.4(11)
O4'	55.0(17)	34.7(15)	52.8(16)	-2.1(12)	22.5(14)	-16.3(13)
O5'	37.0(14)	34.0(15)	45.4(15)	0.7(12)	6.6(12)	9.9(11)
O6'	41.4(15)	26.5(14)	43.6(15)	4.3(11)	0.3(12)	4.3(11)
O7'	26.8(12)	37.8(14)	37.7(13)	-10.8(11)	7.9(11)	4.3(11)
S1'	27.9(4)	27.1(5)	34.7(5)	3.7(4)	5.8(4)	-3.6(4)
S2'	33.2(5)	26.6(5)	35.9(5)	0.7(4)	8.5(4)	-1.9(4)
S3'	27.8(4)	24.7(5)	32.2(4)	-3.7(4)	4.3(4)	1.4(4)
Co1'	22.7(2)	23.9(2)	30.9(2)	-0.63(19)	8.43(19)	-0.04(18)
C1D	39(2)	17.6(18)	36.7(19)	-1.2(14)	9.3(16)	-1.7(15)
C2D	55(2)	29(2)	45(2)	-5.4(17)	18.8(19)	-4.9(18)
C3D	53(2)	33(2)	45(2)	-8.5(17)	15.1(19)	0.1(19)
C4D	88(4)	65(3)	68(3)	-31(3)	42(3)	-18(3)
C5D	33.7(19)	26.9(19)	40(2)	-0.2(15)	16.1(16)	-3.0(15)
C6D	38(2)	29(2)	37.0(19)	-1.1(15)	13.9(16)	-2.9(16)
C7D	44(2)	37(2)	42(2)	-4.4(17)	18.0(18)	-7.2(18)
C8D	57(3)	56(3)	42(2)	1(2)	17(2)	-15(2)
C9D	39(2)	27(2)	41(2)	-6.5(16)	16.8(17)	-12.1(16)
C10D	42(2)	27(2)	46(2)	-9.0(16)	17.5(18)	-6.3(17)
C11D	42(2)	26(2)	45(2)	-3.1(16)	15.3(18)	-9.4(16)
C12D	54(3)	46(3)	49(2)	-6(2)	18(2)	-16(2)
C13D	73(3)	19.4(18)	39(2)	2.9(15)	22.6(18)	5.0(17)
C14D	87(3)	38(2)	40(2)	-0.5(17)	7(2)	19(2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C15D	156(5)	45(3)	45(2)	11(2)	25(3)	44(3)
C16D	167(11)	66(7)	56(5)	-7(5)	23(6)	2(7)
C16E	171(8)	81(7)	43(5)	0(5)	1(5)	70(6)
N1D	39.4(16)	16.9(14)	34.4(15)	-1.8(11)	14.1(13)	-2.0(12)
C1C	42(2)	26(2)	62(2)	2.6(17)	10.0(19)	6.6(16)
C2C	134(5)	43(3)	76(3)	18(2)	51(3)	32(3)
C3C	143(5)	46(3)	85(4)	9(3)	50(4)	47(3)
C4C	254(9)	62(4)	95(4)	3(3)	45(5)	37(5)
C5C	28.3(17)	30(2)	56(2)	4.1(17)	13.7(16)	-4.9(15)
C6C	38(2)	35(2)	55(2)	2.2(18)	12.3(18)	2.7(17)
C7C	37(2)	75(3)	73(3)	23(2)	10(2)	-9(2)
C8C	52(3)	64(3)	49(2)	-6(2)	4(2)	7(2)
C9C	28.8(19)	33(2)	79(3)	9.9(19)	22.9(19)	0.5(16)
C10C	49(2)	46(3)	84(3)	10(2)	34(2)	11(2)
C11C	42(2)	101(4)	77(3)	22(3)	24(2)	8(3)
C12C	89(4)	133(5)	91(4)	34(4)	50(3)	57(4)
C13C	41(2)	20.7(18)	62(2)	3.2(16)	9.8(18)	5.9(15)
C14C	59(3)	36(2)	103(4)	-17(2)	-27(3)	17(2)
C15C	82(3)	47(3)	84(3)	-15(2)	-14(3)	39(2)
C16C	151(6)	80(5)	166(6)	-46(4)	-69(5)	47(4)
N1C	30.8(15)	20.6(15)	59.2(19)	5.3(13)	13.7(14)	0.9(12)

Table S19: Bond Lengths in Å for **sad_sq**.

Atom	Atom	Length/Å
C1	C2	1.512(5)
C1	N1	1.471(4)
C2	N2	1.478(4)
C3	C4	1.521(5)
C3	N1	1.482(4)
C4	N3	1.473(4)
C5	C6	1.524(5)
C5	N1	1.469(4)
C6	N4	1.470(4)
C7	C8	1.541(5)
C7	C9	1.527(5)
C7	C10	1.522(5)
C7	S1	1.815(4)
C11	C12	1.522(5)
C11	C13	1.540(5)
C11	C14	1.522(5)
C11	S2	1.822(4)
C15	C16	1.531(5)
C15	C17	1.519(6)
C15	C18	1.532(6)
C15	S3	1.831(4)
N1	Co1	2.246(3)
N2	S1	1.582(3)
N2	Co1	2.038(3)
N3	S2	1.586(3)
N3	Co1	2.014(3)
N4	S3	1.570(3)
N4	Co1	2.030(3)
O1	Co1	2.134(3)
O2	S1	1.450(3)
O3	S1	1.459(3)
O4	S2	1.458(3)
O5	S2	1.449(3)
O6	S3	1.442(3)
O7	S3	1.456(3)
C1'	C2'	1.510(5)
C1'	N1'	1.474(4)
C2'	N2'	1.488(4)
C3'	C4'	1.511(5)
C3'	N1'	1.477(4)
C4'	N3'	1.481(4)
C5'	C6'	1.514(5)
C5'	N1'	1.483(4)
C6'	N4'	1.474(4)
C7'	C8'	1.531(5)
C7'	C9'	1.533(5)
C7'	C10'	1.529(5)
C7'	S1'	1.824(3)
C11'	C12'	1.531(5)
C11'	C13'	1.530(5)
C11'	C14'	1.527(5)
C11'	S2'	1.821(4)
C15'	C16'	1.530(5)
C15'	C17'	1.524(5)
C15'	C18'	1.519(5)
C15'	S3'	1.824(3)
N1'	Co1'	2.241(3)
N2'	S1'	1.573(3)
N2'	Co1'	2.043(3)
N3'	S2'	1.577(3)
N3'	Co1'	2.023(3)
N4'	S3'	1.578(3)
N4'	Co1'	2.032(3)
O1'	Co1'	2.125(2)
O2'	S1'	1.454(2)
O3'	S1'	1.454(2)

Atom	Atom	Length/Å
O4'	S2'	1.455(2)
O5'	S2'	1.451(2)
O6'	S3'	1.450(2)
O7'	S3'	1.459(2)
C1D	C2D	1.502(5)
C1D	N1D	1.525(4)
C2D	C3D	1.519(5)
C3D	C4D	1.519(5)
C5D	C6D	1.521(5)
C5D	N1D	1.519(4)
C6D	C7D	1.528(5)
C7D	C8D	1.527(5)
C9D	C10D	1.524(5)
C9D	N1D	1.526(4)
C10D	C11D	1.522(5)
C11D	C12D	1.510(5)
C13D	C14D	1.517(6)
C13D	N1D	1.516(4)
C14D	C15D	1.504(6)
C15D	C16D	1.508(2)
C15D	C16E	1.5144(14)
C1C	C2C	1.510(6)
C1C	N1C	1.531(5)
C2C	C3C	1.568(7)
C3C	C4C	1.410(8)
C5C	C6C	1.514(5)
C5C	N1C	1.513(4)
C6C	C7C	1.495(5)
C7C	C8C	1.491(6)
C9C	C10C	1.517(6)
C9C	N1C	1.499(4)
C10C	C11C	1.521(6)
C11C	C12C	1.488(7)
C13C	C14C	1.521(5)
C13C	N1C	1.526(4)
C14C	C15C	1.537(6)
C15C	C16C	1.432(7)

Table S20: Bond Angles in ° for **sad_sq**.

Atom	Atom	Atom	Angle/°
N1	C1	C2	109.3(3)
N2	C2	C1	108.9(3)
N1	C3	C4	109.3(3)
N3	C4	C3	108.7(3)
N1	C5	C6	110.3(3)
N4	C6	C5	108.5(3)
C8	C7	S1	107.6(3)
C9	C7	C8	110.7(3)
C9	C7	S1	109.6(3)
C10	C7	C8	110.2(3)
C10	C7	C9	110.7(3)
C10	C7	S1	108.0(3)
C12	C11	C13	110.3(3)
C12	C11	S2	109.1(3)
C13	C11	S2	107.5(3)
C14	C11	C12	110.8(3)
C14	C11	C13	110.2(3)
C14	C11	S2	108.9(3)
C16	C15	C18	109.8(4)
C16	C15	S3	106.8(3)
C17	C15	C16	111.7(4)
C17	C15	C18	111.5(3)
C17	C15	S3	108.7(3)
C18	C15	S3	108.2(3)
C1	N1	C3	111.4(3)
C1	N1	Co1	107.49(19)
C3	N1	Co1	106.37(19)
C5	N1	C1	112.4(3)
C5	N1	C3	112.3(3)
C5	N1	Co1	106.44(19)
C2	N2	S1	117.0(2)
C2	N2	Co1	112.5(2)
S1	N2	Co1	130.50(18)
C4	N3	S2	116.3(2)
C4	N3	Co1	111.5(2)
S2	N3	Co1	126.75(16)
C6	N4	S3	118.6(2)
C6	N4	Co1	110.7(2)
S3	N4	Co1	130.51(18)
N2	S1	C7	109.47(16)
O2	S1	C7	105.24(18)
O2	S1	N2	112.37(17)
O2	S1	O3	116.03(19)
O3	S1	C7	104.99(17)
O3	S1	N2	108.30(17)
N3	S2	C11	108.43(16)
O4	S2	C11	105.06(17)
O4	S2	N3	111.60(16)
O5	S2	C11	105.88(17)
O5	S2	N3	108.72(15)
O5	S2	O4	116.67(17)
N4	S3	C15	109.52(16)
O6	S3	C15	106.24(19)
O6	S3	N4	111.88(17)
O6	S3	O7	116.01(18)
O7	S3	C15	103.85(18)
O7	S3	N4	108.86(16)
N2	Co1	N1	80.10(11)
N2	Co1	O1	97.12(12)
N3	Co1	N1	81.18(10)
N3	Co1	N2	119.19(11)
N3	Co1	N4	119.46(11)
N3	Co1	O1	101.67(11)
N4	Co1	N1	81.12(11)
N4	Co1	N2	113.83(11)
N4	Co1	O1	98.63(12)
O1	Co1	N1	176.78(11)
N1'	C1'	C2'	110.0(3)

Atom	Atom	Atom	Angle/°
N2'	C2'	C1'	108.6(3)
N1'	C3'	C4'	109.1(3)
N3'	C4'	C3'	108.5(3)
N1'	C5'	C6'	110.6(3)
N4'	C6'	C5'	109.4(3)
C8'	C7'	C9'	109.9(3)
C8'	C7'	S1'	107.6(2)
C9'	C7'	S1'	108.8(2)
C10'	C7'	C8'	110.5(3)
C10'	C7'	C9'	111.1(3)
C10'	C7'	S1'	108.8(2)
C12'	C11'	S2'	108.4(3)
C13'	C11'	C12'	111.3(3)
C13'	C11'	S2'	107.6(3)
C14'	C11'	C12'	110.9(3)
C14'	C11'	C13'	110.5(3)
C14'	C11'	S2'	108.1(2)
C16'	C15'	S3'	107.3(2)
C17'	C15'	C16'	110.6(3)
C17'	C15'	S3'	108.7(2)
C18'	C15'	C16'	110.6(3)
C18'	C15'	C17'	110.6(3)
C18'	C15'	S3'	109.1(2)
C1'	N1'	C3'	111.5(3)
C1'	N1'	C5'	112.1(3)
C1'	N1'	Co1'	107.20(19)
C3'	N1'	C5'	112.1(3)
C3'	N1'	Co1'	107.0(2)
C5'	N1'	Co1'	106.6(2)
C2'	N2'	S1'	116.4(2)
C2'	N2'	Co1'	111.9(2)
S1'	N2'	Co1'	131.21(16)
C4'	N3'	S2'	117.0(2)
C4'	N3'	Co1'	111.5(2)
S2'	N3'	Co1'	125.64(15)
C6'	N4'	S3'	118.3(2)
C6'	N4'	Co1'	110.8(2)
S3'	N4'	Co1'	130.85(15)
N2'	S1'	C7'	109.12(15)
O2'	S1'	C7'	105.53(15)
O2'	S1'	N2'	112.16(15)
O3'	S1'	C7'	104.72(15)
O3'	S1'	N2'	109.08(14)
O3'	S1'	O2'	115.75(15)
N3'	S2'	C11'	108.52(16)
O4'	S2'	C11'	105.10(16)
O4'	S2'	N3'	111.78(15)
O5'	S2'	C11'	105.71(16)
O5'	S2'	N3'	108.76(15)
O5'	S2'	O4'	116.47(16)
N4'	S3'	C15'	109.65(15)
O6'	S3'	C15'	105.49(15)
O6'	S3'	N4'	112.55(15)
O6'	S3'	O7'	115.72(15)
O7'	S3'	C15'	104.25(14)
O7'	S3'	N4'	108.70(14)
N2'	Co1'	N1'	80.55(10)
N2'	Co1'	O1'	97.25(10)
N3'	Co1'	N1'	80.68(11)
N3'	Co1'	N2'	118.30(11)
N3'	Co1'	N4'	120.52(11)
N3'	Co1'	O1'	102.02(10)
N4'	Co1'	N1'	81.43(10)
N4'	Co1'	N2'	113.78(11)
N4'	Co1'	O1'	97.87(10)
O1'	Co1'	N1'	177.14(10)
C2D	C1D	N1D	115.4(3)
C1D	C2D	C3D	111.5(3)
C2D	C3D	C4D	113.3(3)
N1D	C5D	C6D	115.5(3)
C5D	C6D	C7D	110.1(3)
C8D	C7D	C6D	112.1(3)
C10D	C9D	N1D	115.0(3)
C11D	C10D	C9D	111.3(3)
C12D	C11D	C10D	112.8(3)
N1D	C13D	C14D	115.9(3)
C15D	C14D	C13D	110.9(4)
C14D	C15D	C16D	117.9(6)
C14D	C15D	C16E	116.1(6)
C1D	N1D	C9D	108.8(2)
C5D	N1D	C1D	109.0(2)
C5D	N1D	C9D	110.3(2)
C13D	N1D	C1D	110.6(3)
C13D	N1D	C5D	108.8(3)
C13D	N1D	C9D	109.3(3)
C2C	C1C	N1C	116.6(3)
C1C	C2C	C3C	107.6(4)
C4C	C3C	C2C	115.9(5)
N1C	C5C	C6C	116.5(3)
C7C	C6C	C5C	110.9(3)
C8C	C7C	C6C	117.3(4)
N1C	C9C	C10C	115.7(3)
C9C	C10C	C11C	110.2(4)
C12C	C11C	C10C	115.0(5)
C14C	C13C	N1C	116.1(3)
C13C	C14C	C15C	109.2(4)
C16C	C15C	C14C	117.6(5)
C5C	N1C	C1C	111.0(3)
C5C	N1C	C13C	105.5(3)
C9C	N1C	C1C	105.6(3)
C9C	N1C	C5C	112.0(3)
C9C	N1C	C13C	111.4(3)
C13C	N1C	C1C	111.5(3)

Table S21: Hydrogen Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **sad_sq**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}

Atom	x	y	z	U_{eq}
H1C	2640(30)	4264(18)	2470(13)	84(12)
H1D	2590(30)	4764(6)	2090(20)	84(12)
H1A	5818	5183	2675	41
H1B	6137	5247	3390	41
H2A	4798	5475	3429	47
H2B	5003	5825	2926	47
H3A	5995	3910	3042	37
H3B	6518	4382	2915	37
H4A	5545	4523	1965	40
H4B	5799	3936	1991	40
H5A	5422	4770	3980	41
H5B	6103	4351	3967	41
H6A	5062	3723	3638	45
H6B	4909	3986	4218	45
H8A	2610	5992	977	89
H8B	3283	6184	661	89
H8C	3186	6467	1245	89
H9A	4706	6333	1831	74
H9B	4857	6084	1245	74
H9C	5110	5783	1867	74
H10A	4190	5022	1412	64
H10B	4005	5303	779	64
H10C	3254	5120	1021	64
H12A	4687	4113	887	79
H12B	4404	3760	306	79
H12C	5134	3581	876	79
H13A	4341	2759	890	85
H13B	3582	2940	342	85
H13C	3425	2776	962	85
H14A	2725	3621	993	74
H14B	2917	3821	398	74
H14C	3221	4139	1006	74
H16A	1869	4498	4007	116
H16B	2246	4857	4571	116
H16C	2476	4269	4610	116
H17A	3449	5211	3553	88
H17B	2812	5436	3880	88
H17C	2490	5061	3323	88
H18A	4025	4458	4896	88
H18B	3811	5047	4897	88
H18C	4380	4844	4501	88
H1'C	-1970(30)	5038(6)	3044(19)	86(17)
H1'D	-2310(20)	5526(14)	2627(15)	78(16)
H1'A	744	4659	2383	44
H1'B	485	4595	1668	44
H2'A	-865	4338	1645	41
H2'B	-233	3997	2142	41
H3'A	563	5933	2016	44
H3'B	1209	5473	2126	44
H4'A	1029	5311	3081	45
H4'B	1239	5901	3058	45
H5'A	-708	5052	1080	43
H5'B	-55	5495	1092	43
H6'A	-881	6090	1406	41
H6'B	-1482	5801	841	41
H8'A	-1101	3750	4080	64
H8'B	-191	3519	4338	64
H8'C	-804	3300	3732	64

Atom	x	y	z	U_{eq}
H9'A	293	3474	3177	64
H9'B	901	3679	3794	64
H9'C	689	4026	3207	64
H10H	127	4752	3713	53
H10I	404	4437	4325	53
H10J	-531	4631	4072	53
H12J	1054	5742	4158	94
H12K	1189	6074	4752	94
H12L	1448	6295	4191	94
H13F	539	7074	4163	83
H13G	237	6872	4713	83
H13H	-429	7010	4091	83
H14H	-1046	6144	4083	74
H14I	-354	5944	4663	74
H14J	-523	5648	4040	74
H16M	-4293	5166	1080	63
H16N	-4298	4808	525	63
H16O	-4168	5404	481	63
H17D	-2292	4559	1620	50
H17E	-3157	4293	1293	50
H17F	-3104	4697	1814	50
H18D	-2842	5201	194	62
H18E	-2923	4607	296	62
H18F	-2101	4903	654	62
H1DA	3228	7962	3479	38
H1DB	2391	8174	3032	38
H2DA	2488	7550	4057	50
H2DB	1624	7700	3585	50
H3DA	1873	8571	3832	52
H3DB	2764	8439	4278	52
H4DA	2117	8012	4931	105
H4DB	1224	8138	4483	105
H4DC	1800	8585	4837	105
H5DA	3245	7191	2266	39
H5DB	3725	7616	2721	39
H6DA	2928	8260	2154	41
H6DB	2271	7866	1761	41
H7DA	3950	8004	1700	48
H7DB	3397	7536	1378	48
H8DA	2922	8571	1068	77
H8DB	2453	8087	718	77
H8DC	3363	8226	685	77
H9DA	1355	7225	2737	41
H9DB	1465	7674	2308	41
H10D	1959	7047	1714	45
H10E	1707	6616	2112	45
H11A	293	6833	1749	45
H11B	505	7325	1422	45
H12D	793	6323	1054	73
H12E	857	6831	698	73
H12F	-26	6637	734	73
H2	2846	6645	2962	51
H13D	2517	6868	3488	51
H14D	4186	6985	3416	69
H14E	3863	7241	3931	69
H15A	3913	6170	3754	99
H15B	3595	6426	4268	99
H15D	4331	6204	3936	99

Atom	x	y	z	U_{eq}
H16D	3038	6369	4423	147
H16E	3786	6700	4828	147
H16F	3877	6100	4798	147
H16G	5287	6427	4240	157
H16H	4936	6110	4699	157
H16I	4981	6713	4744	157
H1CA	3139	1652	2930	53
H1CB	2261	1792	2478	53
H2CA	3821	2140	2350	96
H2CB	2939	2293	1898	96
H3CA	3565	1257	2090	105
H3CB	2652	1383	1681	105
H4CA	3161	1756	989	207
H4CB	3545	1201	1128	207
H4CC	4089	1684	1408	207
H5CA	3542	2888	3644	45
H5CB	3923	2669	3142	45
H6CA	3859	2101	4181	52
H6CB	4278	1903	3686	52
H7CA	5267	2561	3940	76
H7CB	4845	2769	4425	76
H8CA	6120	2311	4836	86
H8CB	5630	1807	4563	86
H8CC	5366	2118	5069	86
H9CA	2540	1885	3699	54
H9CB	1704	2079	3234	54
H10F	1814	2864	3752	68
H10G	2680	2691	4206	68
H11C	1118	2197	4109	86
H11D	1979	2013	4553	86
H12G	1209	2464	5082	149
H12H	1211	2952	4675	149
H12I	2059	2753	5126	149
H13E	2283	3118	2969	51
H5	2667	2957	2444	51
H14F	1052	2653	2515	92
H14G	1441	2454	2003	92
H15C	1071	3502	2174	95
H15E	1533	3331	1697	95
H16J	374	2992	1097	234
H16K	129	3538	1289	234
H16L	-98	3041	1601	234

Table S22: Hydrogen Bond information for **sad_sq**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O1	H1D	O3	0.977(16)	1.771(16)	2.683(4)	154(4)
O1'	H1'C	O3'	0.957(16)	1.794(15)	2.704(3)	158(4)
O1'	H1'D	O7'	0.941(18)	1.82(2)	2.741(3)	165(4)
C1D	H1DB	O2'[1]	0.97	2.27	3.177(4)	155.1
C9D	H9DA	O4'	0.97	2.28	3.193(4)	157.4
C13D	H2	O2	0.97	2.29	3.118(5)	143.4

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

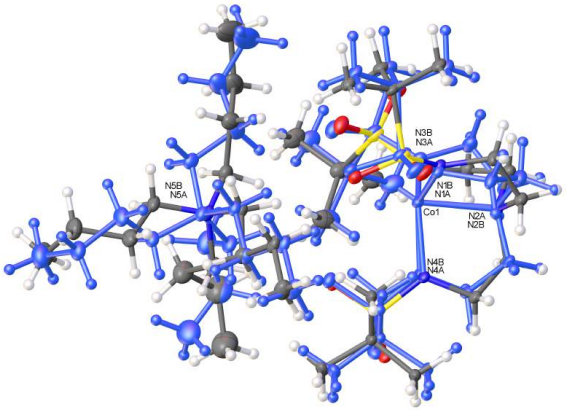
cmw04bucobus

EMORY UNIVERSITY | X-ray Crystallography Center

Submitted by: **Christian Wallen**
Emory University
Solved by: **Thomas C. Pickel**

Sample ID: **CMW04BuCoBus**

Crystal Data and Experimental



Experimental. Single violet prism-shaped crystals of (**cmw04bucobus**) were recrystallised from --•by vapor diffusion. A suitable crystal (0.57×0.48×0.24 mm) was selected and mounted on a loop with paratone oil on a Bruker APEX-II CCD diffractometer. The crystal was cooled to T = 100(2) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program using combined Patterson and dual-space recycling methods and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The crystal structure was refined with version of **ShelXL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{34}H_{75}CoN_5O_6S_3$, M_r = 805.10, monoclinic, $P2_1/c$ (No. 14), a = 19.505(2) Å, b = 11.3473(14) Å, c = 19.833(2) Å, β = 99.185(2)°, $\alpha = \gamma$ = 90°, V = 4333.3(9) Å^3, T = 100(2) K, Z = 4, Z' = 1, μ(MoK$_\alpha$) = 0.585, 51543 reflections measured, 11684 unique (R_{int} = 0.0614) which were used in all calculations. The final wR_2 was 0.2206 (all data) and R_1 was 0.0835 (I > 2σ(I)).

Compound	**cmw04bucobus**
Formula	$C_{34}H_{75}CoN_5O_6S_3$
$D_{calc.}$/ g cm^{-3}	1.234
μ/mm^{-1}	0.585
Formula Weight	805.10
Colour	violet
Shape	prism
Max Size/mm	0.57
Mid Size/mm	0.48
Min Size/mm	0.24
T/K	100(2)
Crystal System	monoclinic
Space Group	$P2_1/c$
a/Å	19.505(2)
b/Å	11.3473(14)
c/Å	19.833(2)
α/°	90
β/°	99.185(2)
γ/°	90
V/Å^3	4333.3(9)
Z	4
Z'	1
Θ_{min}/°	2.074
Θ_{max}/°	29.199
Measured Refl.	51543
Independent Refl.	11684
$I > 2\sigma(I)$	8299
R_{int}	0.0614
Parameters	848
Restraints	1142
Largest Peak	1.584
Deepest Hole	-1.143
GooF	1.080
wR_2 (all data)	0.2206
wR_2	0.1969
R_1 (all data)	0.1176
R_1	0.0835
CCDC #	1434434

Structure Quality Indicators

Reflections:	d min 0.73	I/σ 18.3	Rint 6.14%	complete 100%
Refinement:	Shift 0.004	Max Peak 1.6	Min Peak -1.1	GooF 1.080

A violet prism-shaped crystal with dimensions 0.57×0.48×0.24 mm was mounted on a loop with paratone oil. X-ray diffraction data were collected using a Bruker APEX-II CCD diffractometer equipped with an Oxford Cryosystems low-temperature apparatus operating at T = 100(2) K.

Data were measured using ϕ and ω scans using MoK$_\alpha$ radiation (fine-focus sealed tube, 45 kV, 35 mA). The total number of runs and images was based on the strategy calculation from the program **APEX2** (Bruker, 2014). The maximum resolution achieved was Θ = 29.199°.

Unit cell indexing was performed by using the **APEX2** (Bruker, 2014) software and refined using **SAINT** (Bruker, V8.34A, 2013) on 9806 reflections, 19 percent of the observed reflections. Data reduction, scaling and absorption corrections were performed using **SAINT** (Bruker, V8.34A, 2013) and **SADABS-2014/5** (Bruker,2014) was used for absorption correction. wR_2(int) was 0.0821 before and 0.0579 after correction. The ratio of minimum to maximum transmission is 0.8248. The $\lambda/2$ correction factor is 0.00150. The software also corrects for Lorentz polarisation. The final completeness is 99.9% out to 29.199° in Θ. The absorption coefficient (μ) of this material is 0.585 and the minimum and maximum transmissions are 0.6151 and 0.7458.

The structure was solved in the space group P1 with the **ShelXT** (Sheldrick, 2015) structure solution program using combined Patterson and dual-space recycling methods. The space group P2$_1$/c (# 14) was determined by **ShelXT** (Sheldrick, 2015) structure solution program.The crystal structure was refined by Least Squares using version 2014/7 of **ShelXL** (Sheldrick, 2008). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

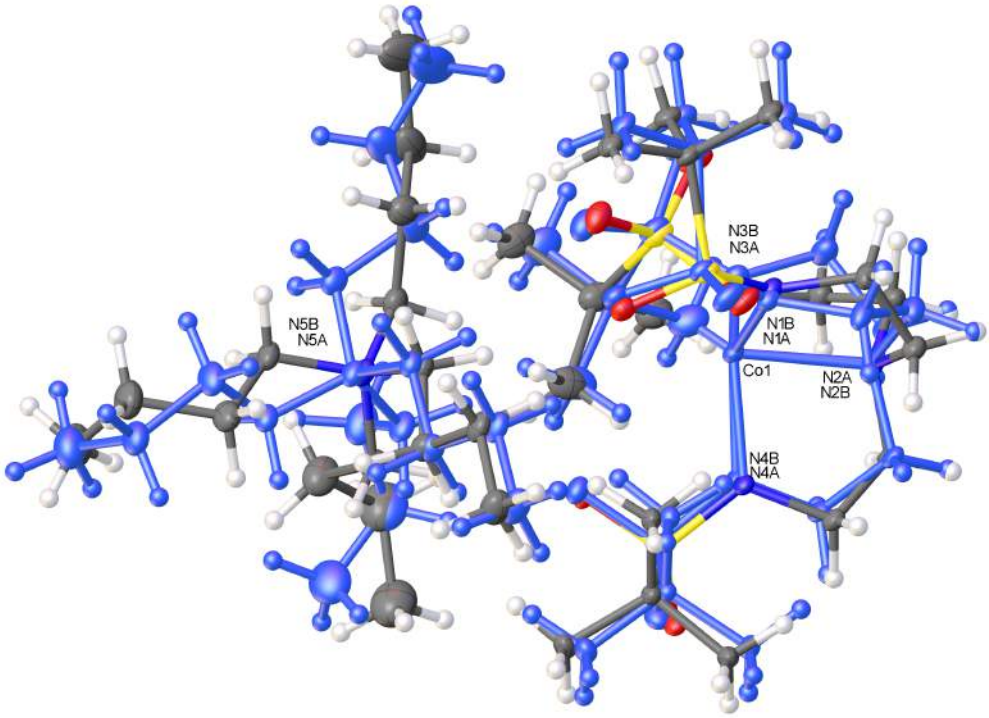
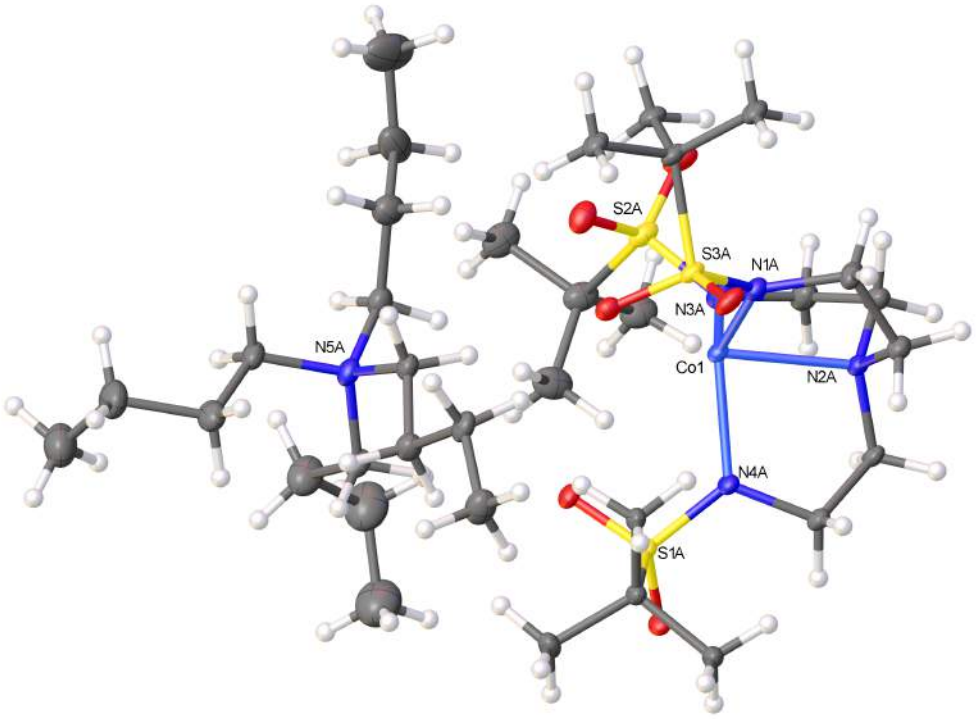


Figure S19: Plot of the asymmetric unit with the second disorder component shown in blue.



FigureS20: Plot of the asymmetric unit with the major disorder component shown only.

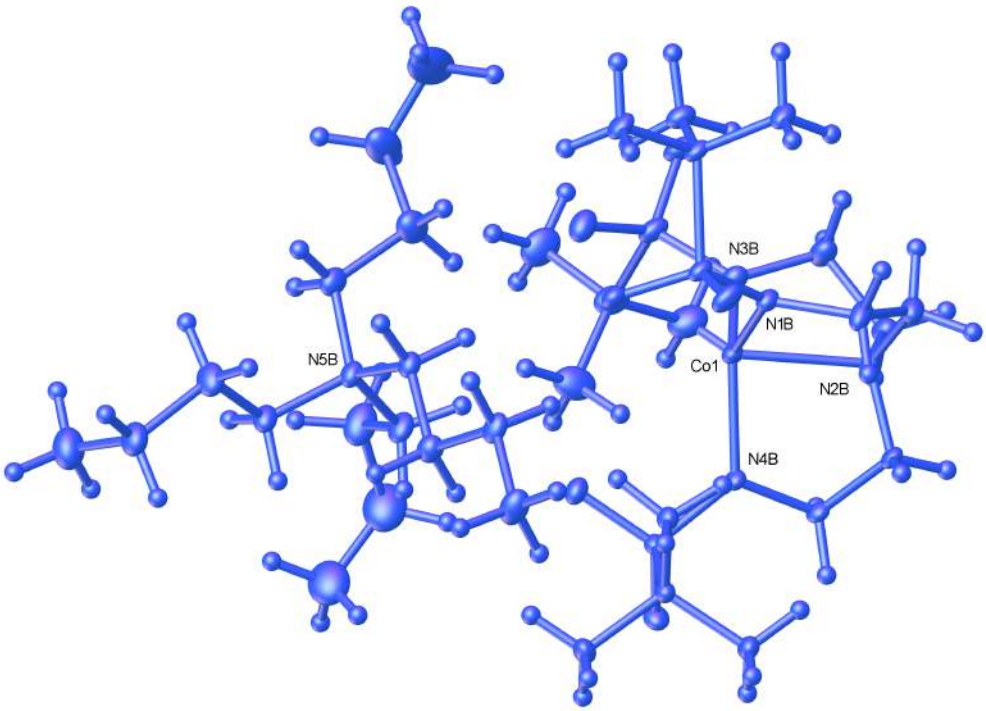
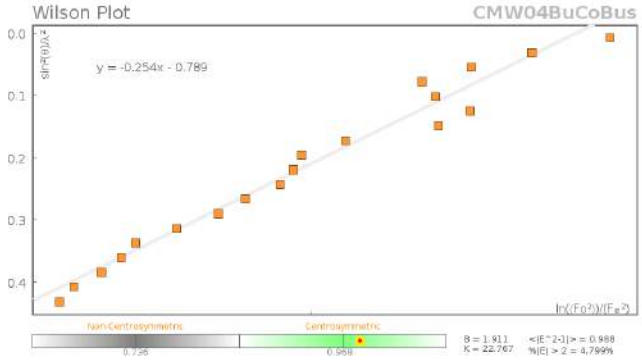
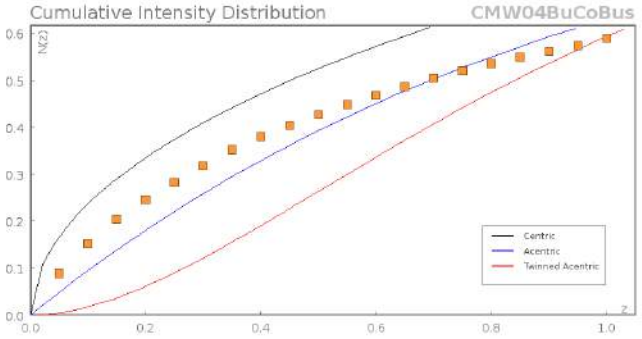


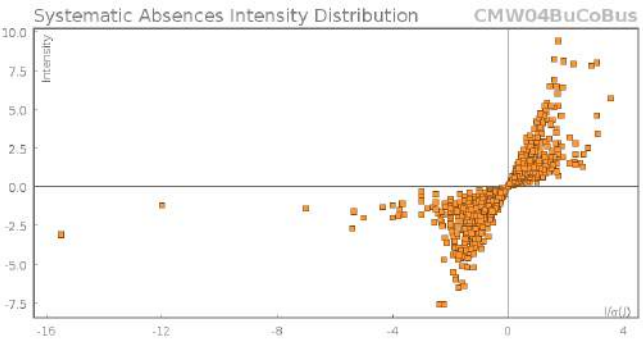
Figure S21: Plot of the asymmetric unit with the minor disorder component shown only.

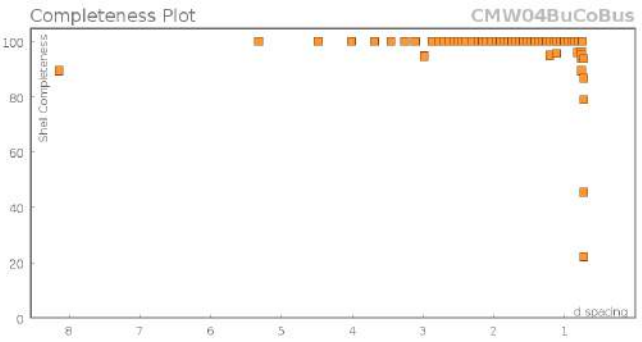
There are two independent molecules in the asymmetric unit.

Data Plots: Diffraction Data

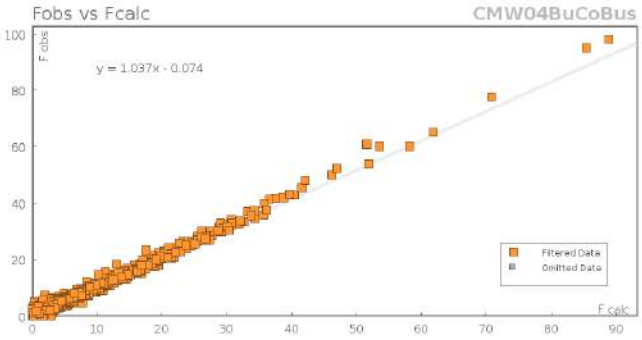


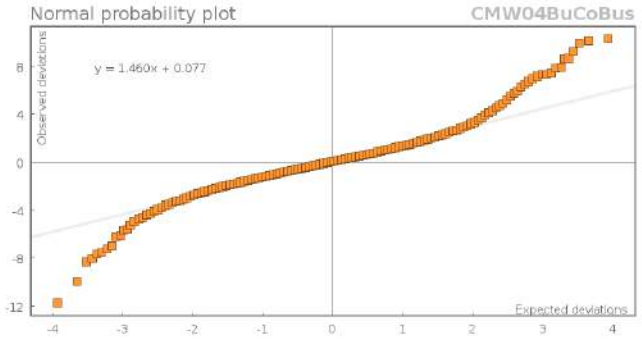






Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	52935	Unique reflections	11684
Completeness	0.995	Mean I/σ	12.23
hklsub>max</sub> collected	(24, 15, 27)	hklsub>min</sub> collected	(-26, -15, -27)
hkl_{max} used	(26, 15, 27)	hkl_{min} used	(-26, 0, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.36
d_{max} used	14.98	d_{min} used	0.73
Friedel pairs	13977	Friedel pairs merged	1
Inconsistent equivalents	0	R_{int}	0.0614
R_{sigma}	0.0547	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	0

Multiplicity	(22662, 12930, 1471)	Maximum multiplicity	12
Removed systematic absences	1392	Filtered off (Shel/OMIT)	0

Images of the Crystal on the Diffractometer

Table S23: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **cmw04bucobus**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
C1B	9408(3)	3687(6)	4595(3)	35.8(15)
C2B	9146(3)	2693(5)	4989(3)	34.9(13)
C3B	8039(3)	2114(5)	5367(3)	32.8(13)
C4B	7575(4)	1840(5)	4687(3)	40.3(15)
C5B	8730(3)	3741(5)	5930(2)	23.9(10)
C6B	8160(3)	4594(5)	6022(2)	24.9(11)
C7B	8428(3)	7551(4)	5446(3)	25.3(8)
C8B	8823(4)	7311(7)	4855(4)	27.1(17)
C9B	8142(4)	8808(5)	5410(5)	34.7(16)
C10B	8902(4)	7359(7)	6129(4)	29.3(15)
C11B	5902(3)	3361(7)	4296(4)	41.2(13)
C12B	5231(3)	3208(10)	3784(5)	56(2)
C13B	5995(4)	4625(8)	4536(6)	54.3(19)
C14B	5905(5)	2527(10)	4906(4)	53.3(19)
C15B	8858(4)	3991(6)	2763(2)	24.9(10)
C16B	8191(6)	3260(9)	2715(4)	31.5(18)
C17B	9497(6)	3206(9)	2844(4)	33.0(17)
C18B	8840(6)	4787(8)	2139(3)	32.9(17)
N1B	8810(2)	4209(5)	4147(2)	24.5(7)
N2B	8528(2)	3076(3)	5284.9(18)	24.6(6)
N3B	7307(2)	2958(4)	4390(2)	29.3(9)
N4B	7968(3)	5244(4)	5377(2)	23.8(8)
O1B	7293(3)	6769(5)	4707(3)	29.9(13)
O2B	7356(3)	6795(5)	5965(3)	32.9(14)
O3B	6651(3)	3897(6)	3367(3)	39.6(10)
O4B	6463(3)	1784(5)	3581(3)	40.6(11)
O5B	8311(4)	5730(5)	3357(3)	31.0(13)
O6B	9590(3)	5513(7)	3577(3)	36.4(14)
S1B	7692.5(19)	6555(2)	5375(2)	24.1(6)
S2B	6614.9(15)	2960(4)	3851.0(15)	31.4(3)
S3B	8911(2)	4965(3)	3501.6(15)	24.6(6)
C1A	9299(6)	3193(10)	4430(5)	32(2)
C2A	9274(4)	3122(10)	5184(4)	29.6(17)
C3A	8195(5)	1943(6)	5163(5)	32.3(18)
C4A	7406(5)	2100(10)	4996(5)	37.4(19)
C5A	8477(5)	3535(7)	6001(3)	23.9(10)
C6A	8551(6)	4856(7)	6014(4)	25.6(17)
C7A	8383(6)	7724(7)	5392(6)	25.3(8)
C8A	8752(9)	7489(16)	4783(8)	26(3)
C9A	7994(9)	8898(7)	5309(10)	34(3)
C10A	8906(7)	7732(13)	6054(8)	29(3)
C11A	5860(4)	3524(12)	4193(6)	41.9(17)

Atom	x	y	z	U_{eq}
C12A	5287(5)	3550(20)	3565(8)	50(3)
C13A	6004(8)	4743(13)	4490(12)	52(3)
C14A	5659(8)	2678(18)	4733(8)	47(3)
C15A	8862(8)	4156(11)	2734(4)	25.7(16)
C16A	8184(11)	3447(18)	2633(8)	28(3)
C17A	9488(12)	3358(18)	2739(8)	30(3)
C18A	8849(12)	5101(16)	2184(5)	30(3)
N1A	8776(4)	4051(9)	4116(3)	24.5(7)
N2A	8546(3)	3084(5)	5314(3)	24.6(6)
N3A	7264(3)	3079(7)	4517(5)	29.3(9)
N4A	8112(5)	5334(5)	5401(4)	23.8(8)
O1A	7250(6)	6685(9)	4806(6)	27(2)
O2A	7487(7)	6743(10)	6070(6)	30(2)
O3A	6759(6)	3759(14)	3366(5)	39.6(10)
O4A	6505(6)	1740(10)	3726(7)	40.6(11)
O5A	8383(8)	5795(10)	3457(6)	29(2)
O6A	9644(7)	5377(14)	3685(6)	33(2)
S1A	7745(4)	6573(5)	5428(4)	24.7(12)
S2A	6639(3)	2968(8)	3904(3)	31.4(3)
S3A	8938(5)	4935(7)	3548(3)	24.6(12)
Co1	7977.5(3)	4271.8(5)	4576.9(2)	20.73(14)
C25B	5785(7)	7943(9)	4189(5)	85(2)
C21B	8854(3)	8915(13)	3199(10)	33(3)
C29B	6240(5)	5503(9)	1777(7)	68(3)
C33B	6540(5)	11488(6)	1896(6)	46(2)
C23B	6703(4)	8007(8)	3440(3)	36.8(15)
C27B	6514(4)	7542(6)	2190(3)	34.0(13)
C31B	6574(4)	9615(6)	2582(3)	32.5(13)
C20B	8091(3)	9180(20)	3216(16)	34.5(17)
N5B	6859(2)	8391(5)	2741(2)	28.2(10)
C22B	9322(5)	9762(17)	3624(12)	46(4)
C24B	5940(4)	7755(9)	3463(4)	55.0(19)
C26B	5705(7)	9217(9)	4332(5)	76(3)
C28B	6735(5)	6268(7)	2264(6)	50(2)
C30B	6602(7)	4584(14)	1442(9)	101(4)
C32B	6724(5)	10176(6)	1936(4)	44.9(17)
C34B	5781(6)	11681(13)	1835(9)	63(3)
C19B	7642(3)	8329(7)	2743(4)	27.5(13)
C25A	5766(9)	7981(13)	4167(7)	86(2)
C21A	8800(4)	9090(20)	3108(16)	33(3)
C29A	6328(9)	5246(12)	1903(9)	62(3)
C33A	6292(5)	11018(8)	1711(5)	60(2)
C23A	6676(5)	8660(11)	3497(4)	36.7(17)
C27A	6571(5)	6958(7)	2685(4)	35.1(15)
C31A	6494(5)	9003(7)	2244(4)	33.0(16)
C20A	8038(5)	9220(30)	3190(20)	34.2(19)
N5A	6842(3)	8217(5)	2812(3)	29.8(13)
C22A	9248(7)	9960(30)	3535(19)	48(5)
C24A	5904(6)	8683(14)	3543(5)	60(2)
C26A	5884(12)	8720(20)	4795(5)	94(4)
C28A	6787(7)	6323(10)	2085(9)	46(2)
C30A	6437(11)	4699(19)	1253(10)	97(5)
C32A	6717(6)	10269(7)	2267(5)	43.0(19)
C34A	5636(10)	11440(30)	1915(13)	72(4)
C19A	7630(3)	8178(8)	2843(5)	28.3(16)

Table S24: Anisotropic Displacement Parameters ($\times 10^4$) **cmw04bucobus**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1B	32(2)	53(3)	22(2)	7(2)	2.2(18)	13(2)
C2B	40(2)	40(3)	24(2)	2(2)	4.4(19)	15(2)
C3B	46(2)	26(2)	24(2)	0.1(18)	-1.9(19)	0.7(19)
C4B	54(3)	29(2)	33(3)	-1(2)	-10(2)	-3(2)
C5B	30(2)	26.4(17)	13.9(14)	1.0(12)	-1.9(14)	0.9(15)
C6B	34(3)	27(2)	13.9(17)	0.5(15)	2.6(18)	1.9(19)
C7B	34.2(16)	21.5(16)	18.7(15)	-0.5(13)	-0.2(12)	6.7(14)
C8B	34(3)	24(3)	22(2)	1(2)	0(2)	5(3)
C9B	44(4)	24(2)	33(3)	-3(2)	-5(3)	10(2)
C10B	38(3)	27(4)	21(2)	0(2)	-2.7(19)	7(3)
C11B	35(2)	54(3)	36(2)	-8(2)	9.2(18)	-8.2(19)
C12B	35(3)	78(6)	53(4)	0(3)	5(3)	-14(3)
C13B	38(3)	61(3)	68(4)	-16(3)	20(3)	-8(3)
C14B	56(5)	67(4)	39(3)	-5(3)	15(3)	-10(4)
C15B	27(2)	33(2)	13.0(16)	-1.7(15)	-0.2(15)	-0.8(18)
C16B	34(2)	37(4)	22(3)	-6(3)	2(2)	-5(3)
C17B	36(3)	43(3)	19(3)	1(3)	2(2)	7(2)
C18B	38(3)	43(4)	16(2)	2(2)	1(2)	1(3)
N1B	25.0(12)	31.0(14)	16.9(10)	-0.2(10)	1.5(9)	3.1(11)
N2B	32.6(13)	24.1(12)	15.8(11)	-0.3(10)	-0.5(10)	4.4(10)
N3B	32.1(13)	28.8(14)	25.2(14)	-0.5(11)	-0.9(11)	-4.8(11)
N4B	31(2)	25.1(13)	14.3(12)	0.1(10)	2.3(12)	5.3(13)
O1B	30(2)	37(3)	22(2)	4.1(17)	0.4(17)	4.9(19)
O2B	42(3)	34(2)	25(2)	0.0(18)	11(2)	12(2)
O3B	35(2)	54(2)	29.0(13)	6.6(13)	4.0(14)	5.4(17)
O4B	43.9(19)	51.8(16)	24(3)	-8.6(16)	-0.9(16)	-9.4(14)
O5B	36(2)	33(2)	21(2)	-4.4(18)	-4.6(19)	2.7(18)
O6B	34(2)	49(3)	23(3)	-1(2)	-4.2(18)	-9(2)
S1B	29.9(10)	24.0(9)	18.4(11)	-1.5(7)	3.7(8)	6.8(8)
S2B	29.9(5)	42.9(6)	20.0(6)	-3.8(5)	-0.3(4)	-6.6(5)
S3B	25.9(10)	31.4(10)	15.0(9)	-1.7(7)	-0.9(7)	-1.1(8)
C1A	32(3)	44(4)	21(3)	4(3)	4(2)	11(3)
C2A	35(3)	33(4)	20(3)	1(3)	3(2)	5(2)
C3A	45(3)	27(3)	23(4)	-1(2)	0(3)	-2(2)
C4A	47(3)	31(3)	32(3)	3(3)	-3(3)	-4(2)
C5A	30(2)	26.4(17)	13.9(14)	1.0(12)	-1.9(14)	0.9(15)
C6A	33(4)	28(2)	15(3)	1(2)	0(3)	3(2)
C7A	34.2(16)	21.5(16)	18.7(15)	-0.5(13)	-0.2(12)	6.7(14)
C8A	34(4)	22(5)	19(4)	2(3)	-2(3)	6(4)
C9A	41(5)	23(3)	35(5)	-3(3)	-4(4)	9(3)
C10A	40(4)	24(6)	21(3)	-2(3)	-2(3)	10(4)
C11A	35(3)	54(3)	38(3)	-7(3)	8(2)	-6(2)
C12A	33(4)	73(7)	45(5)	-3(4)	7(3)	-8(4)
C13A	38(5)	59(4)	61(5)	-15(4)	15(4)	-5(3)
C14A	41(6)	61(5)	42(5)	-7(4)	13(4)	-6(4)
C15A	28(3)	34(3)	14(2)	-2(2)	0(2)	-1(2)
C16A	32(3)	34(5)	17(5)	-5(4)	3(3)	-1(4)
C17A	34(4)	40(5)	15(5)	0(4)	3(3)	4(4)
C18A	35(5)	39(5)	16(3)	1(3)	3(3)	1(4)
N1A	25.0(12)	31.0(14)	16.9(10)	-0.2(10)	1.5(9)	3.1(11)
N2A	32.6(13)	24.1(12)	15.8(11)	-0.3(10)	-0.5(10)	4.4(10)
N3A	32.1(13)	28.8(14)	25.2(14)	-0.5(11)	-0.9(11)	-4.8(11)
N4A	31(2)	25.1(13)	14.3(12)	0.1(10)	2.3(12)	5.3(13)
O1A	31(4)	31(4)	17(3)	3(3)	0(3)	5(3)
O2A	40(5)	33(4)	17(3)	0(3)	5(3)	12(3)
O3A	35(2)	54(2)	29.0(13)	6.6(13)	4.0(14)	5.4(17)
O4A	43.9(19)	51.8(16)	24(3)	-8.6(16)	-0.9(16)	-9.4(14)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O5A	31(3)	30(3)	23(3)	-3(2)	-2(2)	0(2)
O6A	32(3)	48(5)	17(4)	2(4)	-4(3)	-7(3)
S1A	33(2)	25.8(19)	14.0(19)	-0.7(14)	-0.6(15)	7.8(15)
S2A	29.9(5)	42.9(6)	20.0(6)	-3.8(5)	-0.3(4)	-6.6(5)
S3A	26.5(19)	32.2(19)	13.6(17)	-3.1(14)	-1.2(14)	-0.1(15)
Co1	24.3(3)	23.2(3)	14.0(2)	-0.44(18)	0.72(17)	1.5(2)
C25B	85(5)	106(5)	69(4)	17(3)	32(3)	12(4)
C21B	36(2)	36(5)	25(5)	11(4)	0(2)	-2(2)
C29B	50(4)	54(4)	90(6)	-20(4)	-19(4)	1(3)
C33B	57(5)	46(4)	35(5)	11(3)	5(3)	12(3)
C23B	41(3)	47(4)	23(2)	10(2)	5.8(18)	7(3)
C27B	26(3)	44(2)	30(2)	-1.2(19)	0(2)	2(2)
C31B	36(3)	39(2)	23(2)	4.8(18)	6(2)	10(2)
C20B	38(2)	31(3)	32(3)	1(3)	-1(2)	0(2)
N5B	29.2(19)	35(2)	19.9(19)	4.6(16)	2.2(15)	4.6(16)
C22B	46(4)	43(7)	45(6)	8(6)	-8(4)	-9(4)
C24B	42(3)	78(5)	47(3)	19(3)	13(2)	4(3)
C26B	89(7)	87(5)	58(5)	16(4)	31(5)	9(4)
C28B	41(3)	46(3)	59(5)	-8(3)	-8(3)	1(2)
C30B	55(7)	116(7)	115(8)	-60(7)	-36(6)	17(5)
C32B	56(4)	48(3)	33(3)	14(2)	13(3)	14(3)
C34B	61(5)	68(7)	60(6)	14(5)	10(4)	18(5)
C19B	29.7(19)	30(3)	22(3)	5(2)	1.8(16)	3.8(17)
C25A	85(5)	111(5)	70(4)	20(4)	31(4)	8(4)
C21A	37(3)	35(5)	24(6)	11(5)	-1(3)	-1(3)
C29A	44(4)	48(4)	84(6)	-15(4)	-19(4)	3(4)
C33A	76(5)	58(4)	45(4)	16(3)	2(3)	18(3)
C23A	45(3)	43(4)	22(2)	5(2)	4(2)	8(3)
C27A	31(3)	38(3)	33(3)	4(2)	-3(3)	1(2)
C31A	35(3)	42(3)	22(3)	6(2)	4(2)	11(2)
C20A	37(3)	31(3)	32(4)	1(3)	0(3)	0(3)
N5A	31(2)	35(2)	22(2)	5.1(19)	-0.2(18)	3.3(18)
C22A	47(5)	43(8)	49(8)	4(8)	-5(5)	-7(5)
C24A	49(3)	83(5)	49(4)	7(4)	15(3)	8(3)
C26A	98(9)	119(8)	68(5)	9(5)	26(5)	14(7)
C28A	40(3)	50(3)	45(5)	-9(3)	-2(3)	1(3)
C30A	50(8)	127(8)	104(7)	-56(7)	-21(6)	5(7)
C32A	58(4)	43(3)	29(4)	8(3)	9(4)	9(3)
C34A	74(6)	77(9)	64(7)	15(6)	7(5)	24(6)
C19A	32(2)	30(3)	22(3)	4(3)	-1(2)	3.8(19)

Table S25: Bond Lengths in Å for **cmw04bucobus**.

Atom	Atom	Length/Å
C1B	C2B	1.508(7)
C1B	N1B	1.474(6)
C2B	N2B	1.486(6)
C3B	C4B	1.532(7)
C3B	N2B	1.476(6)
C4B	N3B	1.459(7)
C5B	C6B	1.507(7)
C5B	N2B	1.484(5)
C6B	N4B	1.472(6)
C7B	C8B	1.526(6)
C7B	C9B	1.529(7)
C7B	C10B	1.530(6)
C7B	S1B	1.814(5)
C11B	C12B	1.534(8)
C11B	C13B	1.512(8)
C11B	C14B	1.535(9)
C11B	S2B	1.820(5)
C15B	C16B	1.533(6)
C15B	C17B	1.519(6)
C15B	C18B	1.528(6)
C15B	S3B	1.824(4)
N1B	S3B	1.579(4)
N1B	Co1	1.952(4)
N2B	Co1	2.118(4)
N3B	S2B	1.583(4)
N3B	Co1	1.978(4)
N4B	S1B	1.582(4)
N4B	Co1	1.934(4)

Atom	Atom	Length/Å
O1B	S1B	1.446(3)
O2B	S1B	1.456(3)
O3B	S2B	1.442(4)
O4B	S2B	1.450(4)
O5B	S3B	1.448(3)
O6B	S3B	1.449(4)
C1A	C2A	1.506(7)
C1A	N1A	1.473(6)
C2A	N2A	1.484(6)
C3A	C4A	1.531(7)
C3A	N2A	1.473(6)
C4A	N3A	1.459(7)
C5A	C6A	1.506(7)
C5A	N2A	1.481(5)
C6A	N4A	1.473(6)
C7A	C8A	1.526(6)
C7A	C9A	1.529(7)
C7A	C10A	1.530(6)
C7A	S1A	1.814(5)
C11A	C12A	1.534(8)
C11A	C13A	1.513(8)
C11A	C14A	1.535(9)
C11A	S2A	1.820(6)
C15A	C16A	1.533(6)
C15A	C17A	1.519(6)
C15A	C18A	1.528(6)
C15A	S3A	1.824(4)
N1A	S3A	1.579(4)
N1A	Co1	1.944(7)
N2A	Co1	2.160(5)
N3A	S2A	1.584(4)
N3A	Co1	1.932(7)
N4A	S1A	1.583(4)
N4A	Co1	2.013(6)
O1A	S1A	1.445(4)
O2A	S1A	1.456(4)
O3A	S2A	1.442(4)

Atom	Atom	Length/Å
O4A	S2A	1.450(4)
O5A	S3A	1.448(4)
O6A	S3A	1.450(4)
C25B	C24B	1.533(4)
C25B	C26B	1.486(7)
C21B	C20B	1.525(4)
C21B	C22B	1.491(6)
C29B	C28B	1.523(4)
C29B	C30B	1.475(6)
C33B	C32B	1.530(4)
C33B	C34B	1.482(7)
C23B	N5B	1.529(7)
C23B	C24B	1.525(9)
C27B	N5B	1.530(7)
C27B	C28B	1.508(10)
C31B	N5B	1.510(7)
C31B	C32B	1.501(8)
C20B	C19B	1.522(7)
N5B	C19B	1.529(6)
C25A	C24A	1.531(3)
C25A	C26A	1.486(6)
C21A	C20A	1.525(3)
C21A	C22A	1.490(6)
C29A	C28A	1.524(3)
C29A	C30A	1.477(6)
C33A	C32A	1.528(3)
C33A	C34A	1.482(6)
C23A	N5A	1.530(7)
C23A	C24A	1.525(9)
C27A	N5A	1.530(7)
C27A	C28A	1.508(10)
C31A	N5A	1.511(7)
C31A	C32A	1.500(8)
C20A	C19A	1.522(7)
N5A	C19A	1.529(6)

Table S26: Bond Angles in ° for **cmw04bucobus**.

Atom	Atom	Atom	Angle/°
N1B	C1B	C2B	108.2(4)
N2B	C2B	C1B	110.4(4)
N2B	C3B	C4B	110.8(4)
N3B	C4B	C3B	107.6(4)
N2B	C5B	C6B	109.4(3)
N4B	C6B	C5B	107.9(4)
C8B	C7B	C9B	110.9(4)
C8B	C7B	C10B	110.3(4)
C8B	C7B	S1B	108.6(3)
C9B	C7B	C10B	109.7(4)
C9B	C7B	S1B	107.5(3)
C10B	C7B	S1B	109.8(4)
C12B	C11B	C14B	110.3(6)
C12B	C11B	S2B	106.7(4)
C13B	C11B	C12B	111.3(6)
C13B	C11B	C14B	110.6(5)

Atom	Atom	Atom	Angle/°
C13B	C11B	S2B	109.1(4)
C14B	C11B	S2B	108.8(5)
C16B	C15B	S3B	108.5(3)
C17B	C15B	C16B	111.2(4)
C17B	C15B	C18B	110.2(4)
C17B	C15B	S3B	109.3(3)
C18B	C15B	C16B	111.1(4)
C18B	C15B	S3B	106.5(4)
C1B	N1B	S3B	121.2(3)
C1B	N1B	Co1	112.6(3)
S3B	N1B	Co1	123.7(2)
C2B	N2B	Co1	106.5(3)
C3B	N2B	C2B	113.9(4)
C3B	N2B	C5B	111.6(4)
C3B	N2B	Co1	106.2(3)
C5B	N2B	C2B	111.6(4)

Atom	Atom	Atom	Angle/°
C5B	N2B	Co1	106.4(3)
C4B	N3B	S2B	119.0(4)
C4B	N3B	Co1	113.4(3)
S2B	N3B	Co1	126.3(3)
C6B	N4B	S1B	120.8(3)
C6B	N4B	Co1	113.1(3)
S1B	N4B	Co1	125.6(2)
N4B	S1B	C7B	108.8(2)
O1B	S1B	C7B	105.7(2)
O1B	S1B	N4B	107.1(2)
O1B	S1B	O2B	117.3(3)
O2B	S1B	C7B	105.9(2)
O2B	S1B	N4B	111.7(2)
N3B	S2B	C11B	107.9(2)
O3B	S2B	C11B	105.1(3)
O3B	S2B	N3B	108.9(2)
O3B	S2B	O4B	117.5(2)
O4B	S2B	C11B	106.4(2)
O4B	S2B	N3B	110.5(2)
N1B	S3B	C15B	108.9(2)
O5B	S3B	C15B	105.3(2)
O5B	S3B	N1B	106.6(2)
O5B	S3B	O6B	117.3(3)
O6B	S3B	C15B	106.0(2)
O6B	S3B	N1B	112.3(2)
N1A	C1A	C2A	108.9(5)
N2A	C2A	C1A	111.0(4)
N2A	C3A	C4A	111.1(5)
N3A	C4A	C3A	108.1(5)
N2A	C5A	C6A	109.7(4)
N4A	C6A	C5A	108.1(4)
C8A	C7A	C9A	110.9(5)
C8A	C7A	C10A	110.3(4)
C8A	C7A	S1A	108.6(3)
C9A	C7A	C10A	109.8(5)
C9A	C7A	S1A	107.4(4)
C10A	C7A	S1A	109.8(4)
C12A	C11A	C14A	110.2(6)
C12A	C11A	S2A	106.8(5)
C13A	C11A	C12A	111.2(6)
C13A	C11A	C14A	110.6(5)
C13A	C11A	S2A	109.1(4)
C14A	C11A	S2A	108.8(5)
C16A	C15A	S3A	108.5(3)
C17A	C15A	C16A	111.3(5)
C17A	C15A	C18A	110.1(5)
C17A	C15A	S3A	109.3(3)
C18A	C15A	C16A	111.1(4)
C18A	C15A	S3A	106.4(4)
C1A	N1A	S3A	121.1(4)
C1A	N1A	Co1	116.1(4)
S3A	N1A	Co1	121.4(4)
C2A	N2A	Co1	105.4(4)
C3A	N2A	C2A	114.7(5)
C3A	N2A	C5A	112.5(4)
C3A	N2A	Co1	103.9(4)
C5A	N2A	C2A	112.3(4)
C5A	N2A	Co1	107.1(4)

Atom	Atom	Atom	Angle/°
C4A	N3A	S2A	118.9(4)
C4A	N3A	Co1	115.7(4)
S2A	N3A	Co1	124.2(4)
C6A	N4A	S1A	120.3(4)
C6A	N4A	Co1	115.7(3)
S1A	N4A	Co1	123.9(4)
N4A	S1A	C7A	108.7(3)
O1A	S1A	C7A	105.8(3)
O1A	S1A	N4A	107.1(3)
O1A	S1A	O2A	117.3(3)
O2A	S1A	C7A	105.9(3)
O2A	S1A	N4A	111.7(3)
N3A	S2A	C11A	108.0(3)
O3A	S2A	C11A	105.1(3)
O3A	S2A	N3A	108.9(3)
O3A	S2A	O4A	117.5(3)
O4A	S2A	C11A	106.4(3)
O4A	S2A	N3A	110.4(3)
N1A	S3A	C15A	109.1(3)
O5A	S3A	C15A	105.2(3)
O5A	S3A	N1A	106.6(3)
O5A	S3A	O6A	117.3(3)
O6A	S3A	C15A	106.0(3)
O6A	S3A	N1A	112.2(3)
N1B	Co1	N2B	84.08(16)
N1B	Co1	N3B	117.5(2)
N3B	Co1	N2B	83.77(16)
N4B	Co1	N1B	119.76(19)
N4B	Co1	N2B	83.79(15)
N4B	Co1	N3B	119.4(2)
N1A	Co1	N2A	82.8(2)
N1A	Co1	N4A	116.6(3)
N3A	Co1	N1A	120.3(4)
N3A	Co1	N2A	83.8(2)
N3A	Co1	N4A	117.9(4)
N4A	Co1	N2A	80.7(2)
C26B	C25B	C24B	110.9(5)
C22B	C21B	C20B	111.8(4)
C30B	C29B	C28B	112.9(5)
C34B	C33B	C32B	111.8(5)
C24B	C23B	N5B	114.6(5)
C28B	C27B	N5B	116.6(5)
C32B	C31B	N5B	116.9(4)
C19B	C20B	C21B	109.2(4)
C23B	N5B	C27B	109.9(5)
C31B	N5B	C23B	109.3(5)
C31B	N5B	C27B	109.0(3)
C31B	N5B	C19B	112.2(4)
C19B	N5B	C23B	109.1(4)
C19B	N5B	C27B	107.3(4)
C23B	C24B	C25B	110.0(6)
C27B	C28B	C29B	110.0(7)
C31B	C32B	C33B	112.4(6)
C20B	C19B	N5B	116.6(4)
C26A	C25A	C24A	111.1(5)
C22A	C21A	C20A	111.8(4)
C30A	C29A	C28A	112.5(5)
C34A	C33A	C32A	111.9(5)

Atom	Atom	Atom	Angle/°
C24A	C23A	N5A	114.3(5)
C28A	C27A	N5A	116.3(5)
C32A	C31A	N5A	116.7(4)
C19A	C20A	C21A	109.2(4)
C23A	N5A	C27A	109.6(5)
C31A	N5A	C23A	109.5(5)
C31A	N5A	C27A	109.0(4)
C31A	N5A	C19A	112.2(5)
C19A	N5A	C23A	109.1(4)
C19A	N5A	C27A	107.4(4)
C23A	C24A	C25A	110.1(6)
C27A	C28A	C29A	110.0(7)
C31A	C32A	C33A	112.9(6)
C20A	C19A	N5A	116.5(4)

Table S27: Hydrogen Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **cmw04bucobus**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H1BA	9639	4290	4914	43
H1BB	9750	3385	4318	43
H2BA	9020	2012	4682	42
H2BB	9517	2439	5361	42
H3BA	7747	2344	5710	39
H3BB	8303	1398	5536	39
H4BA	7846	1433	4375	48
H4BB	7186	1322	4763	48
H5BA	9167	4176	5915	29
H5BB	8809	3188	6321	29
H6BA	7753	4162	6136	30
H6BB	8324	5149	6399	30
H8BA	8500	7337	4423	41
H8BB	9039	6530	4912	41
H8BC	9184	7911	4851	41
H9BA	8529	9370	5451	52
H9BB	7878	8934	5785	52
H9BC	7838	8926	4973	52
H10A	9089	6556	6147	44
H10B	8635	7472	6503	44
H10C	9286	7926	6175	44
H12A	4831	3393	4007	83
H12B	5196	2392	3620	83
H12C	5237	3742	3396	83
H13A	5988	5145	4141	81
H13B	6441	4707	4840	81
H13C	5617	4842	4783	81
H14A	5517	2726	5145	80
H14B	6344	2610	5220	80
H14C	5854	1712	4742	80
H16A	8129	2793	2294	47
H16B	7793	3787	2711	47
H16C	8225	2731	3110	47
H17A	9511	2719	3254	50
H17B	9915	3696	2887	50
H17C	9475	2696	2442	50
H18A	8828	4301	1729	49
H18B	9255	5287	2198	49
H18C	8424	5285	2090	49
H1AA	9767	3443	4355	39
H1AB	9201	2409	4217	39
H2AA	9522	2407	5375	36
H2AB	9511	3817	5416	36
H3AA	8308	1415	5563	39
H3AB	8366	1568	4771	39

Atom	x	y	z	U_{eq}
H4AA	7188	1370	4789	45
H4AB	7213	2269	5418	45
H5AA	8840	3180	6347	29
H5AB	8018	3312	6113	29
H6AA	8401	5179	6431	31
H6AB	9042	5078	6016	31
H8AA	8428	7619	4358	39
H8AB	8918	6673	4799	39
H8AC	9148	8026	4800	39
H9AA	8324	9538	5274	51
H9AB	7763	9033	5707	51
H9AC	7645	8876	4895	51
H10D	9155	6979	6105	44
H10E	8660	7848	6443	44
H10F	9239	8375	6040	44
H12D	4849	3798	3705	75
H12E	5233	2767	3360	75
H12F	5414	4115	3231	75
H13D	6189	5243	4158	78
H13E	6344	4690	4910	78
H13F	5572	5086	4594	78
H14D	5251	2986	4906	71
H14E	6047	2606	5111	71
H14F	5550	1902	4527	71
H16D	8100	3121	2169	42
H16E	7798	3963	2699	42
H16F	8222	2802	2965	42
H17D	9499	2771	3104	45
H17E	9913	3831	2820	45
H17F	9455	2957	2298	45
H18D	8829	4723	1737	45
H18E	9271	5583	2281	45
H18F	8440	5604	2180	45
H25A	5353	7521	4243	102
H25B	6168	7612	4522	102
H21A	8961	8104	3368	39
H21B	8942	8954	2721	39
H29A	5905	5122	2034	81
H29B	5974	6011	1422	81
H33A	6778	11889	2312	56
H33B	6709	11841	1497	56
H23A	6976	7289	3583	44
H23B	6863	8634	3776	44
H27A	6005	7578	2181	41
H27B	6607	7828	1742	41
H31A	6064	9584	2561	39
H31B	6761	10136	2969	39
H20A	7992	9094	3687	41
H20B	7984	10001	3066	41
H22A	9228	10563	3448	69
H22B	9807	9558	3606	69
H22C	9238	9723	4098	69
H24A	5829	6933	3318	66
H24B	5645	8287	3143	66
H26A	5533	9632	3905	113
H26B	6155	9545	4536	113
H26C	5373	9315	4650	113
H28A	6734	6006	2740	60

Atom	x	y	z	U_{eq}
H28B	7213	6184	2161	60
H30A	6918	4956	1168	151
H30B	6260	4106	1145	151
H30C	6868	4079	1791	151
H32A	6455	9765	1540	54
H32B	7223	10081	1909	54
H34A	5536	11123	1504	95
H34B	5670	12489	1680	95
H34C	5636	11560	2281	95
H19A	7799	7517	2869	33
H19B	7729	8470	2271	33
H25C	5280	7695	4089	104
H25D	6076	7286	4230	104
H21C	8959	8282	3243	39
H21D	8847	9202	2623	39
H29C	6428	4658	2274	74
H29D	5835	5482	1869	74
H33C	6572	11706	1611	72
H33D	6184	10546	1287	72
H23C	6916	8148	3865	44
H23D	6866	9466	3577	44
H27C	6728	6488	3101	42
H27D	6057	6983	2618	42
H31C	6576	8664	1804	40
H31D	5987	8980	2247	40
H20C	7995	9242	3677	41
H20D	7850	9964	2973	41
H22D	9127	10758	3368	71
H22E	9736	9802	3506	71
H22F	9175	9892	4011	71
H24C	5636	8339	3124	72
H24D	5750	9509	3581	72
H26D	6317	9162	4810	141
H26E	5918	8207	5198	141
H26F	5495	9266	4790	141
H28C	7279	6074	2200	55
H28D	6747	6861	1687	55
H30D	6477	5316	916	146
H30E	6042	4187	1084	146
H30F	6865	4230	1328	146
H32C	7213	10310	2215	52
H32D	6673	10603	2719	52
H34D	5257	11359	1529	109
H34E	5686	12267	2053	109
H34F	5532	10964	2300	109
H19C	7806	7451	3088	34
H19D	7730	8115	2371	34

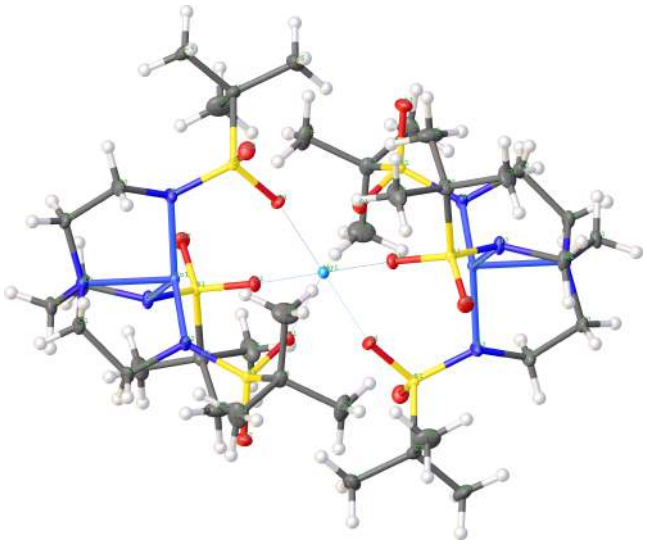
MgCoBus

EMORY UNIVERSITY | X-ray Crystallography Center

Submitted by: **Christian Wallen**
Emory University
Solved by: **John Bacsa**

Sample ID: **MgCoBus**

Crystal Data and Experimental



Experimental. Single violet prism-shaped crystals of (**MgCoBus**) were recrystallised from a mixture of CH_2Cl_2 and methanol by vapor diffusion. A suitable crystal (0.32×0.24×0.21) was selected and mounted on a MITIGEN holder with paratone oil on a Bruker APEX-II CCD diffractometer. The crystal was cooled to T = 100(2) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program using combined Patterson and dual-space recycling methods and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The crystal structure was refined with version 2014/7 of **ShelXL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{36}H_{78}Co_2MgN_8O_{12}S_6$, M_r = 1149.59, trigonal, R-3 (No. 148), a = 12.684(2) Å, b = 12.684(2) Å, c = 27.867(6) Å, α = 90°, β = 90°, γ = 120°, V = 3882.7(16) Å^3, T = 100(2) K, Z = 3, Z' = 1/6, μ(MoK$_\alpha$) = 0.957, 39376 reflections measured, 7192 unique (R_{int} = 0.0362) which were used in all calculations. The final wR_2 was 0.0856 (all data) and R_1 was 0.0325 (I > 2σ(I)).

Compound	**MgCoBus**
Formula	$C_{36}H_{78}Co_2MgN_8O_{12}S_6$
$D_{calc.}$/ g cm^{-3}	1.475
μ/mm^{-1}	0.957
Formula Weight	1149.59
Colour	violet
Shape	prism
Max Size/mm	0.32
Mid Size/mm	0.24
Min Size/mm	0.21
T/K	100(2)
Crystal System	trigonal
Space Group	R-3
a/Å	12.684(2)
b/Å	12.684(2)
c/Å	27.867(6)
α/°	90
β/°	90
γ/°	120
V/Å^3	3882.7(16)
Z	3
Z'	1/6
Θ_{min}/°	2.361
Θ_{max}/°	45.276
Measured Refl.	39376
Independent Refl.	7192
Reflections Used	6105
R_{int}	0.0362
Parameters	115
Restraints	6
Largest Peak	1.467
Deepest Hole	-0.810
GooF	1.060
wR_2 (all data)	0.0856
wR_2	0.0797
R_1 (all data)	0.0418
R_1	0.0325
CCDC #	1434438

Structure Quality Indicators

Reflections:	d min	0.50	I/σ	24.5	Rint	3.62%	complete	99%
Refinement:	Shift	0.003	Max Peak	1.5	Min Peak	-0.8	GooF	1.060

A violet prism-shaped crystal with dimensions 0.32×0.24×0.21 mm was mounted on a MITIGEN holder with paratone oil.X-ray diffraction data were collected using a Bruker APEX-II CCD diffractometer equipped with an Oxford Cryosystems low-temperature apparatus operating at T = 100(2) K.

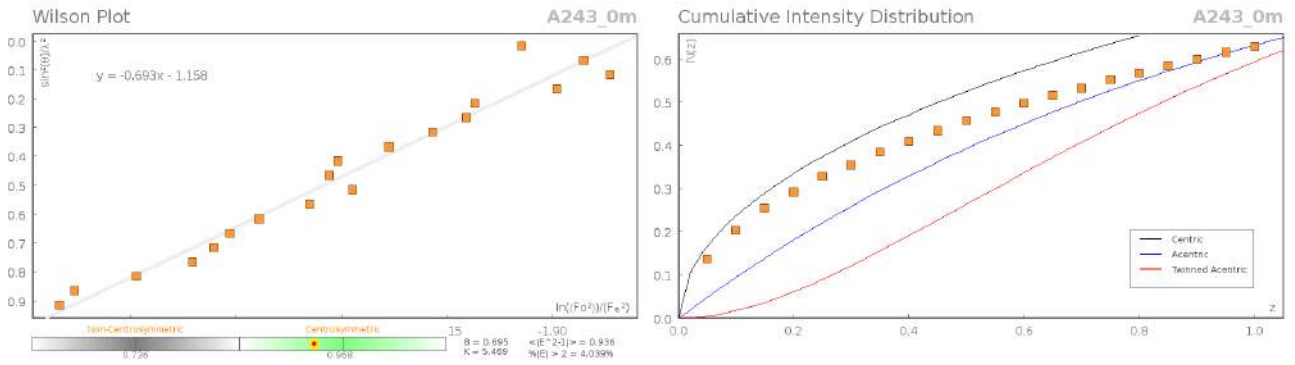
Data were measured using ϕ and ω scans and MoK$_\alpha$ radiation (fine-focus sealed tube, 45 kV, 35 mA). The total number of runs and images was based on the strategy calculation from the program **APEX2** (Bruker, 2014). The maximum resolution achieved was was Θ = 45.27°.

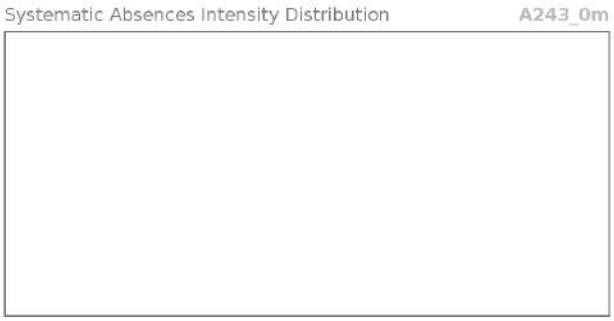
Unit cell indexing was performed by using the **APEX2** (Bruker, 2014) software and refined using **SAINT** (Bruker, V8.34A, 2013) on 9896 reflections, 25% of the observed reflections. Data reduction, scaling and absorption corrections were performed using **SAINT** (Bruker, V8.34A, 2013) and **SADABS-2014/5** (Bruker,2014/5) was used for absorption correction. wR_2(int) was 0.0848 before and 0.0460 after correction. The Ratio of minimum to maximum transmission is 0.8857. The $\lambda/2$ correction factor is 0.00150. This software which corrects for Lorentz polarisation. The final completeness is 99.4% out to 45.276° in Θ. The absorption coefficient (μ) of this material is 0.957 mm^{-1} and the minimum and maximum transmissions are 0.6633 and 0.7489.

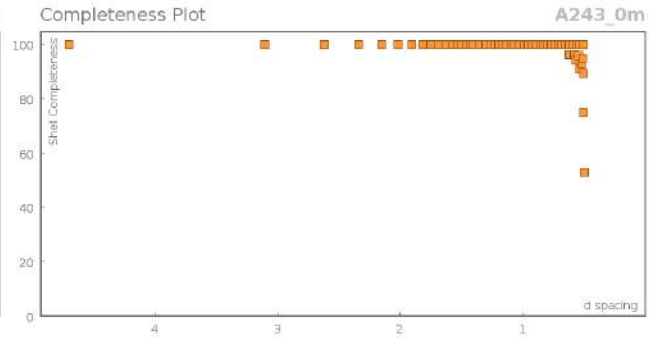
The structure was solved in the space group P1 with the **ShelXT** (Sheldrick, 2015) structure solution program using combined Patterson and dual-space recycling methods. The space group R-3 (# 148) was determined by the **ShelXT** (Sheldrick, 2015) structure solution program. The crystal structure was refined by Least Squares using version 2014/7 of **ShelXL** (Sheldrick, 2008). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

The value of Z' is 0.16667.

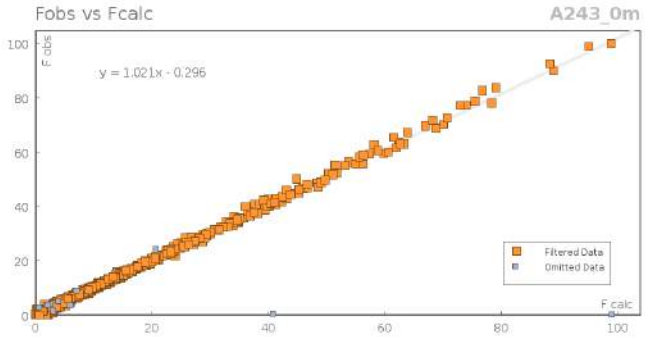
Data Plots: Diffraction Data

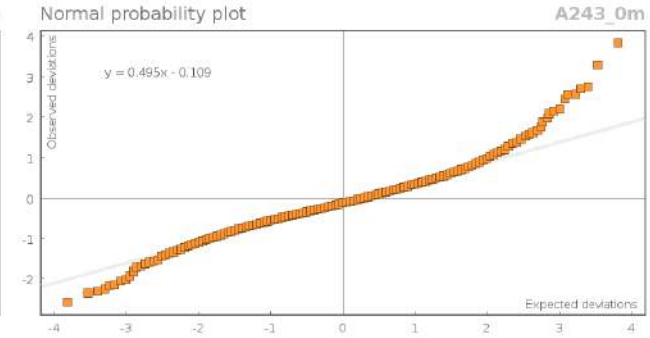






Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	39443	Unique reflections	7192
Completeness	0.994	Mean I/σ	24.51
hklsub>max</sub> collected	(25, 25, 48)	hklsub>min</sub> collected	(-24, -24, -54)
hkl_{max} used	(12, 25, 54)	hkl_{min} used	(-25, 0, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.36
d_{max} used	10.22	d_{min} used	0.5
Friedel pairs	5706	Friedel pairs merged	1
Inconsistent equivalents	0	R_{int}	0.0362
R_{sigma}	0.0271	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	67
Multiplicity	(11601, 7142, 2536, 1280, 166)	Maximum multiplicity	15
Removed systematic absences	0	Filtered off (Shel/OMIT)	0

Images of the Crystal on the Diffractometer

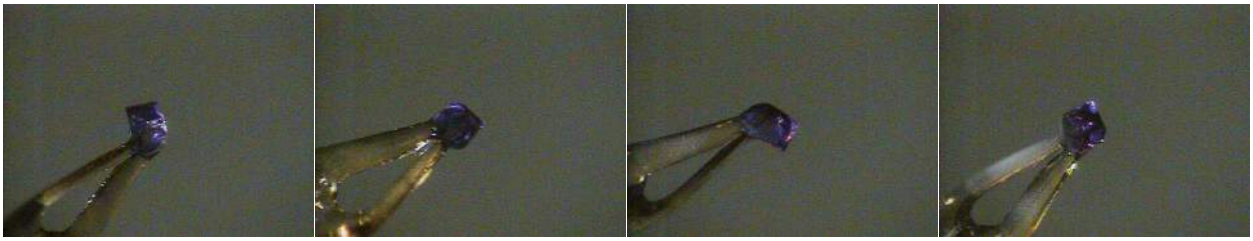


Table S28: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **A243_0m**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Co1	10000	10000	3776.3(2)	7.76(3)
S1	7905.3(2)	10125.5(2)	4196.7(2)	8.52(3)
Mg1	10000	10000	5000	7.35(8)
O1	8670.3(4)	10104.4(5)	4588.3(2)	10.92(7)
O2	6675.2(5)	9104.6(5)	4182.2(2)	15.15(8)
N1	10000	10000	3020.3(3)	10.42(12)
N2	8656.8(5)	10319.6(6)	3723.6(2)	11.79(8)
C1	9115.9(6)	10383.2(7)	2878.7(2)	13.71(10)
C2	8086.2(6)	9942.6(8)	3246.8(2)	15.81(11)
C3	7791.7(6)	11483.1(6)	4298.8(3)	13.65(10)
C6	7130.4(10)	11343.4(10)	4773.6(3)	24.75(16)
C4	7069.4(10)	11600.5(9)	3883.3(3)	24.26(16)
C5	9081.2(9)	12566.6(8)	4322.4(4)	27.57(18)

Table S29: Anisotropic Displacement Parameters (×10⁴) **A243_0m**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	8.37(4)	8.37(4)	6.55(5)	0	0	4.19(2)
S1	7.79(5)	10.11(5)	8.11(6)	0.16(4)	-0.82(4)	4.82(4)
Mg1	7.60(11)	7.60(11)	6.83(19)	0	0	3.80(6)
O1	11.43(16)	13.89(17)	9.47(17)	-0.03(13)	-2.53(12)	7.84(14)
O2	9.28(16)	15.26(19)	16.0(2)	0.50(15)	-1.88(14)	2.44(14)
N1	11.63(19)	11.63(19)	8.0(3)	0	0	5.82(9)
N2	11.34(18)	18.6(2)	7.75(18)	-1.17(15)	-0.86(14)	9.24(17)
C1	16.8(2)	18.9(3)	8.2(2)	1.01(18)	-1.02(17)	10.9(2)
C2	13.3(2)	25.9(3)	9.3(2)	-2.2(2)	-2.58(17)	10.6(2)
C3	17.3(2)	15.2(2)	13.1(2)	1.14(18)	0.23(18)	11.7(2)
C6	37.5(4)	33.5(4)	17.1(3)	1.6(3)	6.7(3)	28.1(4)
C4	35.1(4)	31.8(4)	19.5(3)	1.3(3)	-4.9(3)	27.0(4)
C5	25.2(4)	12.0(3)	42.9(5)	-1.0(3)	-2.6(3)	7.4(3)

Table S30: Bond Lengths in Å for **A243_0m**.

Atom	Atom	Length/Å
Co1	N1	2.1069(10)
Co1	N2[1]	1.9440(6)
Co1	N2	1.9440(7)
Co1	N2[2]	1.9440(7)
S1	O1	1.4694(5)
S1	O2	1.4465(6)
S1	N2	1.5725(6)
S1	C3	1.8208(7)
Mg1	O1[3]	2.0981(5)
Mg1	O1	2.0981(5)
Mg1	O1[4]	2.0981(5)
Mg1	O1[5]	2.0981(5)
Mg1	O1[1]	2.0981(5)
Mg1	O1[2]	2.0981(5)
N1	C1[1]	1.4814(8)
N1	C1[2]	1.4814(8)
N1	C1	1.4814(7)
N2	C2	1.4735(9)
C1	C2	1.5300(10)
C3	C6	1.5290(11)
C3	C4	1.5291(11)
C3	C5	1.5232(12)

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[1]2-Y,1+X-Y,+Z; [2]1+Y-X,2-X,+Z; [3]2-X,2-Y,1-Z; [4]1-Y+X,+X,1-Z; [5]+Y,1-X+Y,1-Z

Table S31: Bond Angles in ° for **A243_0m**.

Atom	Atom	Atom	Angle/°
N2	Co1	N1	85.662(17)
N2[1]	Co1	N1	85.662(17)
N2[2]	Co1	N1	85.662(17)
N2	Co1	N2[1]	119.433(5)

Atom	Atom	Atom	Angle/°
N2[1]	Co1	N2[2]	119.434(5)
N2	Co1	N2[2]	119.434(4)
O1	S1	N2	105.75(3)
O1	S1	C3	105.45(3)
O2	S1	O1	115.52(3)
O2	S1	N2	114.51(3)
O2	S1	C3	106.92(3)
N2	S1	C3	108.14(3)
O1[3]	Mg1	O1[2]	180.0
O1[4]	Mg1	O1[5]	92.95(2)
O1[3]	Mg1	O1[5]	92.95(2)
O1[5]	Mg1	O1[1]	180.0
O1[3]	Mg1	O1[1]	87.05(2)
O1[2]	Mg1	O1[1]	92.95(2)
O1[3]	Mg1	O1	87.05(2)
O1[3]	Mg1	O1[4]	92.95(2)
O1[4]	Mg1	O1	180.0
O1[2]	Mg1	O1	92.95(2)
O1[1]	Mg1	O1	92.95(2)
O1[4]	Mg1	O1[1]	87.05(2)
O1[2]	Mg1	O1[5]	87.05(2)
O1[5]	Mg1	O1	87.05(2)

Atom	Atom	Atom	Angle/°
O1[2]	Mg1	O1[4]	87.05(2)
S1	O1	Mg1	165.08(3)
C1[1]	N1	Co1	105.45(4)
C1	N1	Co1	105.45(4)
C1[2]	N1	Co1	105.45(4)
C1[2]	N1	C1	113.17(4)
C1[1]	N1	C1	113.18(4)
C1[2]	N1	C1[1]	113.18(4)
S1	N2	Co1	115.45(3)
C2	N2	Co1	109.88(4)
C2	N2	S1	122.97(5)
N1	C1	C2	110.45(6)
N2	C2	C1	107.16(6)
C6	C3	S1	108.90(5)
C6	C3	C4	110.24(7)
C4	C3	S1	107.96(5)
C5	C3	S1	107.64(5)
C5	C3	C6	110.27(8)
C5	C3	C4	111.73(7)

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[1]1+Y-X,2-X,+Z; [2]2-Y,1+X-Y,+Z; [3]+Y,1-X+Y,1-Z; [4]2-X,2-Y,1-Z; [5]1-Y+X,+X,1-Z

Table S32: Hydrogen Fractional Atomic Coordinates (×10[4]) and Equivalent Isotropic Displacement Parameters (Å[2]×10[3]) for **A243_0m**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

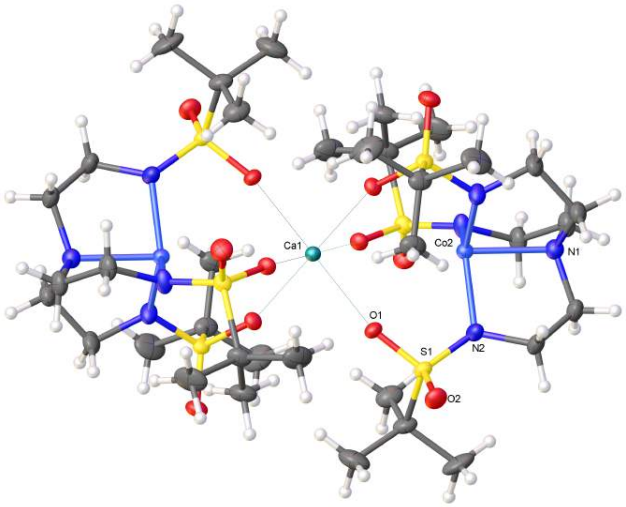
Atom	x	y	z	U_{eq}
H1A	8805(13)	10072(13)	2575(3)	20.4(16)
H1B	9532(13)	11230(7)	2853(5)	20.4(16)
H2A	7630(12)	9096(7)	3229(5)	20.4(16)
H2B	7599(11)	10276(12)	3169(5)	20.4(16)
H6A	7616	11299	5038	37
H6B	6335	10596	4766	37
H6C	7016	12045	4821	37
H4A	6290	10842	3851	36
H4B	7535	11760	3585	36
H4C	6921	12275	3947	36
H5A	9502	12634	4019	41
H5B	9523	12450	4586	41
H5C	9049	13313	4377	41

CMW_03_020

EMORY UNIVERSITY | X-ray Crystallography Center

Submitted by: **Christian Wallen**
Emory University
Solved by: **John Bacsa**
Sample ID: **CMW-03-020**

Crystal Data and Experimental



Experimental. Single violet prism-shaped crystals of (**CMW-03-020**) were recrystallised from a mixture of diethyl ether and CH_2Cl_2 by slow evaporation. A suitable crystal (0.41×0.18×0.11 mm) was selected and mounted on a loop with paratone oil on a Bruker APEX-II CCD diffractometer. The crystal was kept at T = 100(2) K during data collection. Using **Olex2** (Dolomanov et al., 2009), the structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program, using the Charge Flipping solution method. The model was refined with version 2013-4 of **ShelXL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{36}H_{78}CaCo_2N_8O_{12}S_6$, M_r = 1165.36, trigonal, R-3 (No. 148), a = 12.601(3) Å, b = 12.601(3) Å, c = 29.273(8) Å, α = 90°, β = 90°, γ = 120°, V = 4025(2) Å^3, T = 100(2) K, Z = 3, Z' = 0.16667, μ(MoK$_\alpha$) = 1.007, 17386 reflections measured, 4461 unique (R_{int} = 0.0389) which were used in all calculations. The final wR_2 was 0.1085 (all data) and R_1 was 0.0409 (I > 2(I)).

Compound	**CMW-03-020**
Formula	$C_{36}H_{78}CaCo_2N_8O_{12}S_6$
$D_{calc.}$/ g cm^{-3}	1.442
μ/mm^{-1}	1.007
Formula Weight	1165.36
Colour	violet
Shape	prism
Max Size/mm	0.41
Mid Size/mm	0.18
Min Size/mm	0.11
T/K	100(2)
Crystal System	trigonal
Space Group	R-3
a/Å	12.601(3)
b/Å	12.601(3)
c/Å	29.273(8)
α/°	90
β/°	90
γ/°	120
V/Å^3	4025(2)
Z	3
Z'	1/6
Θ_{min}/°	2.087
Θ_{max}/°	37.068
Measured Refl.	17386
Independent Refl.	4461
Reflections Used	3518
R_{int}	0.0389
Parameters	118
Restraints	45
Largest Peak	0.906
Deepest Hole	-0.604
GooF	1.032
wR_2 (all data)	0.1085
wR_2	0.0988
R_1 (all data)	0.0580
R_1	0.0409
CCDC #	1434436

Structure Quality Indicators

Reflections:	d min	0.59	I/σ	16.9	Rint	3.89%	complete 97%
Refinement:	Shift	-0.002	Max Peak	0.9	Min Peak	-0.6	GooF 1.032

A violet prism-shaped crystal with dimensions 0.41×0.18×0.11mm was mounted on a loop with paratone oil. Data were collected using a Bruker APEX-II CCD diffractometer equipped with an Oxford Cryosystems low-temperature apparatus operating at T = 100(2) K.

Data were measured using ϕ and ω scans with a narrow frame width with MoK$_\alpha$ radiation (fine-focus sealed tube, 45 kV, 35 mA). The total number of runs and images was based on the strategy calculation from the program **APEX2** (Bruker). The actually achieved resolution was Θ = 37.068°.

Cell parameters were retrieved using the **SAINT** (Bruker, V8.34A, 2013) software and refined using **SAINT** (Bruker, V8.34A, 2013) on 9971 reflections, 57% of the observed reflections. Data reduction was performed using the **SAINT** (Bruker, V8.34A, 2013) software which corrects for Lorentz polarisation. The final completeness is 99.70 out to 37.068 in Θ. The absorption coefficient (μ) of this material is 1.007 mm^{-1} and the minimum and maximum transmissions are 0.3299 and 0.4389.

The structure was solved in the space group R-3 (# 148) by Charge Flipping using the **ShelXT** (Sheldrick, 2015) structure solution program and refined by Least Squares using version 2013-4 of **ShelXL** (Sheldrick, 2008). All non-hydrogen atoms were refined anisotropically. The value of Z' is 1/6.

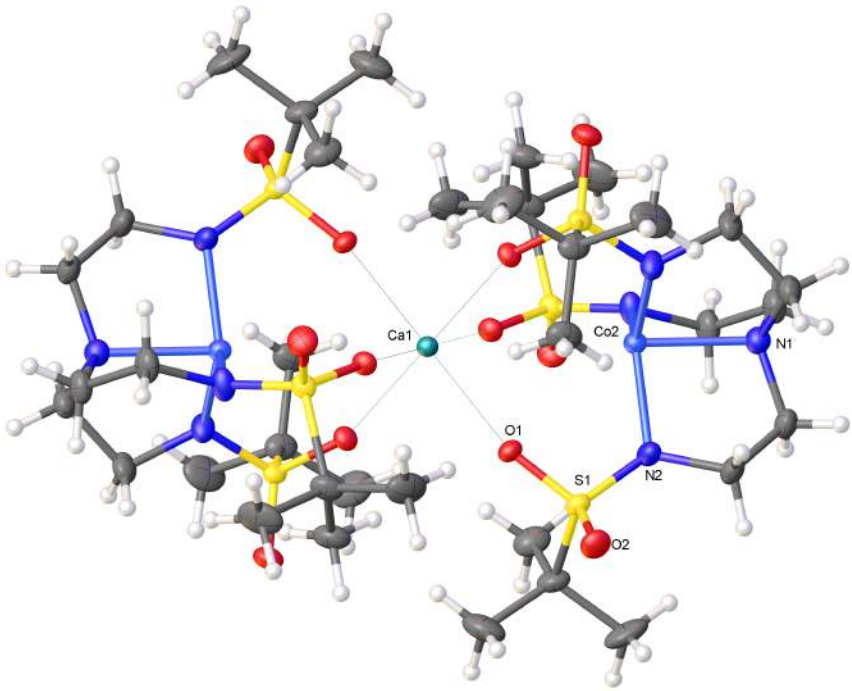


Figure S22: Plot of the dimeric Co^{2+} complex $[C_{36}H_{78}CaCo_2N_8O_{12}S_6]$. The molecule resides on a 3-fold rotation axis through the atoms Ca(1), Co(2) and N(1).

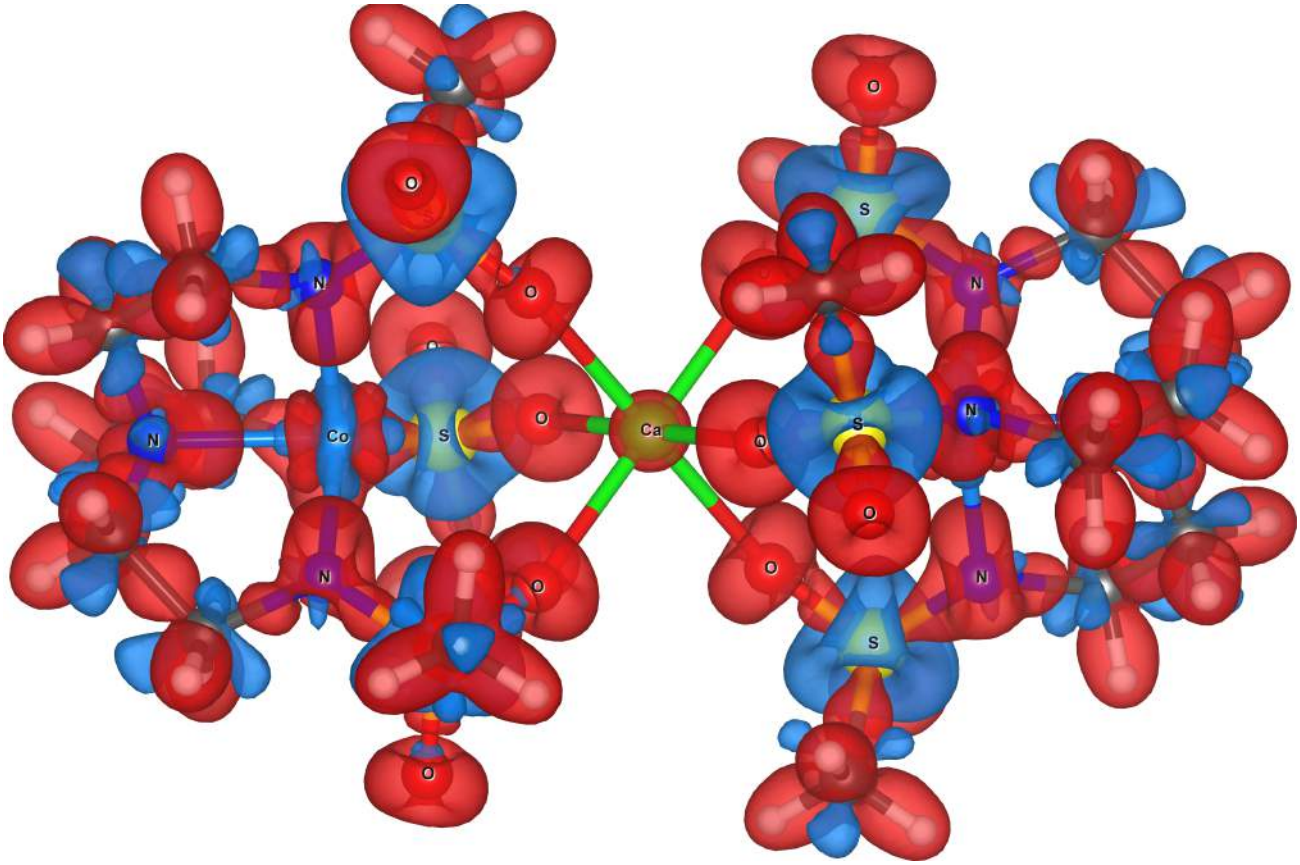


Figure S23: Positive and negative deformation density isosurfaces (0.01 e $Å^{-3}$) of the dimeric Co^{2+} complex $[C_{36}H_{78}CaCo_2N_8O_{12}S_6]$ from refinements with the predicted multipolar parameters. Charge concentrations are shown in red and depletions in blue. There are concentrations of charge corresponding to nitrogen and lone pair electrons. The density about Ca^{2+} is spherical and lobes of electron density from N to

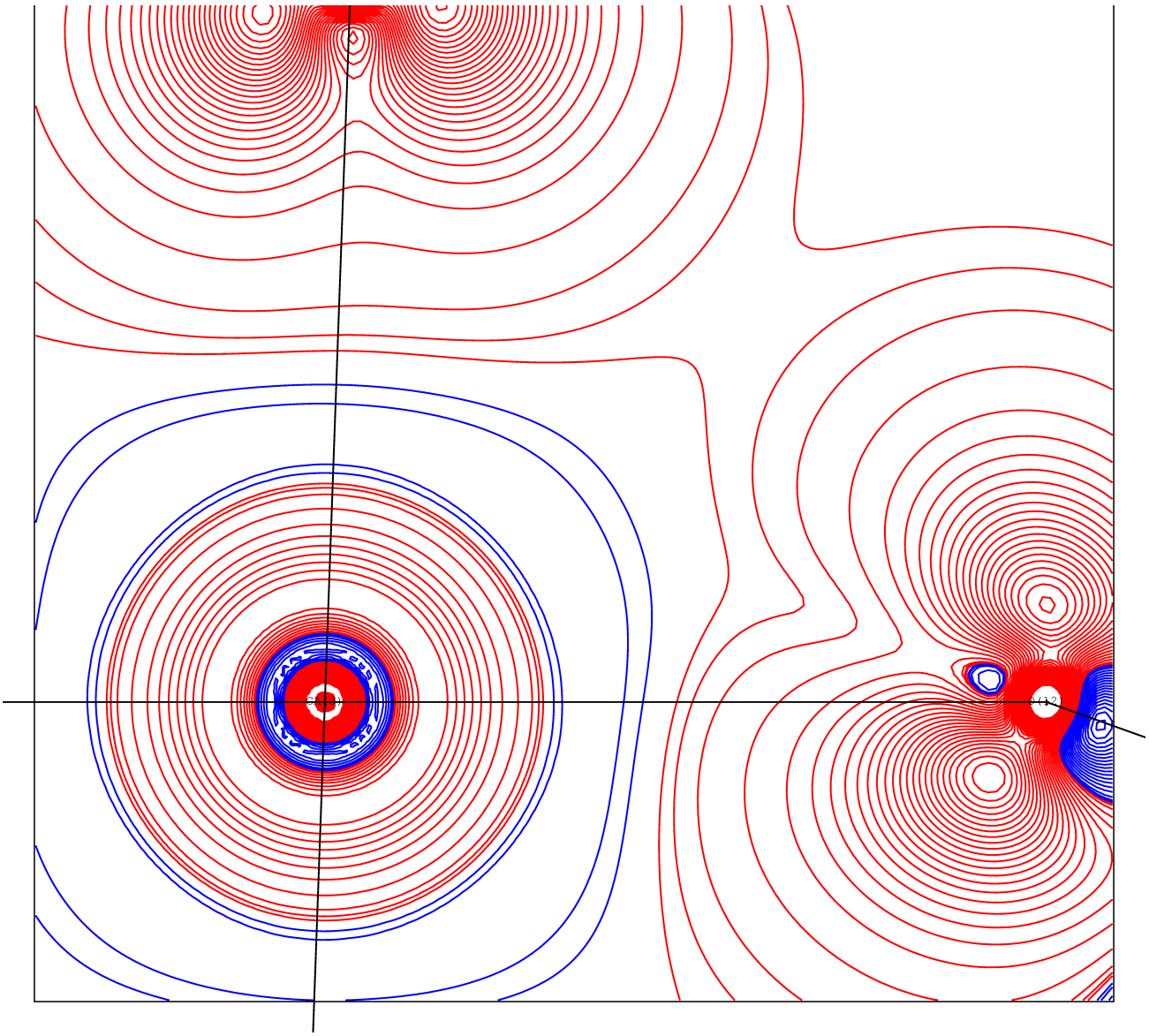
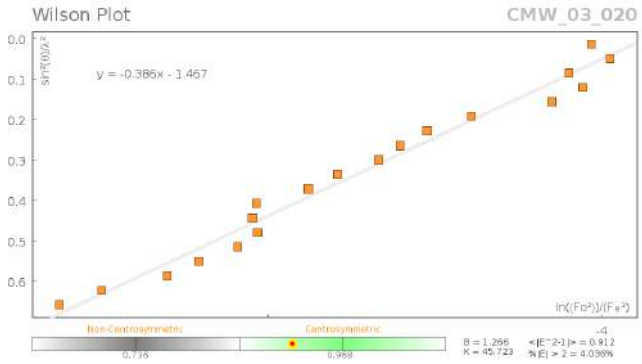
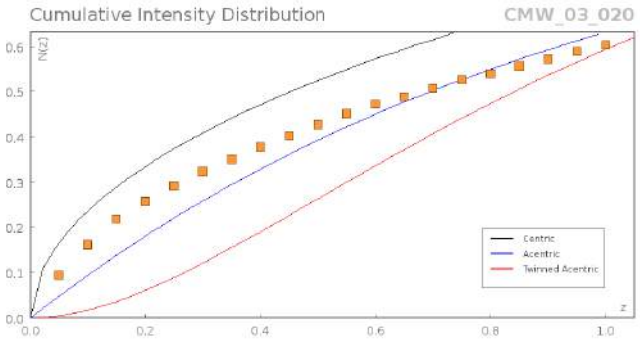
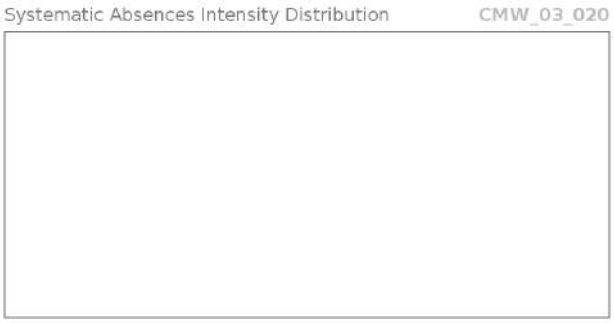


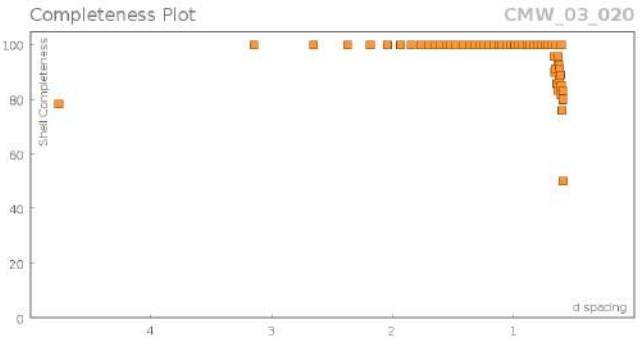
Figure S24: A deformation ED maps in the plane of the atoms Ca(1), O(1) and O(3) as calculated from the refinements with the theoretically predicted multipolar parameters. Red lines represent positive contours and blue lines negative contours. Contours are drawn at 0.1 e $Å^{-3}$ intervals.

Data Plots: Diffraction Data

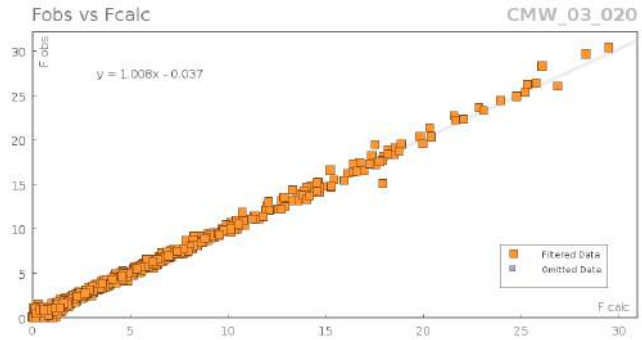


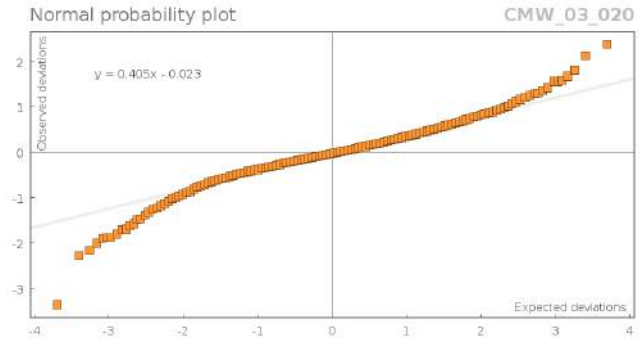






Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	17386	Unique reflections	4461
Completeness	0.972	Mean I/σ	16.87
hklsub>max</sub> collected	(17, 18, 49)	hklsub>min</sub> collected	(-21, -17, -44)
hkl_{max} used	(10, 21, 49)	hkl_{min} used	(-21, 0, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.36
d_{max} used	9.76	d_{min} used	0.59
Friedel pairs	3041	Friedel pairs merged	1
Inconsistent equivalents	0	R_{int}	0.0389
R_{sigma}	0.0407	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	0
Multiplicity	(9146, 3694, 284)	Maximum multiplicity	11
Removed systematic absences	0	Filtered off (Shel/OMIT)	0

Images of the Crystal on the Diffractometer

Table S33: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **CMW_03_020**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
C1	1273.4(18)	871(2)	2922.5(6)	26.6(4)
C2	1895(2)	1909.4(19)	3271.4(5)	27.5(4)
C1B	1073(4)	1229(3)	2982.7(18)	26.6(4)
C2B	2214(4)	1551(7)	3267.3(10)	27.5(4)
C3	3679.8(13)	1840.1(14)	4274.0(5)	25.0(3)
C4	4514.4(17)	2303.0(19)	3853.8(7)	43.0(4)
C5	3189.9(16)	474.9(16)	4344.4(6)	31.1(3)
C6	4349.3(17)	2558.7(19)	4701.6(7)	40.9(4)
N1	0	0	3072.1(6)	22.0(3)
N2	1676.0(11)	1322.6(12)	3735.1(3)	24.2(2)
O1	1561.3(8)	1499.2(9)	4557.4(3)	17.64(16)
O2	2890.9(10)	3381.5(9)	4120.4(3)	25.3(2)
S1	2394.8(3)	2078.0(3)	4168.6(2)	17.47(7)
Ca1	0	0	5000	13.52(10)
Co2	0	0	3787.8(2)	16.00(7)

Table S34: Anisotropic Displacement Parameters (×10⁴) **CMW_03_020**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	28.2(9)	28.3(10)	17.2(6)	1.8(6)	3.4(5)	9.6(7)
C2	26.1(9)	29.6(10)	18.6(6)	3.2(6)	4.9(5)	7.7(7)
C1B	28.2(9)	28.3(10)	17.2(6)	1.8(6)	3.4(5)	9.6(7)
C2B	26.1(9)	29.6(10)	18.6(6)	3.2(6)	4.9(5)	7.7(7)
C3	16.2(6)	23.0(6)	34.8(6)	0.3(5)	5.2(5)	9.0(5)
C4	26.5(8)	40.6(10)	59.8(11)	12.8(8)	24.4(8)	15.3(8)
C5	27.3(7)	27.8(8)	43.7(8)	3.5(6)	8.3(6)	18.0(6)
C6	25.0(8)	42.3(10)	56.2(10)	-15.3(8)	-15.9(7)	17.6(8)
N1	22.9(6)	22.9(6)	20.1(7)	0	0	11.5(3)
N2	19.6(5)	25.1(6)	18.2(4)	-1.1(4)	2.1(3)	4.1(4)
O1	14.9(4)	18.6(4)	18.4(3)	2.7(3)	3.7(3)	7.6(3)
O2	26.9(5)	15.7(4)	29.1(4)	4.6(3)	2.9(4)	7.4(4)
S1	14.96(13)	14.96(14)	19.05(12)	0.88(9)	3.00(9)	4.91(11)
Ca1	12.99(15)	12.99(15)	14.57(19)	0	0	6.50(7)
Co2	15.35(10)	15.35(10)	17.31(12)	0	0	7.67(5)

Table S35: Bond Lengths in Å for **CMW_03_020**.

Atom	Atom	Length/Å
C1	C2	1.531(3)
C1	N1	1.4866(19)
C2	N2	1.5035(19)
C1B	C2B	1.531(3)
C1B	N1	1.483(3)
C2B	N2	1.491(3)

Atom	Atom	Length/Å
C3	C4	1.532(2)
C3	C5	1.523(2)
C3	C6	1.528(2)
C3	S1	1.8145(16)
N1	Co2	2.0949(19)
N2	S1	1.5731(12)

Atom	Atom	Length/Å
N2	Co2	1.9343(13)
O1	S1	1.4712(9)
O1	Ca1	2.3241(10)
O2	S1	1.4428(11)
Ca1	O1[1]	2.3240(10)
Ca1	O1[2]	2.3240(10)
Ca1	O1[3]	2.3240(10)
Ca1	O1[4]	2.3240(10)
Ca1	O1[5]	2.3240(10)
Ca1	Co2	3.5486(10)
Ca1	Co2[2]	3.5486(10)
Co2	N2[1]	1.9343(13)
Co2	N2[3]	1.9343(13)

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[1]+Y-X,-X,+Z; [2]-X,-Y,1-Z; [3]-Y,+X-Y,+Z; [4]-Y+X,+X,1-Z; [5]+Y,-X+Y,1-Z

Table S36: Bond Angles in ° for **CMW_03_020**.

Atom	Atom	Atom	Angle/°
N1	C1	C2	109.66(15)
N2	C2	C1	106.99(15)
N1	C1B	C2B	115.2(4)
N2	C2B	C1B	99.9(3)
C4	C3	S1	107.46(11)
C5	C3	C4	110.62(13)
C5	C3	C6	110.51(14)
C5	C3	S1	108.56(10)
C6	C3	C4	111.20(15)
C6	C3	S1	108.38(11)
C1	N1	Co2	107.14(9)
C1B	N1	Co2	100.2(2)
C2	N2	S1	121.46(11)
C2	N2	Co2	110.41(10)
C2B	N2	S1	123.7(2)
C2B	N2	Co2	115.8(2)
S1	N2	Co2	120.48(6)
S1	O1	Ca1	159.82(6)
N2	S1	C3	109.19(7)
O1	S1	C3	105.14(6)
O1	S1	N2	105.77(6)
O2	S1	C3	106.87(7)
O2	S1	N2	113.62(7)
O2	S1	O1	115.82(6)
O1[1]	Ca1	O1[2]	88.06(3)
O1[3]	Ca1	O1	91.94(3)
O1[3]	Ca1	O1[4]	88.06(3)
O1[5]	Ca1	O1[1]	88.06(3)
O1[1]	Ca1	O1	91.94(3)
O1[4]	Ca1	O1[2]	91.94(3)
O1[2]	Ca1	O1	180.00(3)
O1[5]	Ca1	O1[2]	91.94(3)
O1[4]	Ca1	O1[1]	180.0
O1[3]	Ca1	O1[1]	91.94(3)
O1[3]	Ca1	O1[2]	88.06(3)
O1[5]	Ca1	O1	88.06(3)
O1[5]	Ca1	O1[3]	180.0
O1[5]	Ca1	O1[4]	91.94(3)
O1[4]	Ca1	O1	88.06(3)
O1[5]	Ca1	Co2	123.88(2)
O1[2]	Ca1	Co2	123.88(2)
Co2	Ca1	Co2[2]	180.0
N1	Co2	Ca1	180.0
N2[1]	Co2	N1	85.43(3)
N2	Co2	N1	85.42(3)
N2[3]	Co2	N1	85.43(3)
N2	Co2	N2[3]	119.370(9)
N2	Co2	N2[1]	119.371(9)
N2[3]	Co2	N2[1]	119.371(9)
N2[3]	Co2	Ca1	94.57(3)
N2[1]	Co2	Ca1	94.57(3)
N2	Co2	Ca1	94.58(3)

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[1]-Y,+X-Y,+Z; [2]-X,-Y,1-Z; [3]+Y-X,-X,+Z; [4]+Y,-X+Y,1-Z; [5]-Y+X,+X,1-Z

Table S37: Hydrogen Fractional Atomic Coordinates (×10[4]) and Equivalent Isotropic Displacement Parameters (Å[2]×10[3]) for **CMW_03_020**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H1A	1259	1214	2620	32
H1B	1741	435	2894	32
H2B	2785	2402	3209	33
H2A	1542	2455	3256	33
H1BA	831	1853	3041	32
H1BB	1291	1279	2655	32
H2BA	2551	1009	3196	33
H2BB	2861	2417	3225	33
H4A	4080	1794	3589	65
H4C	5256	2256	3911	65

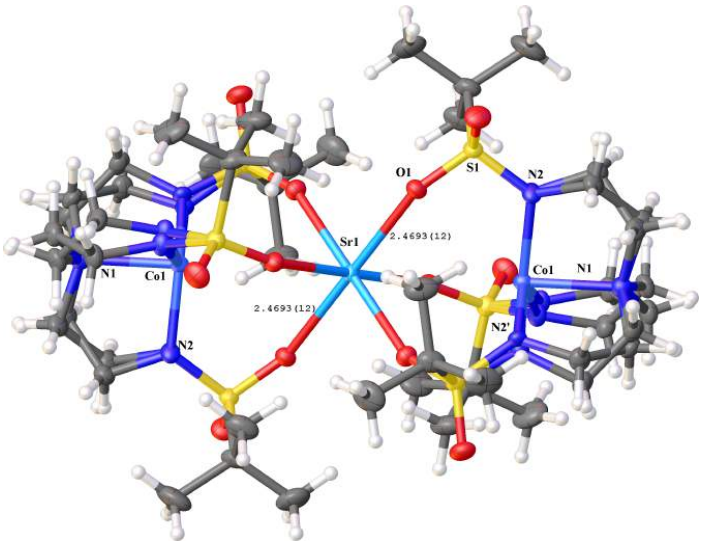
Atom	x	y	z	U_{eq}
H4B	4741	3155	3792	65
H5B	2710(20)	210(20)	4607(8)	47
H5A	2710(20)	20(20)	4099(9)	47
H6B	4601	3425	4660	61
H6A	5075	2480	4753	61
H6C	3801	2232	4966	61
H5C	3920(20)	370(20)	4381(8)	46(6)

CMW-03-050

EMORY UNIVERSITY | X-ray Crystallography Center

Submitted by: **Christian Wallen**
Emory University
Solved by: **John Bacsa**
Sample ID: **CMW-03-050**

Crystal Data and Experimental



Experimental. Single violet prism-shaped crystals of (**CMW-03-050**) were recrystallised from a mixture of CH_2Cl_2, diethyl ether and methanol by vapor diffusion. A suitable crystal (0.36×0.29×0.20 mm) was selected and mounted on a loop with paratone oil on a Bruker APEX-II CCD diffractometer. The crystal was cooled to T = 100(2) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program using combined Patterson and dual-space recycling methods and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The crystal structure was refined with version of **ShelXL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{36}H_{78}Co_2N_8O_{12}S_6Sr$, M_r = 1212.90, trigonal, R-3 (No. 148), a = 12.638(4) Å, b = 12.638(4) Å, c = 29.797(8) Å, α = 90°, β = 90°, γ = 120°, V = 4122(3) Å^3, T = 100(2) K, Z = 3, Z' = 1/6, μ(MoK$_\alpha$) = 1.850, 16290 reflections measured, 2798 unique (R_{int} = 0.0343) which were used in all calculations. The final wR_2 was 0.0937 (all data) and R_1 was 0.0363 (I > 2σ(I)).

Compound	**CMW-03-050**
Formula	$C_{36}H_{78}Co_2N_8O_{12}S_6Sr$
$D_{calc.}$/ g cm^{-3}	1.466
μ/mm^{-1}	1.850
Formula Weight	1212.90
Colour	violet
Shape	prism
Max Size/mm	0.36
Mid Size/mm	0.29
Min Size/mm	0.20
T/K	100(2)
Crystal System	trigonal
Space Group	R-3
a/Å	12.638(4)
b/Å	12.638(4)
c/Å	29.797(8)
α/°	90
β/°	90
γ/°	120
V/Å^3	4122(3)
Z	3
Z'	0.16667
Θ_{min}/°	1.982
Θ_{max}/°	30.513
Measured Refl.	16290
Independent Refl.	2798
$I > 2\sigma(I)$	2518
R_{int}	0.0343
Parameters	118
Restraints	3
Largest Peak	0.933
Deepest Hole	-0.441
GooF	1.066
wR_2 (all data)	0.0937
wR_2	0.0904
R_1 (all data)	0.0413
R_1	0.0363
CCDC #	1434439

Structure Quality Indicators

Reflections:	d min	0.70	I/σ	30.6	Rint	3.43%	complete 100%
Refinement:	Shift	0.000	Max Peak	0.9	Min Peak	-0.4	GooF 1.066

A violet prism-shaped crystal with dimensions 0.36×0.29×0.20 mm was mounted on a loop with paratone oil. X-ray diffraction data were collected using a Bruker APEX-II CCD diffractometer equipped with an Oxford Cryosystems low-temperature apparatus operating at T = 100(2) K.

Data were measured using ω scans using MoK$_\alpha$ radiation (fine-focus sealed tube, 45 kV, 35 mA). The total number of runs and images was based on the strategy calculation from the program **APEX2** (Bruker, 2014). The maximum resolution achieved was Θ = 30.513°.

Unit cell indexing was performed by using the **APEX2** (Bruker, 2014) software and refined using **SAINT** (Bruker, V8.34A, 2013) on 5438 reflections, 33% of the observed reflections. Data reduction, scaling and absorption corrections were performed using **SAINT** (Bruker, V8.34A, 2013) and **SADABS-2014/5** (Bruker, 2014) was used for absorption correction. wR_2(int) was 0.0685 before and 0.0489 after correction. The ratio of minimum to maximum transmission is 0.7793. The $\lambda/2$ correction factor is 0.00150. The software also corrects for Lorentz polarisation. The final completeness is 100.00 out to 30.513 in Θ. The absorption coefficient (μ) of this material is 1.850 and the minimum and maximum transmissions are 0.5814 and 0.7461.

The structure was solved in the space group P1 with the **ShelXT** (Sheldrick, 2015) structure solution program using combined Patterson and dual-space recycling methods. The space group R-3 (# 148) was determined by **ShelXT** (Sheldrick, 2015) structure solution program. The crystal structure was refined by Least Squares using version 2014/7 of **ShelXL** (Sheldrick, 2008). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

The value of Z' is 1/6.

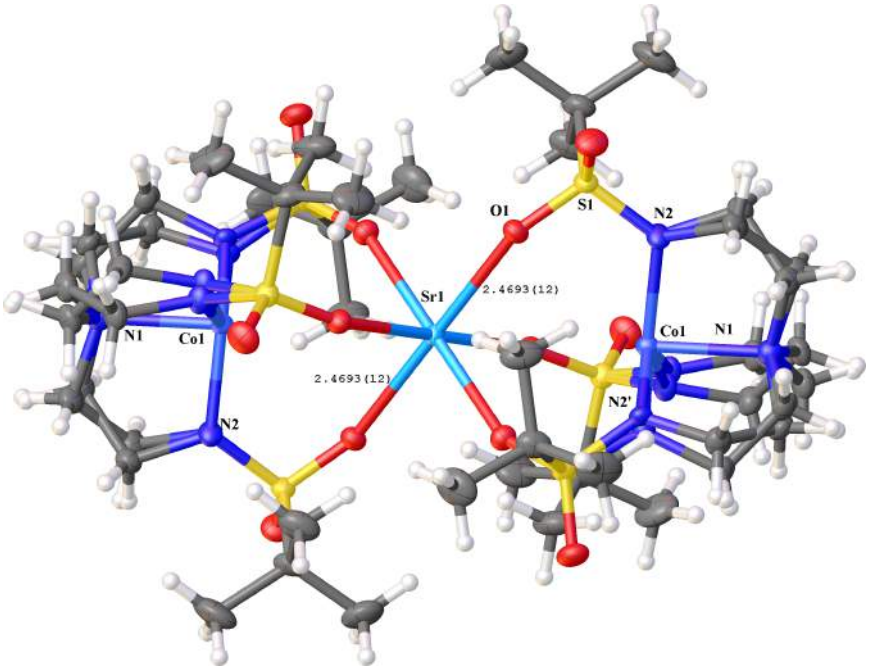


Figure S25:

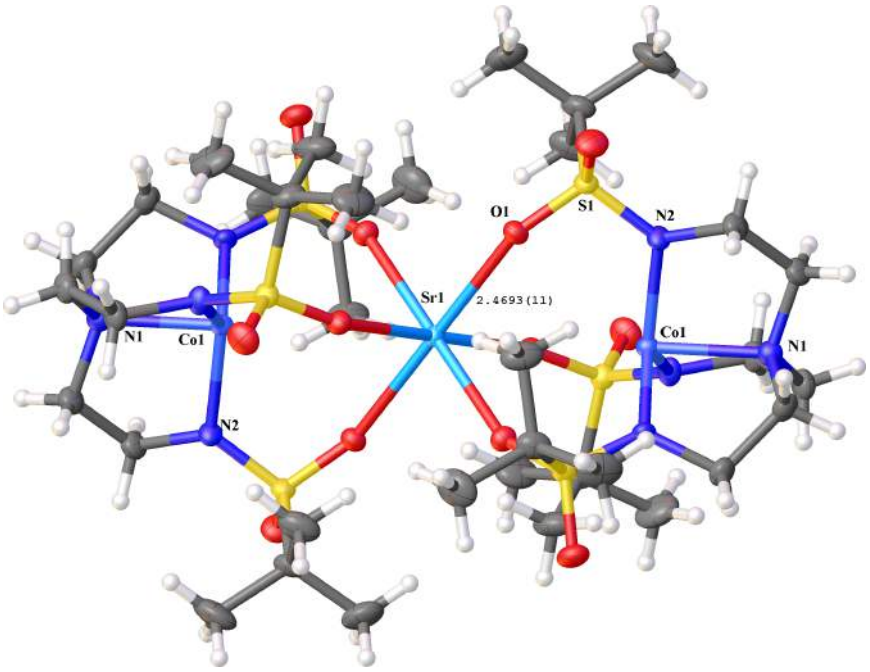
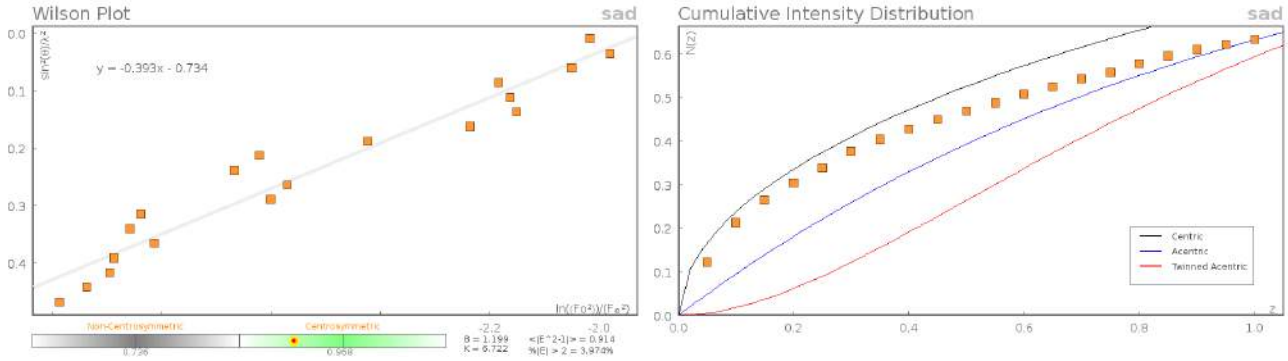
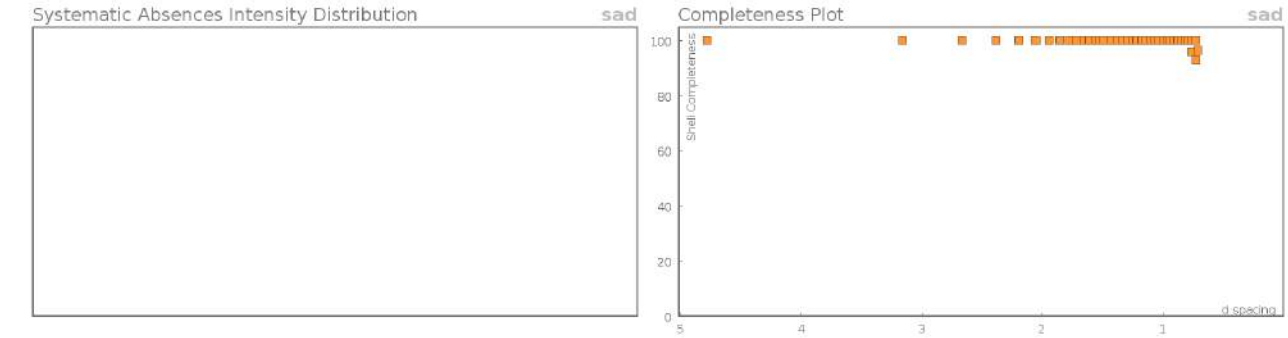


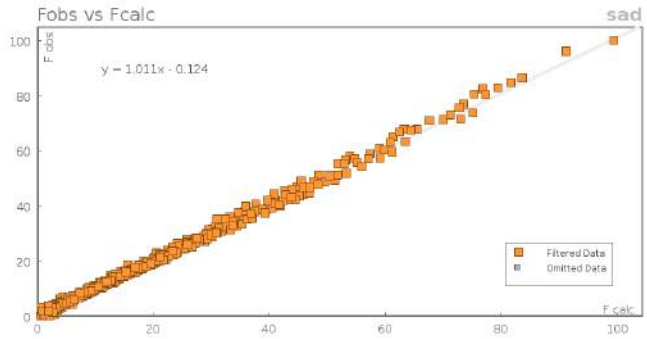
Figure S26:

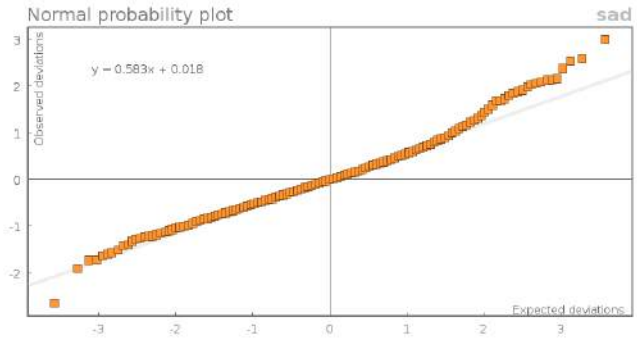
Data Plots: Diffraction Data





Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	16290	Unique reflections	2798
Completeness	0.999	Mean I/σ	30.63
hklsub>max</sub> collected	(17, 17, 42)	hklsub>min</sub> collected	(-18, -18, -42)
hkl_{max} used	(9, 18, 42)	hkl_{min} used	(-18, 0, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.36
d_{max} used	10.27	d_{min} used	0.7
Friedel pairs	5028	Friedel pairs merged	1
Inconsistent equivalents	0	R_{int}	0.0343
R_{sigma}	0.023	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	0
Multiplicity	(9327, 2816, 409, 26)	Maximum multiplicity	14
Removed systematic absences	0	Filtered off (Shel/OMIT)	0

Images of the Crystal on the Diffractometer

Table S38: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **CMW-03-050**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
C1	2932(4)	7540(3)	-403.6(12)	24.2(7)
C2	3377(4)	8594(3)	-68.9(10)	24.2(7)
N2	3053(7)	8057(6)	386.7(9)	18.9(12)
C1'	3440(5)	7857(5)	-368.4(16)	22.1(10)
C2'	2666(5)	8172(5)	-62.4(13)	22.3(12)
N2'	2801(11)	7835(9)	401.6(11)	18.9(12)
C3	1426.8(16)	8441.7(17)	921.2(7)	25.8(4)
C4	979(2)	8815(2)	506.3(9)	44.6(6)
C5	1481(2)	9191(2)	1330.9(9)	41.7(5)
C6	608.0(18)	7073.0(19)	1011.7(9)	35.2(5)
N1	3333	6667	-255.7(8)	19.5(5)
O1	3292.9(11)	8256.3(11)	1197.0(4)	18.8(2)

Atom	x	y	z	U_{eq}
O2	3707.2(13)	10050.4(12)	735.6(5)	27.4(3)
S1	2965.5(4)	8746.4(3)	806.9(2)	17.51(10)
Co1	3333	6667	444.7(2)	14.58(10)
Sr1	3333	6667	1667	14.27(10)

Table S39: Anisotropic Displacement Parameters (×10⁴) **CMW-03-050**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	30.6(18)	24.2(13)	19.7(11)	5.9(9)	2.9(10)	15.2(12)
C2	30.6(18)	24.2(13)	19.7(11)	5.9(9)	2.9(10)	15.2(12)
N2	27(3)	13(2)	17.0(7)	2.3(7)	1.3(8)	10(3)
C1'	27(2)	18(2)	19(2)	6.5(16)	6.6(19)	9.8(19)
C2'	28(3)	25(2)	18.3(19)	2.3(15)	-0.3(16)	17(2)
N2'	27(3)	13(2)	17.0(7)	2.3(7)	1.3(8)	10(3)
C3	21.1(8)	23.0(8)	37.5(10)	-0.3(7)	-5.2(7)	14.1(7)
C4	38.6(12)	37.7(11)	63.4(16)	7.0(11)	-17.4(11)	23.5(10)
C5	34.0(11)	44.9(12)	55.8(14)	-11.7(11)	4.5(10)	26.9(10)
C6	19.1(8)	28.6(9)	54.9(14)	6.8(9)	-3.2(8)	9.6(7)
N1	19.0(6)	19.0(6)	20.6(12)	0	0	9.5(3)
O1	19.1(5)	20.1(5)	19.1(6)	2.0(4)	-1.0(4)	11.1(4)
O2	31.9(7)	17.0(6)	31.9(7)	5.4(5)	5.1(5)	11.3(5)
S1	21.37(19)	15.38(18)	18.43(19)	1.18(13)	-0.20(14)	11.18(15)
Co1	13.93(12)	13.93(12)	15.89(19)	0	0	6.97(6)
Sr1	14.74(12)	14.74(12)	13.33(17)	0	0	7.37(6)

Table S40: Bond Lengths in Å for **CMW-03-050**.

Atom	Atom	Length/Å
C1	C2	1.529(3)
C1	N1	1.493(4)
C2	N2	1.481(3)
N2	S1	1.561(4)
N2	Co1	1.965(6)
C1'	C2'	1.529(4)
C1'	N1	1.480(5)
C2'	N2'	1.481(3)
N2'	S1	1.609(7)
N2'	Co1	1.909(9)
C3	C4	1.529(3)
C3	C5	1.526(3)
C3	C6	1.532(3)
C3	S1	1.8158(19)
N1	C1[1]	1.493(4)
N1	C1[2]	1.493(4)
N1	C1'[1]	1.480(5)
N1	C1'[2]	1.480(5)
N1	Co1	2.087(3)
O1	S1	1.4706(12)
O1	Sr1[3]	2.4697(13)
O1	Sr1	2.4697(13)
O2	S1	1.4474(14)
Co1	N2[2]	1.965(6)
Co1	N2[1]	1.965(6)
Co1	N2'[2]	1.909(9)
Co1	N2'[1]	1.909(9)
Co1	Sr1[3]	3.6411(10)
Co1	Sr1	3.6411(10)
Sr1	O1[4]	2.4697(13)
Sr1	O1[5]	2.4697(13)
Sr1	O1[3]	2.4697(13)
Sr1	O1[2]	2.4697(13)
Sr1	Sr1[3]	0.0000

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[1]+Y-X,1-X,+Z; [2]1-Y,1+X-Y,+Z; [3]2/3-X,4/3-Y,1/3-Z; [4]2/3-Y+X,1/3+X,1/3-Z; [5]-1/3+Y,1/3-X+Y,1/3-Z

Table S41: Bond Angles in ° for **CMW-03-050**.

Atom	Atom	Atom	Angle/°
N1	C1	C2	109.8(3)
N2	C2	C1	107.5(3)
C2	N2	S1	124.0(4)
C2	N2	Co1	111.0(3)
S1	N2	Co1	121.6(2)
N1	C1'	C2'	112.6(3)

Atom	Atom	Atom	Angle/°
N2'	C2'	C1'	107.6(3)
C2'	N2'	S1	119.2(5)
C2'	N2'	Co1	114.9(4)
S1	N2'	Co1	122.3(4)
C4	C3	C6	110.19(17)
C4	C3	S1	107.79(15)
C5	C3	C4	111.34(18)
C5	C3	C6	110.82(19)
C5	C3	S1	107.93(13)
C6	C3	S1	108.65(12)
C1	N1	C1[1]	111.67(15)
C1[2]	N1	C1[1]	111.67(15)
C1	N1	C1[2]	111.67(15)
C1[2]	N1	Co1	107.17(16)
C1	N1	Co1	107.17(16)
C1[1]	N1	Co1	107.17(16)
C1'	N1	C1'[1]	115.01(16)
C1'	N1	C1'[2]	115.01(16)
C1'[2]	N1	C1'[1]	115.01(16)
C1'[2]	N1	Co1	103.1(2)
C1'[1]	N1	Co1	103.1(2)
C1'	N1	Co1	103.1(2)
S1	O1	Sr1[3]	156.23(7)
S1	O1	Sr1	156.23(7)
Sr1[3]	O1	Sr1	0.0
N2	S1	C3	113.6(3)
N2'	S1	C3	104.3(4)
O1	S1	N2	106.6(2)
O1	S1	N2'	104.8(2)
O1	S1	C3	105.04(8)
O2	S1	N2	109.4(2)
O2	S1	N2'	118.9(3)
O2	S1	C3	106.51(8)
O2	S1	O1	115.93(8)
N2	Co1	N2[2]	119.23(2)
N2	Co1	N2[1]	119.24(2)
N2[2]	Co1	N2[1]	119.24(2)
N2	Co1	N1	84.96(8)
N2[2]	Co1	N1	84.96(8)
N2[1]	Co1	N1	84.96(8)

Atom	Atom	Atom	Angle/°
N2	Co1	Sr1[3]	95.04(8)
N2[1]	Co1	Sr1[3]	95.04(8)
N2[2]	Co1	Sr1[3]	95.04(8)
N2[1]	Co1	Sr1	95.04(8)
N2	Co1	Sr1	95.04(8)
N2[2]	Co1	Sr1	95.04(8)
N2'[2]	Co1	N2'[1]	119.55(2)
N2'	Co1	N2'[2]	119.55(2)
N2'	Co1	N2'[1]	119.55(2)
N2'[2]	Co1	N1	86.14(10)
N2'	Co1	N1	86.14(10)
N2'[1]	Co1	N1	86.14(10)
N2'[1]	Co1	Sr1[3]	93.86(10)
N2'[1]	Co1	Sr1	93.86(10)
N2'[2]	Co1	Sr1	93.86(10)
N2'[2]	Co1	Sr1[3]	93.86(10)
N2'	Co1	Sr1	93.86(10)
N2'	Co1	Sr1[3]	93.86(10)
N1	Co1	Sr1	180.0
N1	Co1	Sr1[3]	180.0
Sr1[3]	Co1	Sr1	0.0
O1[4]	Sr1	O1[5]	91.05(4)
O1[4]	Sr1	O1[3]	91.05(4)
O1[5]	Sr1	O1[2]	180.00(6)
O1	Sr1	O1[2]	91.05(4)
O1[5]	Sr1	O1	88.95(4)
O1[4]	Sr1	O1[2]	88.95(4)
O1[5]	Sr1	O1[3]	91.05(4)
O1[4]	Sr1	O1	88.95(4)
O1	Sr1	O1[3]	180.0
O1[3]	Sr1	O1[2]	88.95(4)
Sr1[3]	Sr1	O1[2]	0(10)
Sr1[3]	Sr1	O1	0(10)
Sr1[3]	Sr1	O1[3]	0(10)
Sr1[3]	Sr1	O1[4]	0(10)
Sr1[3]	Sr1	O1[5]	0(10)

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[1]+Y-X,1-X,+Z; [2]1-Y,1+X-Y,+Z; [3]2/3-X,4/3-Y,1/3-Z; [4]2/3-Y+X,1/3+X,1/3-Z; [5]-1/3+Y,1/3-X+Y,1/3-Z

Table S42: Hydrogen Fractional Atomic Coordinates (×10[4]) and Equivalent Isotropic Displacement Parameters (Å[2]×10[3]) for **CMW-03-050**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H1A	2048	7120	-423	29
H1B	3263	7857	-699	29
H2A	4255	9123	-94	29
H2B	2989	9075	-129	29
H1'A	3187	7836	-677	27
H1'B	4290	8493	-344	27
H2'B	2944	9038	-80	27
H2'A	1816	7721	-154	27
H4A	200	8743	569	67
H4C	897	8289	260	67
H4B	1557	9645	429	67
H5A	2035	10041	1274	63

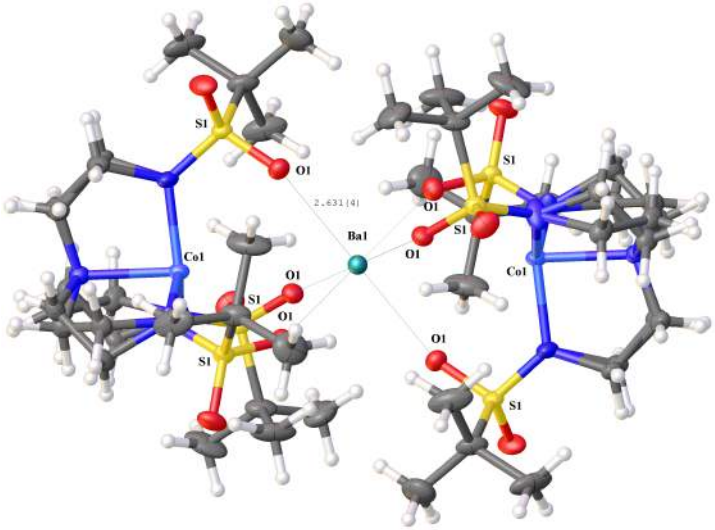
Atom	x	y	z	U_{eq}
H5C	1759	8934	1586	63
H5B	681	9070	1391	63
H6A	-223	6888	1046	53
H6B	871	6858	1282	53
H6C	663	6616	764	53

CoBaCoBus

EMORY UNIVERSITY | X-ray Crystallography Center

Submitted by: **Christian Wallen**
Emory University
Solved by: **John Bacsa**
Sample ID: **[Co2Ba] cluster**

Crystal Data and Experimental



Experimental. Single violet prism-shaped crystals of (**CoBaCoBus**) were recrystallised from a mixture of CH_2Cl_2 and methanol by vapor diffusion. A suitable crystal (0.38×0.30×0.30) was selected and mounted on a loop with paratone oil on a Bruker APEX-II CCD diffractometer. The crystal was cooled to T = 100(2) K during data collection. The structure was solved with the **Superflip** (L. Palatinus & G. Chapuis, 2007) structure solution program using a charge flipping algorithm and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The crystal structure was refined with version 2013-4 of **SHELXL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{36}H_{78}BaCo_2N_8O_{12}S_6$, M_r = 1262.62, trigonal, R-3 (No. 148), a = 12.6571(8) Å, b = 12.6571(8) Å, c = 30.388(2) Å, α = 90°, β = 90°, γ = 120°, V = 4216.0(6) Å^3, T = 100(2) K, Z = 3, Z' = 1/6, μ(MoK$_\alpha$) = 1.556, 36251 reflections measured, 5154 unique (R_{int} = 0.0276) which were used in all calculations. The final wR_2 was 0.1500 (all data) and R_1 was 0.0627 (I > 2(I)).

Compound	**CoBaCoBus**
Formula	$C_{36}H_{78}BaCo_2N_8O_{12}S_6$
$D_{calc.}$/ g cm^{-3}	1.492
μ/mm^{-1}	1.556
Formula Weight	1262.62
Colour	violet
Shape	prism
Max Size/mm	0.38
Mid Size/mm	0.30
Min Size/mm	0.30
T/K	100(2)
Crystal System	trigonal
Space Group	R-3
a/Å	12.6571(8)
b/Å	12.6571(8)
c/Å	30.388(2)
α/°	90
β/°	90
γ/°	120
V/Å^3	4216.0(6)
Z	3
Z'	1/6
Θ_{min}/°	2.011
Θ_{max}/°	38.564
Measured Refl.	36251
Independent Refl.	5154
$I > 2\sigma(I)$	4927
R_{int}	0.0276
Parameters	120
Restraints	0
Largest Peak	1.686
Deepest Hole	-1.346
GooF	1.357
wR_2 (all data)	0.1500
wR_2	0.1493
R_1 (all data)	0.0645
R_1	0.0627
CCDC #	1434435

Structure Quality Indicators

Reflections:	d min 0.57	I/σ 43.9	Rint 2.76%	complete 97%
Refinement:	Shift -0.002	Max Peak 1.7	Min Peak -1.4	GooF 1.357

A violet prism-shaped crystal with dimensions 0.38×0.30×0.30 mm was mounted on a loop with paratone oil. X-ray diffraction data were collected using a Bruker APEX-II CCD diffractometer equipped with an Oxford Cryosystems low-temperature apparatus operating at T = 100(2) K.

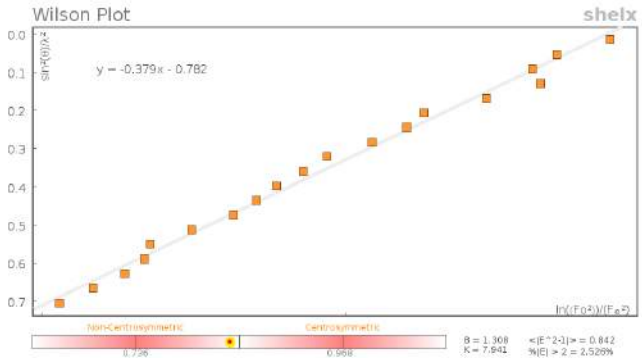
Data were measured using ω scans with MoK$_\alpha$ radiation (fine-focus sealed tube, 45 kV, 35 mA). The total number of runs and images was based on the strategy calculation from the program **APEX2** (Bruker). The maximum resolution achieved was Θ = 38.5°.

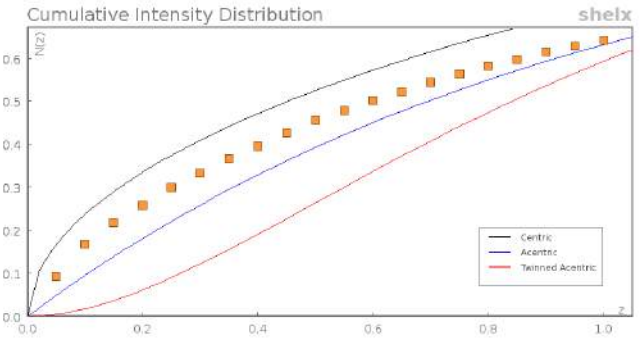
Unit cell indexing was performed by using the **APEX2** (Bruker) software and refined using **SAINT** (Bruker, V8.34A, 2013) on 9797 reflections, 27% of the observed reflections. Data reduction, scaling and absorption corrections were performed using **SAINT** (Bruker, V8.34A, 2013) and **SADABS-2014/2** (Bruker, 2014) was used for absorption correction.wR_2(int) was 0.0693 before and 0.0471 after correction.The Ratio of minimum to maximum transmission is 0.8416.The $\lambda/2$ correction factor is 0.00150. software which corrects for Lorentz polarisation. The final completeness is 98.5% out to 38.564 in Θ. The absorption coefficient (μ) of this material is 1.556 and the minimum and maximum transmissions are 0.6292 and 0.7476.

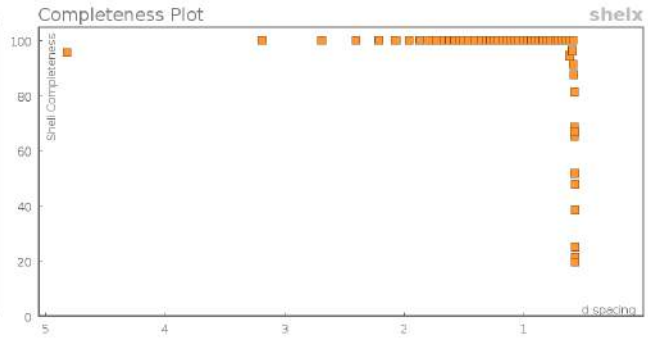
The structure was solved in the space group P1 with the **Superflip** (L. Palatinus & G. Chapuis, 2007) structure solution program using charge flipping methods. The space group R-3 (# 148) was determined by **Superflip** (L. Palatinus & G. Chapuis, 2007) structure solution program. The crystal structure was refined by Least Squares using version 2013-4 of **CoBaCoBusL** (Sheldrick, 2008). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

The value of Z' is 1/6.

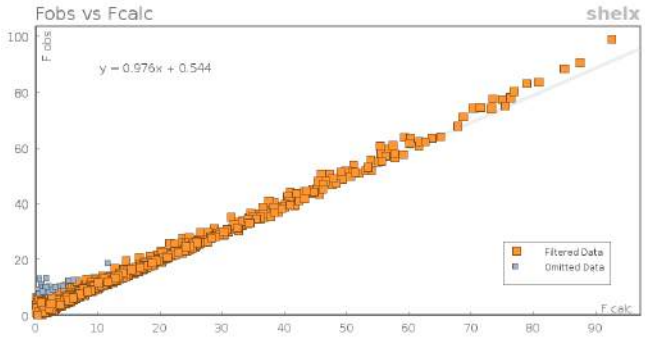
Data Plots: Diffraction Data

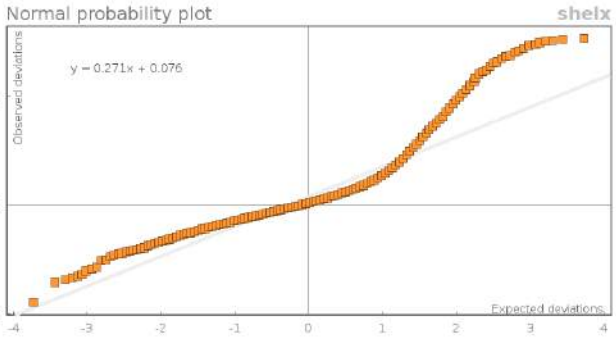






Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	36588	Unique reflections	5154
Completeness	0.97	Mean I/σ	43.9
hklsub>max</sub> collected	(21, 19, 51)	hklsub>min</sub> collected	(-20, -21, -52)
hkl_{max} used	(11, 22, 52)	hkl_{min} used	(-21, 0, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.36
d_{max} used	10.13	d_{min} used	0.57
Friedel pairs	8101	Friedel pairs merged	1
Inconsistent equivalents	0	R_{int}	0.0276
R_{sigma}	0.0187	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	337
Multiplicity	(10906, 5268, 4107, 540, 133)	Maximum multiplicity	22
Removed systematic absences	0	Filtered off (Shel/OMIT)	0

Images of the Crystal on the Diffractometer

Table S43: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **CoBaCoBus**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Ba1	10000	10000	5000	18.19(9)
Co1	10000	10000	6233.7(2)	15.98(12)
S1	7513.0(6)	7895.8(6)	5891.0(2)	18.66(13)
O2	6905(2)	6604(2)	5983.4(10)	29.8(5)
O1	8309(2)	8310(2)	5502.9(8)	22.1(4)
C6	5594(4)	7452(5)	5380.3(19)	46.1(11)
C4	6900(4)	9602(4)	5659(2)	49.7(14)
C5	5499(4)	7933(4)	6172(2)	51.0(14)
N1	10000	10000	6920.4(15)	19.0(7)
N2	8311(3)	8710(3)	6284.5(10)	30.7(6)
C3	6315(3)	8246(3)	5766.7(15)	30.2(7)
C1	10900(8)	9638(8)	7071(3)	24.2(14)
C2B	11458(6)	9288(6)	6729(2)	22(1)
C1B	11174(8)	10085(8)	7032(3)	22.1(12)
C2	11951(6)	10094(7)	6744(2)	26.2(12)

Table S44: Anisotropic Displacement Parameters (×10⁴) **CoBaCoBus**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ba1	18.25(11)	18.25(11)	18.07(16)	0	0	9.12(6)
Co1	13.00(15)	13.00(15)	21.9(3)	0	0	6.50(8)
S1	14.6(3)	15.2(3)	22.2(3)	0.2(2)	0.8(2)	4.5(2)
O2	25.6(11)	16.2(9)	40.0(14)	6.4(9)	-3.9(10)	4.7(8)
O1	19.5(9)	25.2(10)	22.3(9)	2.3(8)	3.1(7)	11.7(8)
C6	26.8(17)	52(3)	59(3)	0(2)	-13.3(18)	18.9(18)
C4	26.8(17)	28.0(17)	101(4)	15(2)	14(2)	18.8(15)
C5	25.2(17)	33(2)	86(4)	-3(2)	27(2)	8.6(15)
N1	17.2(10)	17.2(10)	22.6(18)	0	0	8.6(5)
N2	17.3(11)	31.7(14)	23.3(12)	-3.6(10)	3.6(9)	-2.7(10)
C3	15.5(11)	22.4(13)	52(2)	2.4(13)	4.8(12)	9(1)
C1	25(4)	29(4)	23(3)	-5(3)	-5(3)	16(3)
C2B	23(2)	26(3)	23(2)	2(2)	-1.2(19)	16(2)
C1B	20(3)	25(3)	23(3)	-3(3)	-4(2)	13(3)
C2	21(2)	34(3)	28(3)	-6(2)	-5(2)	17(2)

Table S45: Bond Lengths in Å for **CoBaCoBus**.

Atom	Atom	Length/Å
Ba1	Co1	3.7490(7)
Ba1	Co1[1]	3.7489(7)
Ba1	O1	2.629(2)
Ba1	O1[1]	2.629(2)
Ba1	O1[2]	2.629(2)
Ba1	O1[3]	2.629(2)
Ba1	O1[4]	2.629(2)
Ba1	O1[5]	2.629(2)
Co1	N1	2.087(5)
Co1	N2[5]	1.942(3)
Co1	N2[3]	1.942(3)
Co1	N2	1.942(3)
S1	O2	1.444(2)
S1	O1	1.467(2)
S1	N2	1.572(3)
S1	C3	1.820(4)
C6	C3	1.518(7)
C4	C3	1.527(5)
C5	C3	1.526(6)
N1	C1[5]	1.497(9)
N1	C1	1.497(9)
N1	C1[3]	1.497(9)
N1	C1B[5]	1.474(8)
N1	C1B[3]	1.474(8)
N1	C1B	1.474(8)
N2	C2B[3]	1.453(7)
N2	C2[3]	1.587(7)
C1	C2	1.524(12)
C2B	N2[5]	1.453(7)
C2B	C1B	1.535(11)
C2	N2[5]	1.587(7)

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[1]2-X,2-Y,1-Z; [2]1-Y+X,+X,1-Z; [3]1+Y-X,2-X,+Z; [4]+Y,1-X+Y,1-Z; [5]2-Y,1+X-Y,+Z

Table S46: Bond Angles in ° for **CoBaCoBus**.

Atom	Atom	Atom	Angle/°
Co1[1]	Ba1	Co1	180.0
O1[2]	Ba1	Co1[1]	125.54(5)
O1[3]	Ba1	Co1[1]	125.54(5)
O1	Ba1	Co1[1]	125.54(5)
O1[1]	Ba1	Co1[1]	54.46(5)
O1[4]	Ba1	Co1	125.54(5)
O1[3]	Ba1	Co1	54.46(5)
O1[5]	Ba1	Co1	125.54(5)
O1[2]	Ba1	Co1	54.46(5)
O1[5]	Ba1	Co1[1]	54.46(5)
O1	Ba1	Co1	54.46(5)
O1[1]	Ba1	Co1	125.54(5)
O1[4]	Ba1	Co1[1]	54.46(5)
O1[4]	Ba1	O1[2]	180.00(8)
O1[3]	Ba1	O1[2]	89.61(8)
O1	Ba1	O1[5]	90.39(8)
O1[5]	Ba1	O1[2]	90.39(8)
O1	Ba1	O1[1]	180.00(10)
O1[5]	Ba1	O1[1]	89.61(8)
O1[5]	Ba1	O1[3]	180.0
O1[2]	Ba1	O1[1]	90.39(8)
O1	Ba1	O1[4]	90.39(8)
O1[3]	Ba1	O1[1]	90.39(8)
O1[5]	Ba1	O1[4]	89.61(8)
O1	Ba1	O1[3]	89.61(8)
O1	Ba1	O1[2]	89.61(8)
O1[4]	Ba1	O1[1]	89.61(8)
O1[3]	Ba1	O1[4]	90.39(8)
N1	Co1	Ba1	180.0
N2[2]	Co1	Ba1	94.56(9)
N2	Co1	Ba1	94.56(9)
N2[3]	Co1	Ba1	94.56(9)
N2[3]	Co1	N1	85.44(9)
N2	Co1	N1	85.44(9)
N2[2]	Co1	N1	85.44(9)
N2[3]	Co1	N2	119.38(3)
N2[2]	Co1	N2	119.38(3)
N2[2]	Co1	N2[3]	119.38(3)

Atom	Atom	Atom	Angle/°
O2	S1	O1	116.25(16)
O2	S1	N2	113.48(18)
O2	S1	C3	106.20(16)
O1	S1	N2	106.01(15)
O1	S1	C3	104.70(17)
N2	S1	C3	109.8(2)
S1	O1	Ba1	153.12(15)
C1	N1	Co1	107.8(4)
C1[2]	N1	Co1	107.8(4)
C1[3]	N1	Co1	107.8(4)
C1	N1	C1[3]	111.1(4)
C1	N1	C1[2]	111.1(4)
C1[2]	N1	C1[3]	111.1(4)
C1B	N1	Co1	103.3(4)
C1B[2]	N1	Co1	103.3(4)
C1B[3]	N1	Co1	103.3(4)
C1B[2]	N1	C1B[3]	114.9(3)
C1B	N1	C1B[3]	114.9(3)
C1B	N1	C1B[2]	114.9(3)
S1	N2	Co1	124.55(17)
S1	N2	C2[2]	116.8(3)
C2B[2]	N2	Co1	113.6(3)
C2B[2]	N2	S1	121.8(3)
C2[2]	N2	Co1	108.3(3)
C6	C3	S1	107.3(3)
C6	C3	C4	111.8(4)
C6	C3	C5	110.4(4)
C4	C3	S1	108.9(2)
C5	C3	S1	107.9(3)
C5	C3	C4	110.5(4)
N1	C1	C2	109.8(6)
N2[3]	C2B	C1B	105.3(5)
N1	C1B	C2B	111.9(6)
C1	C2	N2[3]	103.7(5)

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[1]2-X,2-Y,1-Z; [2]1+Y-X,2-X,+Z; [3]2-Y,1+X-Y,+Z; [4]1-Y+X,+X,1-Z; [5]+Y,1-X+Y,1-Z

Table S47: Hydrogen Fractional Atomic Coordinates (×10[4]) and Equivalent Isotropic Displacement Parameters (Å[2]×10[3]) for **CoBaCoBus**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H6A	6121	7681	5120	69
H6B	4899	7567	5320	69
H6C	5298	6593	5452	69
H4A	7404	10084	5908	75
H4B	6260	9807	5604	75
H4C	7411	9786	5396	75
H5A	5192	7079	6253	76
H5B	4811	8056	6106	76
H5C	5972	8462	6417	76

Atom	x	y	z	U_{eq}
H1A	10494	8738	7095	29
H1B	11218	9991	7365	29
H2BA	12306	9467	6773	26
H2BB	10895	8412	6789	26
H1BA	11148	9826	7341	27
H1BB	11835	10945	7007	27
H2A	12491	9759	6813	31
H2B	12439	10996	6745	31

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