SUPPORTING INFORMATION

“New Cyanometalate Building Units:
Synthesis and Characterization of $[\text{Re}(\text{CN})_7]^{3-}$ and $[\text{Re}(\text{CN})_8]^{3-}$ ”

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Figure S1. The X-band EPR spectrum of an undiluted powder of $(\text{Bu}_4\text{N})_3[\text{Re}(\text{CN})_7]$ (**1**) at 20 K. Units along the vertical axis are arbitrary.

Figure S2. A portion of the crystal structure of $[fac\text{-Mn}(\text{H}_2\text{O})_3][cis\text{-Mn}(\text{H}_2\text{O})_2][\text{Re}(\text{CN})_7]\cdot 3\text{H}_2\text{O}$ (**2**). Large black and cross-hatched spheres represent Re and Mn atoms respectively, while smaller highlighted, white, and diagonally shaded spheres represent C, N, and O atoms, respectively. All atoms lie on general positions in the crystal.

Table S1. Crystal data and structure refinement for **1**.

Identification code	mvb54f
Empirical formula	C ₅₅ H ₁₀₈ N ₁₀ Re
Formula weight	1095.71
Temperature	152 K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	P21/c
Unit cell dimensions	$a = 22.9918(3)$ Å $\alpha = 90^\circ$ $b = 23.0860(3)$ Å $\beta = 90.7550(10)^\circ$ $c = 23.0773(5)$ Å $\gamma = 90^\circ$
Volume, Z	12248.1(3) Å ³ , 8
Density (calculated)	1.188 Mg/m ³
Absorption coefficient	2.025 mm ⁻¹
F(000)	4664
Crystal size	0.21 x 0.18 x 0.11 mm
Crystal color and habit	yellow rectangular block
θ range for data collection	1.76 to 24.10°
Limiting indices	$-25 \leq h \leq 26$, $-23 \leq k \leq 26$, $-26 \leq l \leq 16$
Reflections collected	53436
Independent reflections	19272 ($R_{\text{int}} = 0.0850$)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14922 / 0 / 741
Goodness-of-fit on F^2	1.249
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0541$, $wR2 = 0.1250$
R indices (all data)	$R1 = 0.1165$, $wR2 = 0.1489$
Largest diff. peak and hole	2.201 and -1.502 eÅ ⁻³

Table S2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for **1**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Re(1)	5166(1)	7580(1)	2092(1)	24(1)
C(1)	5704(4)	8101(4)	1582(4)	26(2)
N(1)	6012(4)	8361(4)	1280(4)	41(2)
C(2)	4627(4)	7064(4)	2581(4)	30(2)
N(2)	4343(4)	6748(4)	2871(4)	42(2)
C(3)	5834(5)	7179(4)	2576(4)	34(3)
N(3)	6186(3)	6931(4)	2850(4)	45(2)
C(4)	5512(4)	6909(5)	1601(4)	32(3)
N(4)	5716(4)	6532(4)	1326(3)	44(2)
C(5)	4596(4)	7451(4)	1385(4)	31(2)
N(5)	4281(4)	7362(3)	1000(4)	42(2)
C(6)	4513(4)	8201(4)	2126(4)	31(2)
N(6)	4142(4)	8532(4)	2153(4)	49(2)
C(7)	5372(4)	8147(4)	2772(4)	31(2)
N(7)	5488(3)	8471(4)	3143(4)	42(2)
Re(2)	2(1)	7408(1)	7223(1)	32(1)
C(8)	-546(4)	7958(4)	6744(5)	38(3)
N(8)	-867(4)	8247(4)	6471(4)	47(2)
C(9)	557(4)	6842(5)	7676(5)	43(3)
N(9)	872(4)	6523(4)	7927(4)	65(3)
C(10)	-408(4)	6764(4)	6738(4)	34(3)
N(10)	-667(4)	6413(4)	6468(4)	45(2)
C(11)	-644(4)	7040(5)	7743(4)	38(3)
N(11)	-972(4)	6806(4)	8052(4)	49(2)
C(12)	-119(4)	7949(4)	7924(5)	38(3)
N(12)	-213(4)	8252(4)	8305(4)	52(3)
C(13)	645(4)	8039(5)	7210(5)	43(3)
N(13)	1000(4)	8408(4)	7211(5)	71(3)
C(14)	540(4)	7259(4)	6498(5)	37(3)
N(14)	831(4)	7169(4)	6103(4)	54(3)
N(15)	5239(3)	5110(3)	2386(3)	31(2)
N(16)	2576(3)	7453(3)	1854(3)	30(2)
N(17)	2431(3)	2666(3)	3041(4)	42(2)

N(18)	5275(3)	7500(3)	4598(3)	31(2)
N(19)	-215(4)	7778(4)	4824(3)	48(2)
N(20)	117(3)	9951(3)	7697(3)	36(2)
C(15)	5444(4)	4625(4)	1995(4)	31(2)
C(16)	5885(4)	4794(4)	1548(4)	41(3)
C(17)	6071(5)	4264(4)	1202(5)	53(3)
C(18)	6515(5)	4384(5)	738(5)	65(4)
C(19)	4929(4)	5567(4)	2033(4)	39(3)
C(20)	4381(4)	5397(4)	1734(4)	49(3)
C(21)	4163(5)	5902(5)	1362(5)	66(4)
C(22)	3621(5)	5750(6)	1013(6)	89(4)
C(23)	5735(4)	5414(4)	2697(4)	45(3)
C(24)	6133(5)	5006(5)	3045(5)	56(3)
C(25)	6636(5)	5333(5)	3342(5)	75(4)
C(26)	6449(6)	5658(6)	3819(6)	100(5)
C(27)	4820(4)	4830(4)	2822(4)	30(2)
C(28)	4579(4)	5223(4)	3278(4)	37(3)
C(29)	4077(4)	4924(4)	3580(4)	39(3)
C(30)	3870(4)	5269(4)	4098(4)	52(3)
C(31)	2104(4)	7205(4)	1454(4)	37(3)
C(32)	2328(4)	6814(4)	986(4)	43(3)
C(33)	1832(4)	6590(4)	597(4)	49(3)
C(34)	2058(5)	6223(5)	106(4)	61(3)
C(35)	2920(4)	6991(4)	2164(4)	34(2)
C(36)	2561(4)	6596(4)	2559(4)	42(3)
C(37)	2916(4)	6079(4)	2753(4)	44(3)
C(38)	2569(5)	5707(5)	3178(5)	60(3)
C(39)	2273(4)	7854(4)	2278(4)	32(2)
C(40)	2659(4)	8096(4)	2747(4)	45(3)
C(41)	2368(5)	8604(5)	3073(5)	58(3)
C(42)	2341(5)	9152(5)	2711(5)	79(4)
C(43)	3025(4)	7797(4)	1502(4)	36(3)
C(44)	2771(4)	8269(4)	1124(4)	47(3)
C(45)	3242(5)	8555(5)	777(5)	62(3)
C(46)	3008(5)	9019(5)	350(5)	72(4)
C(47)	2092(4)	3086(5)	3426(4)	50(3)
C(48)	2457(5)	3515(5)	3769(5)	60(3)
C(49)	2101(5)	3843(5)	4182(5)	69(4)
C(50)	2453(5)	4294(5)	4515(5)	77(4)
C(51)	2827(4)	2987(4)	2629(4)	44(3)
C(52)	2518(4)	3368(4)	2181(4)	51(3)

C(53)	2964(5)	3741(5)	1854(5)	56(3)
C(54)	3232(5)	4214(5)	2238(5)	67(4)
C(55)	2820(4)	2271(4)	3399(4)	45(3)
C(56)	2501(5)	1941(5)	3861(5)	65(3)
C(57)	2863(7)	1443(7)	4096(7)	111(6)
C(58)	2884(7)	953(7)	3653(6)	119(6)
C(59)	1974(4)	2317(4)	2700(4)	49(3)
C(60)	2209(5)	1841(5)	2322(5)	55(3)
C(61)	1695(5)	1574(5)	1979(5)	65(4)
C(62)	1860(6)	1049(6)	1648(6)	94(5)
C(63)	4758(4)	7557(4)	4176(4)	36(2)
C(64)	4200(4)	7731(4)	4464(4)	46(3)
C(65)	3671(4)	7642(4)	4046(5)	50(3)
C(66)	3479(5)	7015(5)	4026(5)	84(4)
C(67)	5193(4)	6978(4)	4984(4)	32(2)
C(68)	5140(4)	6407(4)	4668(4)	40(3)
C(69)	5234(4)	5887(4)	5089(4)	41(3)
C(70)	4753(4)	5862(4)	5558(4)	44(3)
C(71)	5822(4)	7434(4)	4222(4)	39(3)
C(72)	6378(4)	7258(5)	4559(4)	49(3)
C(73)	6903(5)	7327(5)	4166(5)	56(3)
C(74)	7459(5)	7088(5)	4463(5)	70(4)
C(75)	5335(4)	8020(4)	4989(4)	39(3)
C(76)	5410(5)	8596(5)	4677(5)	51(3)
C(77B)	5296(10)	9085(10)	5074(10)	64(7)
C(77)	6007(15)	8831(16)	4804(14)	119(12)
C(78)	6149(16)	9310(17)	4530(16)	137(13)
C(78B)	5409(11)	9653(11)	4798(11)	77(8)
C(79)	16(4)	8195(4)	5292(4)	44(3)
C(80)	257(5)	8758(4)	5100(4)	48(3)
C(81)	315(5)	9182(4)	5630(4)	50(3)
C(82)	641(4)	9723(4)	5486(4)	51(3)
C(83)	242(5)	7725(5)	4354(5)	54(3)
C(84)	801(5)	7440(5)	4535(5)	61(3)
C(85)	1265(5)	7533(5)	4062(5)	72(4)
C(86)	1844(6)	7278(6)	4210(6)	86(4)
C(87)	-745(5)	8016(6)	4524(5)	72(4)
C(88)	-1282(6)	8048(6)	4938(6)	86(4)
C(89)	-1751(7)	8421(7)	4601(7)	115(6)
C(90)	-1679(8)	9022(8)	4681(7)	148(7)
C(91)	-329(5)	7214(5)	5115(5)	69(4)

C(92)	-613(6)	6740(6)	4729(6)	94(5)
C(93)	-446(7)	6112(7)	5039(7)	117(6)
C(94)	-693(10)	5702(10)	4721(10)	235(12)
C(95)	-222(4)	10403(4)	8038(4)	41(3)
C(96)	-799(5)	10198(5)	8283(5)	58(3)
C(97)	-1032(5)	10677(5)	8673(5)	66(4)
C(98)	-1607(5)	10502(5)	8943(5)	84(4)
C(99)	-265(4)	9638(4)	7265(4)	45(3)
C(100)	-552(4)	10031(4)	6800(4)	47(3)
C(101)	-1095(5)	9757(5)	6551(5)	55(3)
C(102)	-1369(5)	10147(5)	6086(5)	71(4)
C(103)	607(4)	10268(4)	7404(4)	39(3)
C(104)	1047(4)	9888(4)	7109(4)	43(3)
C(105)	1553(5)	10238(5)	6899(5)	57(3)
C(106)	1988(4)	9865(4)	6570(4)	54(3)
C(107)	356(4)	9502(4)	8102(4)	41(3)
C(108)	775(5)	9707(5)	8576(5)	57(3)
C(109)	1002(5)	9186(5)	8936(5)	65(4)
C(110)	1391(5)	9370(6)	9442(5)	87(4)

Table S3. Bond lengths [Å] and angles [°] for **1**.

Re(1)-C(2)	2.064(10)	N(17)-C(55)	1.517(12)	C(41)-C(42)	1.518(14)
Re(1)-C(6)	2.079(10)	N(17)-C(51)	1.518(12)	C(43)-C(44)	1.507(12)
Re(1)-C(4)	2.083(11)	N(17)-C(59)	1.532(12)	C(44)-C(45)	1.510(13)
Re(1)-C(7)	2.092(11)	N(17)-C(47)	1.535(12)	C(45)-C(46)	1.546(14)
Re(1)-C(1)	2.099(10)	N(18)-C(75)	1.507(11)	C(47)-C(48)	1.514(13)
Re(1)-C(5)	2.101(10)	N(18)-C(67)	1.511(10)	C(48)-C(49)	1.476(14)
Re(1)-C(3)	2.103(11)	N(18)-C(63)	1.532(11)	C(49)-C(50)	1.522(14)
C(1)-N(1)	1.165(11)	N(18)-C(71)	1.545(11)	C(51)-C(52)	1.526(12)
C(2)-N(2)	1.191(11)	N(19)-C(91)	1.491(13)	C(52)-C(53)	1.543(13)
C(3)-N(3)	1.169(11)	N(19)-C(87)	1.496(13)	C(53)-C(54)	1.531(14)
C(4)-N(4)	1.179(11)	N(19)-C(83)	1.524(12)	C(55)-C(56)	1.508(14)
C(5)-N(5)	1.158(11)	N(19)-C(79)	1.537(11)	C(56)-C(57)	1.52(2)
C(6)-N(6)	1.147(11)	N(20)-C(107)	1.494(11)	C(57)-C(58)	1.52(2)
C(7)-N(7)	1.166(11)	N(20)-C(99)	1.504(11)	C(59)-C(60)	1.509(13)
Re(2)-C(12)	2.065(11)	N(20)-C(103)	1.511(11)	C(60)-C(61)	1.543(14)
Re(2)-C(13)	2.075(11)	N(20)-C(95)	1.527(11)	C(61)-C(62)	1.49(2)
Re(2)-C(10)	2.080(11)	C(15)-C(16)	1.507(12)	C(63)-C(64)	1.506(13)
Re(2)-C(8)	2.093(11)	C(16)-C(17)	1.525(13)	C(64)-C(65)	1.554(13)
Re(2)-C(9)	2.097(11)	C(17)-C(18)	1.516(13)	C(65)-C(66)	1.514(14)
Re(2)-C(11)	2.103(11)	C(19)-C(20)	1.481(12)	C(67)-C(68)	1.511(12)
Re(2)-C(14)	2.123(11)	C(20)-C(21)	1.528(14)	C(68)-C(69)	1.558(12)
C(8)-N(8)	1.173(11)	C(21)-C(22)	1.52(2)	C(69)-C(70)	1.558(12)
C(9)-N(9)	1.179(12)	C(23)-C(24)	1.533(13)	C(71)-C(72)	1.542(13)
C(10)-N(10)	1.179(11)	C(24)-C(25)	1.536(14)	C(72)-C(73)	1.528(14)
C(11)-N(11)	1.175(11)	C(25)-C(26)	1.40(2)	C(73)-C(74)	1.544(14)
C(12)-N(12)	1.148(12)	C(27)-C(28)	1.500(12)	C(75)-C(76)	1.523(13)
C(13)-N(13)	1.179(12)	C(28)-C(29)	1.522(12)	C(76)-C(77B)	1.48(2)
C(14)-N(14)	1.154(11)	C(29)-C(30)	1.519(12)	C(76)-C(77)	1.50(3)
N(15)-C(19)	1.507(11)	C(31)-C(32)	1.503(12)	C(77B)-C(78B)	1.48(3)
N(15)-C(23)	1.513(11)	C(32)-C(33)	1.533(13)	C(77B)-C(77)	1.85(4)
N(15)-C(15)	1.517(11)	C(33)-C(34)	1.512(13)	C(77)-C(78)	1.32(4)
N(15)-C(27)	1.546(11)	C(35)-C(36)	1.536(12)	C(78)-C(78B)	1.98(4)
N(16)-C(35)	1.503(11)	C(36)-C(37)	1.512(12)	C(79)-C(80)	1.483(13)
N(16)-C(39)	1.522(11)	C(37)-C(38)	1.534(13)	C(80)-C(81)	1.570(13)
N(16)-C(31)	1.527(11)	C(39)-C(40)	1.499(12)	C(81)-C(82)	1.496(13)
N(16)-C(43)	1.543(11)	C(40)-C(41)	1.548(14)	C(83)-C(84)	1.498(14)

C(84)-C(85)	1.55(2)	C(93)-C(94)	1.32(2)	C(103)-C(104)	1.508(12)
C(85)-C(86)	1.49(2)	C(95)-C(96)	1.525(13)	C(104)-C(105)	1.502(13)
C(87)-C(88)	1.57(2)	C(96)-C(97)	1.528(14)	C(105)-C(106)	1.529(13)
C(88)-C(89)	1.58(2)	C(97)-C(98)	1.52(2)	C(107)-C(108)	1.525(12)
C(89)-C(90)	1.41(2)	C(99)-C(100)	1.548(12)	C(108)-C(109)	1.549(14)
C(91)-C(92)	1.55(2)	C(100)-C(101)	1.506(13)	C(109)-C(110)	1.523(14)
C(92)-C(93)	1.66(2)	C(101)-C(102)	1.529(13)		

C(2)-Re(1)-C(6)	86.5(4)	C(10)-Re(2)-C(8)	83.3(4)
C(2)-Re(1)-C(4)	96.0(4)	C(12)-Re(2)-C(9)	94.2(4)
C(6)-Re(1)-C(4)	144.6(4)	C(13)-Re(2)-C(9)	90.9(4)
C(2)-Re(1)-C(7)	94.7(3)	C(10)-Re(2)-C(9)	95.3(4)
C(6)-Re(1)-C(7)	72.3(3)	C(8)-Re(2)-C(9)	178.1(4)
C(4)-Re(1)-C(7)	142.0(4)	C(12)-Re(2)-C(11)	72.1(4)
C(2)-Re(1)-C(1)	179.0(3)	C(13)-Re(2)-C(11)	143.2(4)
C(6)-Re(1)-C(1)	93.3(4)	C(10)-Re(2)-C(11)	72.5(4)
C(4)-Re(1)-C(1)	83.6(4)	C(8)-Re(2)-C(11)	97.0(4)
C(7)-Re(1)-C(1)	86.1(4)	C(9)-Re(2)-C(11)	83.8(4)
C(2)-Re(1)-C(5)	88.3(4)	C(12)-Re(2)-C(14)	143.3(4)
C(6)-Re(1)-C(5)	71.6(3)	C(13)-Re(2)-C(14)	71.3(4)
C(4)-Re(1)-C(5)	73.2(3)	C(10)-Re(2)-C(14)	74.0(4)
C(7)-Re(1)-C(5)	143.5(4)	C(8)-Re(2)-C(14)	92.1(4)
C(1)-Re(1)-C(5)	90.7(3)	C(9)-Re(2)-C(14)	86.3(4)
C(2)-Re(1)-C(3)	84.0(4)	C(11)-Re(2)-C(14)	144.0(4)
C(6)-Re(1)-C(3)	143.8(4)	N(8)-C(8)-Re(2)	177.3(9)
C(4)-Re(1)-C(3)	71.3(4)	N(9)-C(9)-Re(2)	179.3(10)
C(7)-Re(1)-C(3)	73.7(4)	N(10)-C(10)-Re(2)	176.6(8)
C(1)-Re(1)-C(3)	96.8(3)	N(11)-C(11)-Re(2)	174.7(9)
C(5)-Re(1)-C(3)	142.6(4)	N(12)-C(12)-Re(2)	176.8(10)
N(1)-C(1)-Re(1)	175.9(9)	N(13)-C(13)-Re(2)	178.1(9)
N(2)-C(2)-Re(1)	176.3(9)	N(14)-C(14)-Re(2)	179.0(9)
N(3)-C(3)-Re(1)	176.3(9)	C(19)-N(15)-C(23)	106.2(7)
N(4)-C(4)-Re(1)	179.0(8)	C(19)-N(15)-C(15)	110.2(7)
N(5)-C(5)-Re(1)	178.0(9)	C(23)-N(15)-C(15)	112.8(7)
N(6)-C(6)-Re(1)	177.9(9)	C(19)-N(15)-C(27)	110.5(7)
N(7)-C(7)-Re(1)	178.7(9)	C(23)-N(15)-C(27)	110.9(7)
C(12)-Re(2)-C(13)	72.0(4)	C(15)-N(15)-C(27)	106.2(7)
C(12)-Re(2)-C(10)	142.1(4)	C(35)-N(16)-C(39)	111.6(7)
C(13)-Re(2)-C(10)	144.3(4)	C(35)-N(16)-C(31)	112.7(7)
C(12)-Re(2)-C(8)	87.7(4)	C(39)-N(16)-C(31)	106.9(6)
C(13)-Re(2)-C(8)	89.5(4)	C(35)-N(16)-C(43)	105.3(6)

C(39)-N(16)-C(43)	109.9(7)	C(107)-N(20)-C(99)	106.7(7)
C(31)-N(16)-C(43)	110.5(7)	C(107)-N(20)-C(103)	110.3(7)
C(55)-N(17)-C(51)	106.3(7)	C(99)-N(20)-C(103)	111.6(7)
C(55)-N(17)-C(59)	111.0(8)	C(107)-N(20)-C(95)	109.8(7)
C(51)-N(17)-C(59)	110.4(8)	C(99)-N(20)-C(95)	111.8(8)
C(55)-N(17)-C(47)	111.4(8)	C(103)-N(20)-C(95)	106.7(7)
C(51)-N(17)-C(47)	111.6(8)	C(16)-C(15)-N(15)	115.6(7)
C(59)-N(17)-C(47)	106.3(7)	C(15)-C(16)-C(17)	110.2(8)
C(75)-N(18)-C(67)	107.0(6)	C(18)-C(17)-C(16)	114.8(9)
C(75)-N(18)-C(63)	112.0(7)	C(20)-C(19)-N(15)	117.3(8)
C(67)-N(18)-C(63)	110.1(7)	C(19)-C(20)-C(21)	109.2(9)
C(75)-N(18)-C(71)	110.2(7)	C(22)-C(21)-C(20)	112.6(10)
C(67)-N(18)-C(71)	111.2(7)	N(15)-C(23)-C(24)	113.8(8)
C(63)-N(18)-C(71)	106.4(6)	C(23)-C(24)-C(25)	111.8(9)
C(91)-N(19)-C(87)	112.5(9)	C(26)-C(25)-C(24)	112.2(11)
C(91)-N(19)-C(83)	112.2(8)	C(28)-C(27)-N(15)	116.2(7)
C(87)-N(19)-C(83)	105.4(8)	C(27)-C(28)-C(29)	109.5(8)
C(91)-N(19)-C(79)	106.9(8)	C(30)-C(29)-C(28)	111.7(8)
C(87)-N(19)-C(79)	111.5(8)	C(32)-C(31)-N(16)	114.4(8)
C(83)-N(19)-C(79)	108.3(8)	C(31)-C(32)-C(33)	111.4(8)
C(34)-C(33)-C(32)	111.6(9)	C(62)-C(61)-C(60)	112.9(10)
N(16)-C(35)-C(36)	114.8(7)	C(64)-C(63)-N(18)	113.7(7)
C(37)-C(36)-C(35)	110.6(8)	C(63)-C(64)-C(65)	110.8(8)
C(36)-C(37)-C(38)	110.4(8)	C(66)-C(65)-C(64)	111.7(9)
C(40)-C(39)-N(16)	114.8(7)	N(18)-C(67)-C(68)	114.8(7)
C(39)-C(40)-C(41)	112.2(8)	C(67)-C(68)-C(69)	111.2(8)
C(42)-C(41)-C(40)	112.2(10)	C(68)-C(69)-C(70)	111.6(8)
C(44)-C(43)-N(16)	114.8(7)	C(72)-C(71)-N(18)	114.8(8)
C(43)-C(44)-C(45)	110.4(8)	C(73)-C(72)-C(71)	109.3(8)
C(44)-C(45)-C(46)	113.3(9)	C(72)-C(73)-C(74)	110.8(9)
C(48)-C(47)-N(17)	115.7(8)	N(18)-C(75)-C(76)	115.0(8)
C(49)-C(48)-C(47)	111.4(10)	C(77B)-C(76)-C(77)	77(2)
C(48)-C(49)-C(50)	112.4(10)	C(77B)-C(76)-C(75)	110.6(13)
N(17)-C(51)-C(52)	115.4(8)	C(77)-C(76)-C(75)	109(2)
C(51)-C(52)-C(53)	110.2(9)	C(76)-C(77B)-C(78B)	112(2)
C(54)-C(53)-C(52)	112.4(9)	C(76)-C(77B)-C(77)	52.1(13)
C(56)-C(55)-N(17)	113.5(8)	C(78B)-C(77B)-C(77)	89(2)
C(55)-C(56)-C(57)	111.4(11)	C(78)-C(77)-C(76)	116(3)
C(56)-C(57)-C(58)	110.1(12)	C(78)-C(77)-C(77B)	97(3)
C(60)-C(59)-N(17)	115.5(8)	C(76)-C(77)-C(77B)	51.1(13)
C(59)-C(60)-C(61)	108.0(9)	C(77)-C(78)-C(78B)	88(3)

C(77B)-C(78B)-C(78)	86(2)	C(96)-C(95)-N(20)	115.5(8)
C(80)-C(79)-N(19)	117.8(8)	C(95)-C(96)-C(97)	107.9(9)
C(79)-C(80)-C(81)	110.1(8)	C(98)-C(97)-C(96)	111.3(10)
C(82)-C(81)-C(80)	112.7(9)	N(20)-C(99)-C(100)	114.8(8)
C(84)-C(83)-N(19)	115.7(9)	C(101)-C(100)-C(99)	111.3(8)
C(83)-C(84)-C(85)	109.8(9)	C(100)-C(101)-C(102)	110.6(9)
C(86)-C(85)-C(84)	113.8(10)	C(104)-C(103)-N(20)	115.4(8)
N(19)-C(87)-C(88)	112.2(10)	C(105)-C(104)-C(103)	111.2(9)
C(87)-C(88)-C(89)	105.3(11)	C(104)-C(105)-C(106)	111.9(9)
C(90)-C(89)-C(88)	113.3(14)	N(20)-C(107)-C(108)	117.2(8)
N(19)-C(91)-C(92)	115.6(10)	C(107)-C(108)-C(109)	110.4(9)
C(91)-C(92)-C(93)	106.0(11)	C(110)-C(109)-C(108)	112.6(10)
C(94)-C(93)-C(92)	107(2)		

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2U_{11} + \dots + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Re(1)	22(1)	27(1)	24(1)	2(1)	-1(1)	-2(1)
C(1)	25(6)	25(6)	30(7)	-6(5)	-8(5)	1(5)
N(1)	31(5)	51(6)	41(6)	14(5)	-9(5)	-4(4)
C(2)	37(6)	28(6)	24(6)	-9(5)	6(5)	-2(5)
N(2)	52(6)	38(6)	36(6)	-10(4)	10(5)	1(4)
C(3)	44(7)	36(7)	23(6)	1(5)	8(5)	-7(5)
N(3)	35(5)	55(6)	45(6)	-1(5)	-9(5)	3(5)
C(4)	20(6)	52(7)	26(7)	18(5)	12(5)	5(5)
N(4)	43(6)	61(7)	27(6)	2(5)	-2(4)	10(5)
C(5)	27(5)	37(6)	30(6)	-3(5)	11(5)	-5(5)
N(5)	37(5)	51(6)	37(6)	1(5)	0(5)	7(4)
C(6)	24(6)	39(7)	29(7)	-11(5)	-7(5)	6(5)
N(6)	38(6)	41(6)	68(7)	-20(5)	-13(5)	-6(5)
C(7)	31(6)	30(6)	32(7)	13(5)	8(5)	5(5)
N(7)	40(6)	39(6)	46(6)	-9(5)	1(5)	-1(4)
Re(2)	22(1)	29(1)	44(1)	5(1)	2(1)	1(1)
C(8)	29(6)	35(7)	51(8)	3(5)	16(6)	1(5)
N(8)	48(6)	48(6)	46(6)	16(5)	22(5)	16(5)
C(9)	33(7)	48(8)	47(8)	-9(6)	-17(6)	-14(5)
N(9)	51(6)	51(7)	92(9)	-3(6)	-39(6)	-1(5)
C(10)	19(6)	41(7)	41(7)	4(5)	0(5)	-1(5)
N(10)	34(5)	43(6)	58(7)	8(5)	1(5)	1(4)
C(11)	35(7)	48(7)	31(7)	4(5)	-7(5)	-3(5)
N(11)	43(6)	65(7)	38(6)	7(5)	-3(5)	-9(5)
C(12)	41(7)	28(7)	45(8)	8(5)	13(6)	-9(5)
N(12)	57(7)	44(6)	55(7)	4(5)	-11(5)	-18(5)
C(13)	33(6)	38(7)	58(8)	-10(6)	15(6)	-1(5)
N(13)	45(6)	46(7)	122(10)	-32(6)	38(6)	-6(5)
C(14)	31(6)	26(6)	53(8)	-5(5)	5(6)	-4(5)
N(14)	46(6)	45(6)	70(7)	-7(5)	17(5)	1(5)
N(15)	42(5)	23(5)	30(5)	4(4)	-2(4)	3(4)
N(16)	15(4)	45(5)	29(5)	-3(4)	2(3)	-3(4)

N(17)	22(4)	46(6)	59(6)	-6(4)	5(4)	-1(4)
N(18)	35(4)	36(5)	21(4)	1(4)	2(4)	2(4)
N(19)	50(6)	61(7)	33(5)	-25(4)	7(4)	-10(5)
N(20)	48(6)	26(5)	34(6)	-4(4)	2(4)	-2(4)

Table S5. Crystal data and structure refinement for **2**.

Identification code	mvb67s4	
Empirical formula	$\text{C}_7\text{H}_{16}\text{Mn}_2\text{N}_7\text{O}_8\text{Re}$	
Formula weight	622.35	
Temperature	136 K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	$a = 7.5397(3)$ Å	$\alpha = 78.8680(10)^\circ$
	$b = 12.5924(6)$ Å	$\beta = 87.873(2)^\circ$
	$c = 19.7366(11)$ Å	$\gamma = 88.026(2)^\circ$
Volume, Z	1836.6(2) Å ³ , 4	
Density (calculated)	2.251 Mg/m ³	
Absorption coefficient	7.977 mm ⁻¹	
F(000)	1184	
Crystal size	0.11 x 0.21 x 0.02 mm	
Crystal color and habit	pale purple trapezoidal plate	
θ range for data collection	1.78 to 25.51°	
Limiting indices	$-9 \leq h \leq 6$, $-14 \leq k \leq 15$, $-23 \leq l \leq 22$	
Reflections collected	9489	
Independent reflections	5899 ($R_{\text{int}} = 0.0545$)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5898 / 0 / 231	
Goodness-of-fit on F^2	1.034	
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0545$, $wR2 = 0.1358$	
R indices (all data)	$R1 = 0.0887$, $wR2 = 0.1544$	
Largest diff. peak and hole	2.153 and -3.546 eÅ ⁻³	

Table S6. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for **2**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Re(1)	7380(1)	-2774(1)	921(1)	7(1)
C(1)	7853(17)	-1469(11)	125(7)	15(3)
N(1)	11996(12)	721(8)	323(5)	5(2)
C(2)	8994(17)	-1709(11)	1297(7)	16(3)
N(2)	9868(13)	-1113(9)	1515(5)	10(2)
C(3)	5119(17)	-1861(11)	1104(7)	14(3)
N(3)	13915(15)	-1372(10)	1260(6)	19(3)
C(4)	9695(17)	-3728(11)	863(7)	13(3)
N(4)	9148(15)	-5681(10)	-887(6)	18(3)
C(5)	5715(17)	-4083(11)	1173(7)	13(3)
N(5)	5219(14)	-5194(9)	-1339(6)	17(3)
C(6)	6908(17)	-3265(11)	3(7)	13(3)
N(6)	6779(14)	-3554(9)	-514(6)	12(2)
C(7)	7520(16)	-3361(11)	1981(7)	10(3)
N(7)	7609(14)	-3695(9)	-7439(6)	17(3)
Re(2)	7509(1)	-2722(1)	-4023(1)	8(1)
C(8)	7251(21)	-2985(14)	-2955(9)	31(4)
N(8)	7123(18)	-3228(12)	-2347(8)	42(4)
C(9)	9776(17)	-3700(11)	-3908(7)	12(3)
N(9)	9049(15)	-5694(10)	-6180(6)	20(3)
C(10)	7268(17)	-3494(11)	-4856(7)	16(3)
N(10)	7226(14)	-3959(9)	-5305(6)	14(3)
C(11)	5826(16)	-4013(11)	-3733(7)	10(3)
N(11)	5144(14)	-5282(9)	-6421(6)	12(2)
C(12)	9022(17)	-1531(11)	-3722(7)	14(3)
N(12)	10130(13)	865(9)	-6439(5)	10(2)
C(13)	8111(17)	-1634(11)	-4936(7)	13(3)
N(13)	8315(14)	-1030(9)	-5446(6)	16(3)
C(14)	5188(16)	-1797(10)	-4069(7)	9(3)
N(14)	6045(14)	1207(9)	-5941(6)	13(3)
Mn(1)	12154(2)	-41(2)	1418(1)	8(1)
O(1)	14378(12)	1041(8)	1472(5)	18(2)
O(2)	12365(12)	-307(8)	2561(5)	21(2)

O(3)	9875(11)	1161(7)	1561(5)	12(2)
Mn(2)	7632(3)	-4269(2)	-1367(1)	11(1)
O(4)	10264(11)	-3408(8)	-1465(5)	16(2)
O(5)	8839(26)	-5049(17)	-2328(11)	119(7)
Mn(3)	7341(2)	-4232(2)	-6340(1)	8(1)
O(6)	9906(11)	-3183(7)	-6439(5)	13(2)
O(7)	5028(11)	-2932(7)	-6445(5)	13(2)
Mn(4)	7586(2)	64(2)	-6411(1)	8(1)
O(8)	5033(11)	-779(7)	-6450(4)	9(2)
O(9)	7057(11)	1143(7)	-7454(5)	16(2)
O(10)	8635(11)	-1125(7)	-7021(5)	17(2)
O(11)	7681(13)	3290(8)	-4577(5)	25(2)
O(12)	7350(13)	3394(8)	-7423(5)	25(2)
O(13)	7496(12)	1081(8)	-4594(5)	20(2)
O(14)	2719(13)	-3129(8)	-7474(5)	28(3)
O(15)	17351(12)	1201(8)	554(5)	20(2)
O(16)	17381(12)	3479(8)	422(5)	22(2)

Table S7. Bond lengths [Å] and angles [°] for **2**.

Re(1)-C(6)	2.071(13)	C(6)-N(6)	1.16(2)	N(11)-Mn(3)	2.184(11)
Re(1)-C(1)	2.07(2)	N(6)-Mn(2)	2.127(11)	C(12)-N(12)#10	1.17(2)
Re(1)-C(5)	2.078(13)	C(7)-N(7)#6	1.14(2)	N(12)-C(12)#10	1.17(2)
Re(1)-C(3)	2.083(13)	N(7)-C(7)#7	1.14(2)	N(12)-Mn(4)	2.192(10)
Re(1)-C(7)	2.086(13)	N(7)-Mn(3)	2.148(12)	C(13)-N(13)	1.15(2)
Re(1)-C(2)	2.096(13)	Re(2)-C(14)	2.063(12)	N(13)-Mn(4)	2.201(12)
Re(1)-C(4)	2.097(13)	Re(2)-C(9)	2.066(13)	C(14)-N(14)#11	1.17(2)
C(1)-N(1)#1	1.17(2)	Re(2)-C(8)	2.07(2)	N(14)-C(14)#11	1.17(2)
N(1)-C(1)#1	1.17(2)	Re(2)-C(11)	2.076(13)	N(14)-Mn(4)	2.145(11)
N(1)-Mn(1)	2.195(10)	Re(2)-C(10)	2.082(14)	Mn(1)-O(1)	2.215(9)
C(2)-N(2)	1.17(2)	Re(2)-C(13)	2.087(14)	Mn(1)-O(2)	2.226(10)
N(2)-Mn(1)	2.206(10)	Re(2)-C(12)	2.102(13)	Mn(1)-O(3)	2.295(9)
C(3)-N(3)#2	1.15(2)	C(8)-N(8)	1.18(2)	Mn(2)-O(4)	2.279(9)
N(3)-C(3)#3	1.15(2)	N(8)-Mn(2)	2.16(2)	Mn(2)-O(5)	2.43(2)
N(3)-Mn(1)	2.165(12)	C(9)-N(9)#8	1.14(2)	Mn(3)-O(7)	2.337(9)
C(4)-N(4)#4	1.12(2)	N(9)-C(9)#8	1.14(2)	Mn(3)-O(6)	2.360(9)
N(4)-C(4)#4	1.12(2)	N(9)-Mn(3)	2.189(12)	Mn(4)-O(10)	2.205(9)
N(4)-Mn(2)	2.158(12)	C(10)-N(10)	1.15(2)	Mn(4)-O(8)	2.241(8)
C(5)-N(5)#5	1.16(2)	N(10)-Mn(3)	2.134(11)	Mn(4)-O(9)	2.277(10)
N(5)-C(5)#5	1.16(2)	C(11)-N(11)#9	1.16(2)		
N(5)-Mn(2)	2.186(11)	N(11)-C(11)#9	1.16(2)		
C(6)-Re(1)-C(1)	72.6(5)	C(3)-Re(1)-C(2)	90.9(5)		
C(6)-Re(1)-C(5)	73.7(5)	C(7)-Re(1)-C(2)	74.1(5)		
C(1)-Re(1)-C(5)	139.9(5)	C(6)-Re(1)-C(4)	81.7(5)		
C(6)-Re(1)-C(3)	104.4(5)	C(1)-Re(1)-C(4)	101.4(5)		
C(1)-Re(1)-C(3)	83.3(5)	C(5)-Re(1)-C(4)	94.7(5)		
C(5)-Re(1)-C(3)	84.4(5)	C(3)-Re(1)-C(4)	173.3(5)		
C(6)-Re(1)-C(7)	141.7(5)	C(7)-Re(1)-C(4)	84.1(5)		
C(1)-Re(1)-C(7)	145.4(5)	C(2)-Re(1)-C(4)	86.1(5)		
C(5)-Re(1)-C(7)	72.2(5)	N(1)#1-C(1)-Re(1)	175.6(11)		
C(3)-Re(1)-C(7)	89.3(5)	C(1)#1-N(1)-Mn(1)	151.0(10)		
C(6)-Re(1)-C(2)	139.5(5)	N(2)-C(2)-Re(1)	178.8(11)		
C(1)-Re(1)-C(2)	72.2(5)	C(2)-N(2)-Mn(1)	150.9(10)		
C(5)-Re(1)-C(2)	146.1(6)	N(3)#2-C(3)-Re(1)	174.4(12)		

C(3)#3-N(3)-Mn(1)	162.4(11)	C(14)-Re(2)-C(9)	175.9(5)
N(4)#4-C(4)-Re(1)	172.4(12)	C(14)-Re(2)-C(8)	88.4(6)
C(4)#4-N(4)-Mn(2)	153.2(12)	C(9)-Re(2)-C(8)	87.8(6)
N(5)#5-C(5)-Re(1)	177.4(12)	C(14)-Re(2)-C(11)	84.0(5)
C(5)#5-N(5)-Mn(2)	157.2(11)	C(9)-Re(2)-C(11)	93.4(5)
N(6)-C(6)-Re(1)	174.9(11)	C(8)-Re(2)-C(11)	73.6(6)
C(6)-N(6)-Mn(2)	156.6(10)	C(14)-Re(2)-C(10)	101.6(5)
N(7)#6-C(7)-Re(1)	179.1(12)	C(9)-Re(2)-C(10)	80.6(5)
C(7)#7-N(7)-Mn(3)	170.8(11)	C(8)-Re(2)-C(10)	141.8(6)
C(11)-Re(2)-C(10)	71.0(5)	N(3)-Mn(1)-O(2)	96.6(4)
C(14)-Re(2)-C(13)	82.2(5)	N(1)-Mn(1)-O(2)	163.1(4)
C(9)-Re(2)-C(13)	101.8(5)	N(2)-Mn(1)-O(2)	91.4(4)
C(8)-Re(2)-C(13)	147.1(6)	O(1)-Mn(1)-O(2)	81.1(4)
C(11)-Re(2)-C(13)	135.9(5)	N(3)-Mn(1)-O(3)	169.4(4)
C(10)-Re(2)-C(13)	71.1(5)	N(1)-Mn(1)-O(3)	83.8(3)
C(14)-Re(2)-C(12)	93.7(5)	N(2)-Mn(1)-O(3)	79.6(3)
C(9)-Re(2)-C(12)	86.7(5)	O(1)-Mn(1)-O(3)	97.5(3)
C(8)-Re(2)-C(12)	74.4(6)	O(2)-Mn(1)-O(3)	85.7(3)
C(11)-Re(2)-C(12)	147.9(5)	N(6)-Mn(2)-N(8)	112.5(5)
C(10)-Re(2)-C(12)	140.0(5)	N(6)-Mn(2)-N(4)	103.0(4)
C(13)-Re(2)-C(12)	74.9(5)	N(8)-Mn(2)-N(4)	143.1(5)
N(8)-C(8)-Re(2)	174(2)	N(6)-Mn(2)-N(5)	93.7(4)
C(8)-N(8)-Mn(2)	153.4(14)	N(8)-Mn(2)-N(5)	95.2(5)
N(9)#8-C(9)-Re(2)	174.8(12)	N(4)-Mn(2)-N(5)	92.3(4)
C(9)#8-N(9)-Mn(3)	165.0(11)	N(6)-Mn(2)-O(4)	91.6(4)
N(10)-C(10)-Re(2)	175.9(12)	N(8)-Mn(2)-O(4)	84.0(4)
C(10)-N(10)-Mn(3)	158.7(11)	N(4)-Mn(2)-O(4)	85.3(4)
N(11)#9-C(11)-Re(2)	178.4(11)	N(5)-Mn(2)-O(4)	174.5(4)
C(11)#9-N(11)-Mn(3)	158.8(11)	N(6)-Mn(2)-O(5)	175.6(5)
N(12)#10-C(12)-Re(2)	179.3(12)	N(8)-Mn(2)-O(5)	68.4(6)
C(12)#10-N(12)-Mn(4)	149.4(10)	N(4)-Mn(2)-O(5)	75.4(6)
N(13)-C(13)-Re(2)	175.1(11)	N(5)-Mn(2)-O(5)	90.5(6)
C(13)-N(13)-Mn(4)	157.7(10)	O(4)-Mn(2)-O(5)	84.1(5)
N(14)#11-C(14)-Re(2)	173.3(10)	N(10)-Mn(3)-N(7)	152.6(4)
C(14)#11-N(14)-Mn(4)	150.9(10)	N(10)-Mn(3)-N(11)	106.3(4)
N(3)-Mn(1)-N(1)	96.1(4)	N(7)-Mn(3)-N(11)	93.2(4)
N(3)-Mn(1)-N(2)	90.0(4)	N(10)-Mn(3)-N(9)	98.4(4)
N(1)-Mn(1)-N(2)	99.7(4)	N(7)-Mn(3)-N(9)	101.6(4)
N(3)-Mn(1)-O(1)	93.1(4)	N(11)-Mn(3)-N(9)	87.0(4)
N(1)-Mn(1)-O(1)	87.1(4)	N(10)-Mn(3)-O(7)	81.2(4)
N(2)-Mn(1)-O(1)	172.2(4)	N(7)-Mn(3)-O(7)	83.1(4)

N(11)-Mn(3)-O(7)	81.3(4)	N(12)-Mn(4)-O(10)	93.6(4)
N(9)-Mn(3)-O(7)	167.7(4)	N(13)-Mn(4)-O(10)	90.7(4)
N(10)-Mn(3)-O(6)	83.6(4)	N(14)-Mn(4)-O(8)	86.3(4)
N(7)-Mn(3)-O(6)	78.3(4)	N(12)-Mn(4)-O(8)	176.2(4)
N(11)-Mn(3)-O(6)	169.7(4)	N(13)-Mn(4)-O(8)	92.1(4)
N(9)-Mn(3)-O(6)	88.9(4)	O(10)-Mn(4)-O(8)	83.2(3)
O(7)-Mn(3)-O(6)	103.2(3)	N(14)-Mn(4)-O(9)	87.9(4)
N(14)-Mn(4)-N(12)	96.6(4)	N(12)-Mn(4)-O(9)	87.3(4)
N(14)-Mn(4)-N(13)	96.8(4)	N(13)-Mn(4)-O(9)	174.9(4)
N(12)-Mn(4)-N(13)	89.9(4)	O(10)-Mn(4)-O(9)	85.2(3)
N(14)-Mn(4)-O(10)	167.4(4)	O(8)-Mn(4)-O(9)	90.5(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z	#2 x-1,y,z	#3 x+1,y,z	#4 -x+2,-y-1,-z
#5 -x+1,-y-1,-z	#6 x,y,z+1	#7 x,y,z-1	#8 -x+2,-y-1,-z-1
#9 -x+1,-y-1,-z-1	#10 -x+2,-y,-z-1	#11 -x+1,-y,-z-1	

Table S8. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[(h a^*)^2 U_{11} + \dots + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Re(1)	7(1)	6(1)	8(1)	-1(1)	-2(1)	-1(1)
Re(2)	8(1)	8(1)	6(1)	1(1)	-2(1)	-2(1)
Mn(1)	9(1)	7(1)	9(1)	-1(1)	-2(1)	-1(1)
Mn(2)	10(1)	7(1)	14(1)	1(1)	-2(1)	-1(1)
Mn(3)	10(1)	7(1)	7(1)	-1(1)	-3(1)	-2(1)
Mn(4)	9(1)	7(1)	9(1)	-1(1)	-2(1)	-1(1)

Table S9. Crystal data and structure refinement for **4·2MeCN**.

Identification code	mvb76f	
Empirical formula	C ₁₂ H ₆ K ₃ N ₁₀ Re	
Formula weight	593.77	
Temperature	134 K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	Pnma	
Unit cell dimensions	$a = 17.2149(5)$ Å	$\alpha = 90^\circ$
	$b = 10.5170(3)$ Å	$\beta = 90^\circ$
	$c = 9.3391(3)$ Å	$\gamma = 90^\circ$
Volume, Z	1690.84(9) Å ³ , 4	
Density (calculated)	2.333 Mg/m ³	
Absorption coefficient	7.946 mm ⁻¹	
F(000)	1120	
Crystal size	0.31 x 0.22 x 0.07 mm	
Crystal color and habit	clear white plate	
θ range for data collection	2.37 to 25.52°	
Limiting indices	$-14 \leq h \leq 20$, $-12 \leq k \leq 12$, $-11 \leq l \leq 10$	
Reflections collected	7163	
Independent reflections	1570 ($R_{\text{int}} = 0.0502$)	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	1570 / 0 / 123	
Goodness-of-fit on F ²	1.005	
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0194$, $wR2 = 0.0438$	
R indices (all data)	$R1 = 0.0221$, $wR2 = 0.0440$	
Largest diff. peak and hole	0.911 and -1.271 eÅ ⁻³	

Table S10. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 4·2MeCN. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Re(1)	1142(1)	2500	2018(1)	10(1)
C(1)	903(3)	2500	-210(6)	15(1)
N(1)	757(3)	2500	-1406(5)	20(1)
C(2)	164(2)	1313(3)	1924(3)	14(1)
N(2)	-386(2)	699(3)	1806(3)	21(1)
C(3)	1602(2)	808(3)	1167(4)	14(1)
N(3)	1838(2)	-131(3)	708(3)	18(1)
C(4)	2337(3)	2500	2487(5)	14(1)
N(4)	2981(3)	2500	2797(5)	22(1)
C(5)	1182(2)	1323(3)	3827(4)	18(1)
N(5)	1227(2)	664(3)	4816(4)	29(1)
C(6)	3530(4)	2500	8909(6)	22(1)
C(7)	4257(5)	2500	9672(7)	34(2)
N(6)	2956(3)	2500	8274(5)	28(1)
K(1)	3915(1)	2500	5318(1)	20(1)
K(2)	1795(1)	438(1)	7573(1)	17(1)

Table S11. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **4-2MeCN**.

Re(1)-C(5)#1	2.095(4)	C(3)-N(3)	1.151(4)	K(1)-N(3)#8	2.832(3)
Re(1)-C(5)	2.095(4)	C(3)-K(2)#6	3.325(4)	K(1)-N(3)#9	2.832(3)
Re(1)-C(2)#1	2.098(4)	C(3)-K(2)#2	3.395(3)	K(1)-N(2)#10	2.995(3)
Re(1)-C(2)	2.098(4)	N(3)-K(1)#6	2.832(3)	K(1)-N(2)#11	2.995(3)
Re(1)-C(4)	2.103(6)	N(3)-K(2)#6	2.945(3)	K(1)-C(2)#11	3.251(4)
Re(1)-C(3)	2.104(4)	N(3)-K(2)#2	2.989(3)	K(1)-C(2)#10	3.251(4)
Re(1)-C(3)#1	2.104(4)	C(4)-N(4)	1.146(7)	K(1)-N(1)#10	3.330(5)
Re(1)-C(1)	2.121(5)	C(4)-K(2)#7	3.433(3)	K(1)-C(1)#10	3.424(5)
C(1)-N(1)	1.144(6)	C(4)-K(2)#6	3.433(3)	K(1)-K(2)#6	4.197(1)
C(1)-K(2)#2	3.369(4)	N(4)-K(1)	2.851(5)	K(2)-N(2)#5	2.765(3)
C(1)-K(2)#3	3.369(4)	N(4)-K(2)#7	3.121(1)	K(2)-N(3)#8	2.945(3)
C(1)-K(1)#4	3.424(5)	N(4)-K(2)#6	3.121(1)	K(2)-N(1)#12	2.968(3)
N(1)-K(2)#3	2.968(3)	C(5)-N(5)	1.157(5)	K(2)-N(3)#12	2.989(3)
N(1)-K(2)#2	2.968(3)	N(5)-K(2)	2.764(3)	K(2)-N(4)#8	3.121(1)
N(1)-K(1)#4	3.330(5)	C(6)-N(6)	1.152(7)	K(2)-C(3)#8	3.325(4)
C(2)-N(2)	1.152(5)	C(6)-C(7)	1.440(1)	K(2)-C(1)#12	3.369(4)
C(2)-K(1)#4	3.250(4)	C(6)-K(1)	3.419(5)	K(2)-C(3)#12	3.395(3)
N(2)-K(2)#5	2.765(3)	N(6)-K(2)#1	3.020(4)	K(2)-C(4)#8	3.433(3)
N(2)-K(1)#4	2.995(3)	N(6)-K(2)	3.020(4)	K(2)-K(1)#8	4.197(1)
		N(6)-K(1)	3.217(5)		
C(5)#1-Re(1)-C(5)	72.4(2)	C(4)-Re(1)-C(3)	73.19(12)		
C(5)#1-Re(1)-C(2)#1	73.08(13)	C(5)#1-Re(1)-C(3)#1	78.02(13)		
C(5)-Re(1)-C(2)#1	114.34(14)	C(5)-Re(1)-C(3)#1	142.38(14)		
C(5)#1-Re(1)-C(2)	114.34(14)	C(2)#1-Re(1)-C(3)#1	77.44(13)		
C(5)-Re(1)-C(2)	73.07(13)	C(2)-Re(1)-C(3)#1	142.13(13)		
C(2)#1-Re(1)-C(2)	73.0(2)	C(4)-Re(1)-C(3)#1	73.19(12)		
C(5)#1-Re(1)-C(4)	78.4(2)	C(3)-Re(1)-C(3)#1	115.5(2)		
C(5)-Re(1)-C(4)	78.5(2)	C(5)#1-Re(1)-C(1)	142.86(10)		
C(2)#1-Re(1)-C(4)	142.53(10)	C(5)-Re(1)-C(1)	142.86(10)		
C(2)-Re(1)-C(4)	142.54(10)	C(2)#1-Re(1)-C(1)	78.62(14)		
C(5)#1-Re(1)-C(3)	142.38(14)	C(2)-Re(1)-C(1)	78.62(14)		
C(5)-Re(1)-C(3)	78.03(13)	C(4)-Re(1)-C(1)	113.2(2)		
C(2)#1-Re(1)-C(3)	142.13(13)	C(3)-Re(1)-C(1)	72.68(11)		
C(2)-Re(1)-C(3)	77.44(13)	C(3)#1-Re(1)-C(1)	72.68(11)		

N(1)-C(1)-Re(1)	178.6(5)	C(4)-N(4)-K(2)#7	95.89(10)
N(1)-C(1)-K(2)#2	60.0(2)	K(1)-N(4)-K(2)#7	89.18(9)
Re(1)-C(1)-K(2)#2	121.0(2)	C(4)-N(4)-K(2)#6	95.89(10)
N(1)-C(1)-K(2)#3	60.0(2)	K(1)-N(4)-K(2)#6	89.18(9)
Re(1)-C(1)-K(2)#3	121.0(2)	K(2)#7-N(4)-K(2)#6	163.8(2)
K(2)#2-C(1)-K(2)#3	80.13(12)	N(5)-C(5)-Re(1)	177.9(3)
N(1)-C(1)-K(1)#4	75.7(4)	C(5)-N(5)-K(2)	144.9(3)
Re(1)-C(1)-K(1)#4	102.9(2)	N(6)-C(6)-C(7)	178.7(7)
K(2)#2-C(1)-K(1)#4	115.96(13)	N(6)-C(6)-K(1)	70.2(4)
K(2)#3-C(1)-K(1)#4	115.96(13)	C(7)-C(6)-K(1)	108.4(4)
C(1)-N(1)-K(2)#3	100.5(3)	C(6)-N(6)-K(2)#1	132.74(11)
C(1)-N(1)-K(2)#2	100.5(3)	C(6)-N(6)-K(2)	132.74(11)
K(2)#3-N(1)-K(2)#2	93.91(14)	K(2)#1-N(6)-K(2)	91.8(2)
C(1)-N(1)-K(1)#4	84.9(4)	C(6)-N(6)-K(1)	90.1(4)
K(2)#3-N(1)-K(1)#4	132.18(8)	K(2)#1-N(6)-K(1)	98.82(11)
K(2)#2-N(1)-K(1)#4	132.18(8)	K(2)-N(6)-K(1)	98.82(11)
N(2)-C(2)-Re(1)	176.2(3)	N(3)#8-K(1)-N(3)#9	123.21(13)
N(2)-C(2)-K(1)#4	67.0(2)	N(3)#8-K(1)-N(4)	81.25(8)
Re(1)-C(2)-K(1)#4	109.24(12)	N(3)#9-K(1)-N(4)	81.25(8)
C(2)-N(2)-K(2)#5	160.7(3)	N(3)#8-K(1)-N(2)#10	73.30(8)
C(2)-N(2)-K(1)#4	92.2(2)	N(3)#9-K(1)-N(2)#10	145.62(9)
K(2)#5-N(2)-K(1)#4	93.44(10)	N(4)-K(1)-N(2)#10	71.30(10)
N(3)-C(3)-Re(1)	178.5(3)	N(3)#8-K(1)-N(2)#11	145.62(9)
N(3)-C(3)-K(2)#6	61.0(2)	N(3)#9-K(1)-N(2)#11	73.30(8)
Re(1)-C(3)-K(2)#6	119.75(13)	N(4)-K(1)-N(2)#11	71.30(10)
N(3)-C(3)-K(2)#2	59.9(2)	N(2)#10-K(1)-N(2)#11	78.46(12)
Re(1)-C(3)-K(2)#2	120.50(13)	N(3)#8-K(1)-N(6)	69.80(7)
K(2)#6-C(3)-K(2)#2	105.30(10)	N(3)#9-K(1)-N(6)	69.80(7)
C(3)-N(3)-K(1)#6	129.8(3)	N(4)-K(1)-N(6)	114.8(2)
C(3)-N(3)-K(2)#6	99.0(2)	N(2)#10-K(1)-N(6)	140.77(6)
K(1)#6-N(3)-K(2)#6	110.21(10)	N(2)#11-K(1)-N(6)	140.77(6)
C(3)-N(3)-K(2)#2	100.6(2)	N(3)#8-K(1)-C(2)#11	136.35(9)
K(1)#6-N(3)-K(2)#2	92.23(9)	N(3)#9-K(1)-C(2)#11	92.74(9)
K(2)#6-N(3)-K(2)#2	128.39(11)	N(4)-K(1)-C(2)#11	80.86(11)
N(4)-C(4)-Re(1)	177.4(4)	N(2)#10-K(1)-C(2)#11	63.30(9)
N(4)-C(4)-K(2)#7	64.72(9)	N(2)#11-K(1)-C(2)#11	20.74(8)
Re(1)-C(4)-K(2)#7	115.50(9)	N(6)-K(1)-C(2)#11	153.16(8)
N(4)-C(4)-K(2)#6	64.72(9)	N(3)#8-K(1)-C(2)#10	92.74(9)
Re(1)-C(4)-K(2)#6	115.50(9)	N(3)#9-K(1)-C(2)#10	136.35(9)
K(2)#7-C(4)-K(2)#6	128.3(2)	N(4)-K(1)-C(2)#10	80.86(11)
C(4)-N(4)-K(1)	138.9(4)	N(2)#10-K(1)-C(2)#10	20.74(8)

N(2)#11-K(1)-C(2)#10	63.30(9)	N(3)#8-K(1)-C(1)#10	117.48(7)
N(6)-K(1)-C(2)#10	153.16(8)	N(3)#9-K(1)-C(1)#10	117.48(7)
C(2)#11-K(1)-C(2)#10	45.18(13)	N(4)-K(1)-C(1)#10	122.63(14)
N(3)#8-K(1)-N(1)#10	113.38(7)	N(2)#10-K(1)-C(1)#10	65.10(9)
N(3)#9-K(1)-N(1)#10	113.38(7)	N(2)#11-K(1)-C(1)#10	65.10(9)
N(4)-K(1)-N(1)#10	142.08(13)	N(6)-K(1)-C(1)#10	122.58(14)
N(2)#10-K(1)-N(1)#10	79.60(9)	C(2)#11-K(1)-C(1)#10	47.13(10)
N(2)#11-K(1)-N(1)#10	79.60(9)	C(2)#10-K(1)-C(1)#10	47.13(10)
N(6)-K(1)-N(1)#10	103.13(13)	N(1)#10-K(1)-C(1)#10	19.45(11)
C(2)#11-K(1)-N(1)#10	64.30(10)	C(6)-K(1)-C(1)#10	102.9(2)
C(2)#10-K(1)-N(1)#10	64.30(10)	N(3)#8-K(1)-K(2)#6	45.37(6)
N(3)#8-K(1)-C(6)	77.59(8)	N(3)#9-K(1)-K(2)#6	126.35(8)
N(3)#9-K(1)-C(6)	77.59(8)	N(4)-K(1)-K(2)#6	48.03(2)
N(4)-K(1)-C(6)	134.5(2)	N(2)#10-K(1)-K(2)#6	41.13(7)
N(2)#10-K(1)-C(6)	136.69(8)	N(2)#11-K(1)-K(2)#6	100.25(7)
N(2)#11-K(1)-C(6)	136.69(8)	N(6)-K(1)-K(2)#6	112.01(7)
N(6)-K(1)-C(6)	19.70(13)	C(2)#11-K(1)-K(2)#6	94.71(6)
C(2)#11-K(1)-C(6)	139.48(11)	C(2)#10-K(1)-K(2)#6	61.09(7)
C(2)#10-K(1)-C(6)	139.48(11)	N(1)#10-K(1)-K(2)#6	117.63(5)
N(1)#10-K(1)-C(6)	83.43(14)	C(6)-K(1)-K(2)#6	122.87(6)
C(1)#10-K(1)-K(2)#6	105.85(6)	N(6)-K(2)-N(4)#8	127.93(12)
N(5)-K(2)-N(2)#5	85.54(10)	N(5)-K(2)-C(3)#8	87.69(10)
N(5)-K(2)-N(3)#8	74.99(10)	N(2)#5-K(2)-C(3)#8	129.82(9)
N(2)#5-K(2)-N(3)#8	141.02(9)	N(3)#8-K(2)-C(3)#8	19.99(8)
N(5)-K(2)-N(1)#12	91.36(12)	N(1)#12-K(2)-C(3)#8	156.15(10)
N(2)#5-K(2)-N(1)#12	73.77(10)	N(3)#12-K(2)-C(3)#8	106.70(8)
N(3)#8-K(2)-N(1)#12	138.69(9)	N(6)-K(2)-C(3)#8	79.61(10)
N(5)-K(2)-N(3)#12	159.75(10)	N(4)#8-K(2)-C(3)#8	62.22(11)
N(2)#5-K(2)-N(3)#12	74.32(9)	N(5)-K(2)-C(1)#12	110.85(12)
N(3)#8-K(2)-N(3)#12	122.52(5)	N(2)#5-K(2)-C(1)#12	75.49(10)
N(1)#12-K(2)-N(3)#12	81.16(10)	N(3)#8-K(2)-C(1)#12	142.96(9)
N(5)-K(2)-N(6)	111.98(11)	N(1)#12-K(2)-C(1)#12	19.51(11)
N(2)#5-K(2)-N(6)	147.66(11)	N(3)#12-K(2)-C(1)#12	62.50(10)
N(3)#8-K(2)-N(6)	71.25(11)	N(6)-K(2)-C(1)#12	72.91(12)
N(1)#12-K(2)-N(6)	78.68(12)	N(4)#8-K(2)-C(1)#12	130.72(11)
N(3)#12-K(2)-N(6)	85.12(11)	C(3)#8-K(2)-C(1)#12	151.01(11)
N(5)-K(2)-N(4)#8	101.02(11)	N(5)-K(2)-C(3)#12	151.19(11)
N(2)#5-K(2)-N(4)#8	70.50(12)	N(2)#5-K(2)-C(3)#12	75.89(9)
N(3)#8-K(2)-N(4)#8	80.36(11)	N(3)#8-K(2)-C(3)#12	132.50(9)
N(1)#12-K(2)-N(4)#8	140.93(12)	N(1)#12-K(2)-C(3)#12	62.58(10)
N(3)#12-K(2)-N(4)#8	74.52(10)	N(3)#12-K(2)-C(3)#12	19.46(8)

N(6)-K(2)-C(3)#12	76.60(11)	C(3)#12-K(2)-C(4)#8	99.71(10)
N(4)#8-K(2)-C(3)#12	93.40(10)	N(5)-K(2)-K(1)#8	121.95(8)
C(3)#8-K(2)-C(3)#12	121.12(7)	N(2)#5-K(2)-K(1)#8	45.43(7)
C(1)#12-K(2)-C(3)#12	43.45(10)	N(3)#8-K(2)-K(1)#8	120.89(6)
N(5)-K(2)-C(4)#8	102.10(11)	N(1)#12-K(2)-K(1)#8	99.57(7)
N(2)#5-K(2)-C(4)#8	89.86(11)	N(3)#12-K(2)-K(1)#8	42.40(6)
N(3)#8-K(2)-C(4)#8	62.62(10)	N(6)-K(2)-K(1)#8	126.07(9)
N(1)#12-K(2)-C(4)#8	158.02(11)	N(4)#8-K(2)-K(1)#8	42.79(9)
N(3)#12-K(2)-C(4)#8	80.32(10)	C(3)#8-K(2)-K(1)#8	101.13(6)
N(6)-K(2)-C(4)#8	111.31(12)	C(1)#12-K(2)-K(1)#8	88.03(6)
N(4)#8-K(2)-C(4)#8	19.39(11)	C(3)#12-K(2)-K(1)#8	56.76(6)
C(3)#8-K(2)-C(4)#8	43.53(10)	C(4)#8-K(2)-K(1)#8	58.56(9)
C(1)#12-K(2)-C(4)#8	142.38(11)		

Symmetry transformations used to generate equivalent atoms:

#1 $x, -y+1/2, z$ #2 $x, y, z-1$ #3 $x, -y+1/2, z-1$ #4 $x-1/2, y, -z+1/2$
#5 $-x, -y, -z+1$ #6 $-x+1/2, -y, z-1/2$ #7 $-x+1/2, y+1/2, z-1/2$
#8 $-x+1/2, -y, z+1/2$ #9 $-x+1/2, y+1/2, z+1/2$ #10 $x+1/2, y, -z+1/2$
#11 $x+1/2, -y+1/2, -z+1/2$ #12 $x, y, z+1$

Table S12. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 4·2MeCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2U_{11} + \dots + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Re(1)	10(1)	12(1)	10(1)	0	-1(1)	0
C(1)	11(3)	10(2)	24(3)	0	2(2)	0
N(1)	29(3)	17(2)	14(3)	0	-2(2)	0
C(2)	19(2)	14(2)	9(2)	3(1)	0(2)	3(2)
N(2)	17(2)	22(2)	25(2)	1(1)	-2(2)	-1(2)
C(3)	12(2)	18(2)	14(2)	2(2)	-2(2)	-1(2)
N(3)	17(2)	21(2)	16(2)	-1(1)	-3(1)	2(1)
C(4)	17(3)	10(3)	13(3)	0	-1(2)	0
N(4)	19(3)	20(2)	26(3)	0	2(2)	0
C(5)	16(2)	22(2)	15(2)	-1(2)	-3(2)	-3(2)
N(5)	31(2)	30(2)	25(2)	3(2)	-4(2)	-4(2)
C(6)	28(4)	19(3)	20(3)	0	2(3)	0
C(7)	34(5)	33(4)	36(4)	0	-14(3)	0
N(6)	32(4)	25(3)	27(3)	0	-1(3)	0
K(1)	21(1)	20(1)	18(1)	0	4(1)	0
K(2)	17(1)	19(1)	15(1)	-1(1)	2(1)	-1(1)