Supporting Information Available for:

Switchable Cr(II) Ethylene Oligomerization/Polymerization Catalyst

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General Experimental Details: All reactions were carried out under a dry nitrogen atmosphere. Solvents were dried using an aluminum oxide solvent purification system. Infrared spectra were recorded on an ABB Bomem FTIR instrument from Nujol mulls prepared in a drybox. Samples for magnetic susceptibility were pre-weighed inside a drybox equipped with an analytical balance and measured on a Johnson Matthey Magnetic Susceptibility balance. Elemental analyses were carried out with a Perkin-Elmer 2400 CHN analyzer. Data for X-ray crystal structure determination were obtained with a Bruker diffractometer equipped with a 1K Smart CCD area detector.

General Oligomerization Procedure: A Parr reactor was dried in an oven at 80 °C for three hours prior to each run, and then placed under vacuum for 30 minutes. The reactor was then charged with toluene, MAO, 40 bar ethylene and heated to 50 °C with stirring. After 15 minutes the pressure was momentarily released to allow injecting the catalyst solution into the reactor under a stream of ethylene and then the reactor was immediately re-pressurized. The reaction was allowed to run for 1 hour after which the temperature was rapidly reduced to 5 °C, the reactor was de-pressurized and a mixture of MeOH/HCl was injected to quench the reaction. The organic and aqueous phases were then separated from the polymer. Precautions were taken to maintain the T as low as possible during the work up to minimize loss of volatiles. Polymeric materials were sonicated with aqueous solution of HCl, dried at 60 °C for 18 hours under reduced pressure before the final mass was weighed.

Synthesis of Complex 1: 2,5-bis(diphenyl(pyrrol-2-yl)methyl)-1-methylpyrrole : (0.200 g, 0.368 mmol) was dissolved in 5 mL of THF. Potassium Hydride (2.05 eq, 0.030 g, 0.754 mmol) was then added and the suspension was stirred for 4 hours. The resulting solution was added to a solution of $CrCl_3(THF)_3$ (1 eq, 0.137 g, 0.368 mmol) in THF which resulted in a dark green suspension. The solution was then centrifuged to remove KCl leaving a clear dark green solution. The solution was allowed to stand at room temperature for 48 hours after which, X-ray quality dark green crystals of **1** were formed (0.194 g, 0.308 mmol, 83.8%). IR (Nujol mull, cm^{-1}) ν: 1594 (m), 1550 (m), 1227 (m), 1151 (s), 1030 (s), 897 (s), 865 (s), 797 (w) 764, (s), 744 (s), 720 (s), 519 (m). Elemental Analysis Calculated (Found) for $CrClC_{39}H_{31}N_3$: C 74.75 (74.73), H 4.97 (4.65), N 6.68 (6.52). $\mu_{eff} = 3.77\ \mu_{BM}$

Synthesis of Complex 2a: 2,5-bis(diphenyl(1H-pyrrol-2-yl)methyl)-1-methylpyrrole : (0.200 g, 0.368 mmol) was dissolved in 5 mL of THF. Potassium Hydride (2.05 eq, 0.030 g, 0.754 mmol) was added to the solution and stirred for 4 hours. The resulting solution was then added to a solution of $CrCl_3(THF)_3$ (1 eq, 0.137 g, 0.368 mmol) in THF which resulted in a light blue suspension. After stirring for 2 hours the blue suspension was allowed to settle, the supernatant was removed and the solid was dried under reduced pressure to yield the formulated compound $[(C_{39}H_{31}N_3Cr)(THF)_2](KCl)_2$ (0.309 g, 0.350 mmol, 95.1 %) IR (Nujol mull, cm^{-1}) ν: 3053 (m), 1158 (m), 1053 (s), 1027 (s), 875(s).

Synthesis of Complex 2b: The addition of 4 equivalents of pyridine (0.143 g, 1.80 mmol) to a suspension of **2a** (0.400 g, 0.452 mmol) in 20 ml of THF rapidly formed a dark brown/purple solution. Stirring was halted after 5 minutes and dark purple block

crystals started to precipitate (0.335 g, 0.426 mmol, 94.2%). IR (Nujol mull, cm^{-1}) ν: 1604 (s), 1218 (m), 1153 (m), 1043 (m), 751 (s), 692 (s), 632 (s) Elemental Analysis Calculated (Found) for $CrC_{49}H_{41}N_5(THF)_{0.5}$: C 77.74 (77.23), H 5.76 (5.45), N 8.89 (8.52). μ_{eff} = 4.92 μ_{BM}

Synthesis of Complex 3: 2,5-bis(diphenyl(pyrrol-2-yl)methyl)-1-methylpyrrole : (0.200 g, 0.368 mmol) was dissolved in 5 mL of THF and cooled to -30 °C. $LiCH_2Si(CH_3)_3$ (2.05 eq, 0.071 g, 0.754 mmol) was then added to the cooled solution and stirring was continued for 2 hours. The resulting solution was combined with a solution of $CrCl_2(THF)_{1.39}$ (1 eq, 0.082 g, 0.368 mmol) in THF which resulted in the formation of a dark green suspension. After centrifugation to remove LiCl, the solution was layered with hexanes. X-ray quality dark green crystals were formed after 24 hours (0.096 g, 0.113 mmol, 30.8 %). IR (Nujol mull, cm^{-1}) ν: 1594 (w), 1296 (w), 1260 (w), 1227 (w), 1081 (m), 1052 (s), 1026 (s), 866 (s), 782 (s), 762 (s), 753 (s), 741 (s), 708 (s), 631 (s). Elemental Analysis Calculated (Found) for $CrLiClC_{51}H_{55}N_3O_3$: C 71.86 (71.55), H 6.50 (6.38), N 4.93 (4.66). μ_{eff} = 4.69 μ_{BM}

Crystallographic Data Complex 1

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

Identification code	Complex 1
Empirical formula	C39 H31 Cl Cr N3
Formula weight	629.12
Temperature	210(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 8.594(10) A alpha = 90 deg. b = 15.904(19) A beta = 99.04(2) deg. c = 23.14(3) A gamma = 90 deg.
Volume	3124(6) A^3
Z, Calculated density	4, 1.338 Mg/m^3
Absorption coefficient	0.485 mm^-1
F(000)	1308
Crystal size	0.30 x 0.20 x 0.10 mm
Theta range for data collection	1.56 to 24.71 deg.
Limiting indices	-10<=h<=10, -18<=k<=18, -27<=l<=27
Reflections collected / unique	19111 / 5317 [R(int) = 0.1052]
Completeness to theta = 24.71	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9531 and 0.8682
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5317 / 0 / 398
Goodness-of-fit on F^2	1.054
Final R indices [I>2sigma(I)]	R1 = 0.0592, wR2 = 0.1055
R indices (all data)	R1 = 0.1352, wR2 = 0.1233
Largest diff. peak and hole	0.266 and -0.470 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Complex 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cr(1)	4583(1)	-300(1)	7546(1)	29(1)
Cl	2477(1)	-1077(1)	7223(1)	53(1)
N(1)	6104(4)	-771(2)	7087(1)	30(1)
N(2)	6108(3)	804(2)	7737(1)	23(1)
N(3)	5260(4)	-696(2)	8358(1)	32(1)
C(1)	6778(5)	-1558(3)	7132(2)	39(1)
C(2)	8101(5)	-1551(3)	6868(2)	45(1)
C(3)	8272(5)	-727(3)	6648(2)	38(1)
C(4)	7041(5)	-265(3)	6785(2)	28(1)
C(5)	6463(4)	639(3)	6641(2)	25(1)
C(6)	5517(4)	879(2)	7131(2)	23(1)
C(7)	3898(4)	1048(2)	7095(2)	26(1)
C(8)	3503(4)	1085(2)	7666(2)	25(1)
C(9)	4863(4)	938(2)	8069(2)	23(1)
C(10)	7788(4)	675(3)	7983(2)	28(1)
C(11)	5033(4)	771(2)	8731(2)	26(1)
C(12)	5684(4)	-127(2)	8821(2)	26(1)
C(13)	6476(5)	-549(3)	9294(2)	33(1)
C(14)	6549(5)	-1402(3)	9131(2)	40(1)
C(15)	5800(5)	-1470(3)	8558(2)	38(1)
C(16)	5013(5)	1424(3)	5745(2)	35(1)
C(17)	3900(5)	1462(3)	5235(2)	40(1)
C(18)	3016(5)	783(3)	5036(2)	44(1)
C(19)	3243(5)	34(3)	5347(2)	44(1)
C(20)	4368(5)	-24(3)	5848(2)	36(1)
C(21)	5263(4)	672(3)	6056(2)	27(1)
C(22)	8017(5)	2001(3)	6913(2)	36(1)
C(23)	9244(5)	2554(3)	6848(2)	47(1)
C(24)	10280(6)	2366(3)	6474(2)	52(1)
C(25)	10093(5)	1633(3)	6147(2)	50(1)
C(26)	8871(5)	1087(3)	6198(2)	37(1)
C(27)	7832(4)	1258(3)	6599(2)	26(1)
C(28)	6361(4)	1377(3)	9706(2)	31(1)
C(29)	7254(5)	1982(3)	10040(2)	39(1)
C(30)	7846(5)	2660(3)	9769(2)	40(1)
C(31)	7519(5)	2749(3)	9169(2)	36(1)
C(32)	6641(5)	2143(2)	8835(2)	29(1)
C(33)	6074(4)	1442(3)	9090(2)	25(1)
C(34)	2487(5)	86(3)	8977(2)	37(1)
C(35)	1019(5)	140(3)	9168(2)	46(1)
C(36)	419(5)	898(4)	9298(2)	49(1)
C(37)	1257(5)	1623(4)	9227(2)	50(1)
C(38)	2714(5)	1578(3)	9032(2)	40(1)
C(39)	3364(4)	807(3)	8915(2)	27(1)

Table S3. Bond lengths [A] and angles [deg] for Complex 1.

Cr(1)-N(1)	1.958(4)
Cr(1)-N(3)	1.981(4)
Cr(1)-N(2)	2.194(4)
Cr(1)-Cl	2.221(2)
Cr(1)-C(9)	2.304(4)
Cr(1)-C(6)	2.308(4)
Cr(1)-C(7)	2.417(4)
Cr(1)-C(8)	2.424(5)
N(1)-C(1)	1.376(5)
N(1)-C(4)	1.401(5)
N(2)-C(6)	1.421(5)
N(2)-C(9)	1.427(5)
N(2)-C(10)	1.481(5)
N(3)-C(15)	1.372(5)
N(3)-C(12)	1.406(5)
C(1)-C(2)	1.373(6)
C(2)-C(3)	1.422(6)
C(3)-C(4)	1.365(5)
C(4)-C(5)	1.541(6)
C(5)-C(6)	1.544(5)
C(5)-C(27)	1.549(5)
C(5)-C(21)	1.568(5)
C(6)-C(7)	1.406(5)
C(7)-C(8)	1.418(5)
C(8)-C(9)	1.394(5)
C(9)-C(11)	1.540(5)
C(11)-C(12)	1.536(5)
C(11)-C(33)	1.547(5)
C(11)-C(39)	1.561(5)
C(12)-C(13)	1.371(5)
C(13)-C(14)	1.412(6)
C(14)-C(15)	1.384(6)
C(16)-C(21)	1.394(5)
C(16)-C(17)	1.399(6)
C(17)-C(18)	1.358(6)
C(18)-C(19)	1.391(6)
C(19)-C(20)	1.390(6)
C(20)-C(21)	1.391(5)
C(22)-C(27)	1.383(6)
C(22)-C(23)	1.399(6)
C(23)-C(24)	1.369(6)
C(24)-C(25)	1.385(7)
C(25)-C(26)	1.382(6)
C(26)-C(27)	1.413(6)
C(28)-C(29)	1.388(6)
C(28)-C(33)	1.410(5)
C(29)-C(30)	1.385(6)
C(30)-C(31)	1.381(6)
C(31)-C(32)	1.382(5)
C(32)-C(33)	1.385(5)
C(34)-C(39)	1.392(6)
C(34)-C(35)	1.403(6)

C(35)-C(36)	1.362(6)
C(36)-C(37)	1.384(7)
C(37)-C(38)	1.397(6)
C(38)-C(39)	1.391(6)
N(1)-Cr(1)-N(3)	105.74(15)
N(1)-Cr(1)-N(2)	89.28(15)
N(3)-Cr(1)-N(2)	89.15(13)
N(1)-Cr(1)-Cl	100.55(13)
N(3)-Cr(1)-Cl	104.16(11)
N(2)-Cr(1)-Cl	160.42(9)
N(1)-Cr(1)-C(9)	126.04(15)
N(3)-Cr(1)-C(9)	77.42(16)
N(2)-Cr(1)-C(9)	36.88(12)
Cl-Cr(1)-C(9)	131.62(11)
N(1)-Cr(1)-C(6)	77.28(16)
N(3)-Cr(1)-C(6)	125.69(14)
N(2)-Cr(1)-C(6)	36.69(12)
Cl-Cr(1)-C(6)	129.08(11)
C(9)-Cr(1)-C(6)	60.64(15)
N(1)-Cr(1)-C(7)	104.09(15)
N(3)-Cr(1)-C(7)	134.98(14)
N(2)-Cr(1)-C(7)	58.28(14)
Cl-Cr(1)-C(7)	102.61(12)
C(9)-Cr(1)-C(7)	57.77(15)
C(6)-Cr(1)-C(7)	34.53(13)
N(1)-Cr(1)-C(8)	135.29(14)
N(3)-Cr(1)-C(8)	103.88(14)
N(2)-Cr(1)-C(8)	58.43(14)
Cl-Cr(1)-C(8)	103.77(12)
C(9)-Cr(1)-C(8)	34.18(13)
C(6)-Cr(1)-C(8)	58.25(15)
C(7)-Cr(1)-C(8)	34.07(13)
C(1)-N(1)-C(4)	106.9(3)
C(1)-N(1)-Cr(1)	128.1(3)
C(4)-N(1)-Cr(1)	122.4(3)
C(6)-N(2)-C(9)	109.7(3)
C(6)-N(2)-C(10)	124.5(3)
C(9)-N(2)-C(10)	125.6(3)
C(6)-N(2)-Cr(1)	76.0(2)
C(9)-N(2)-Cr(1)	75.8(2)
C(10)-N(2)-Cr(1)	118.8(2)
C(15)-N(3)-C(12)	106.7(3)
C(15)-N(3)-Cr(1)	129.7(3)
C(12)-N(3)-Cr(1)	121.4(3)
C(2)-C(1)-N(1)	109.1(4)
C(1)-C(2)-C(3)	107.8(4)
C(4)-C(3)-C(2)	106.6(4)
C(3)-C(4)-N(1)	109.5(4)
C(3)-C(4)-C(5)	133.3(4)
N(1)-C(4)-C(5)	117.0(3)
C(4)-C(5)-C(6)	105.1(3)
C(4)-C(5)-C(27)	112.6(3)
C(6)-C(5)-C(27)	112.4(3)
C(4)-C(5)-C(21)	111.4(3)
C(6)-C(5)-C(21)	105.9(3)
C(27)-C(5)-C(21)	109.2(3)

C(7)-C(6)-N(2)	105.7(3)
C(7)-C(6)-C(5)	129.4(3)
N(2)-C(6)-C(5)	123.9(3)
C(7)-C(6)-Cr(1)	77.0(2)
N(2)-C(6)-Cr(1)	67.31(19)
C(5)-C(6)-Cr(1)	111.3(2)
C(6)-C(7)-C(8)	109.4(3)
C(6)-C(7)-Cr(1)	68.5(2)
C(8)-C(7)-Cr(1)	73.3(2)
C(9)-C(8)-C(7)	108.5(3)
C(9)-C(8)-Cr(1)	68.2(2)
C(7)-C(8)-Cr(1)	72.7(2)
C(8)-C(9)-N(2)	106.7(3)
C(8)-C(9)-C(11)	129.2(3)
N(2)-C(9)-C(11)	123.2(3)
C(8)-C(9)-Cr(1)	77.6(2)
N(2)-C(9)-Cr(1)	67.36(19)
C(11)-C(9)-Cr(1)	111.2(3)
C(12)-C(11)-C(9)	105.7(3)
C(12)-C(11)-C(33)	113.6(3)
C(9)-C(11)-C(33)	111.9(3)
C(12)-C(11)-C(39)	109.2(3)
C(9)-C(11)-C(39)	108.5(3)
C(33)-C(11)-C(39)	107.8(3)
C(13)-C(12)-N(3)	109.3(4)
C(13)-C(12)-C(11)	133.5(4)
N(3)-C(12)-C(11)	116.7(3)
C(12)-C(13)-C(14)	107.2(4)
C(15)-C(14)-C(13)	107.3(4)
N(3)-C(15)-C(14)	109.6(4)
C(21)-C(16)-C(17)	120.1(4)
C(18)-C(17)-C(16)	121.7(4)
C(17)-C(18)-C(19)	118.6(4)
C(20)-C(19)-C(18)	120.7(4)
C(19)-C(20)-C(21)	120.7(4)
C(20)-C(21)-C(16)	118.2(4)
C(20)-C(21)-C(5)	121.6(4)
C(16)-C(21)-C(5)	120.1(4)
C(27)-C(22)-C(23)	120.4(4)
C(24)-C(23)-C(22)	120.5(5)
C(23)-C(24)-C(25)	119.8(5)
C(26)-C(25)-C(24)	120.5(4)
C(25)-C(26)-C(27)	120.1(4)
C(22)-C(27)-C(26)	118.5(4)
C(22)-C(27)-C(5)	122.5(4)
C(26)-C(27)-C(5)	118.9(4)
C(29)-C(28)-C(33)	120.4(4)
C(30)-C(29)-C(28)	119.8(4)
C(31)-C(30)-C(29)	120.3(4)
C(30)-C(31)-C(32)	119.8(4)
C(31)-C(32)-C(33)	121.4(4)
C(32)-C(33)-C(28)	118.1(4)
C(32)-C(33)-C(11)	122.5(4)
C(28)-C(33)-C(11)	119.1(4)
C(39)-C(34)-C(35)	120.6(4)
C(36)-C(35)-C(34)	120.9(5)
C(35)-C(36)-C(37)	119.3(5)

C(36)-C(37)-C(38)	120.3(5)
C(39)-C(38)-C(37)	121.0(4)
C(38)-C(39)-C(34)	117.8(4)
C(38)-C(39)-C(11)	120.0(4)
C(34)-C(39)-C(11)	122.2(4)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for Complex 1. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cr(1)	31(1)	28(1)	28(1)	-1(1)	4(1)	-2(1)
Cl	45(1)	57(1)	55(1)	-5(1)	2(1)	-20(1)
N(1)	36(2)	24(2)	32(2)	0(2)	7(2)	5(2)
N(2)	26(2)	24(2)	20(2)	-1(2)	6(2)	0(2)
N(3)	36(2)	26(2)	32(2)	-1(2)	4(2)	2(2)
C(1)	49(3)	29(3)	38(3)	3(2)	7(2)	7(2)
C(2)	55(3)	33(3)	47(3)	-7(3)	0(3)	19(3)
C(3)	28(2)	48(3)	38(3)	-2(2)	9(2)	9(2)
C(4)	30(2)	30(3)	23(2)	-4(2)	0(2)	0(2)
C(5)	25(2)	26(2)	24(2)	-1(2)	5(2)	1(2)
C(6)	29(2)	16(2)	23(2)	3(2)	3(2)	-5(2)
C(7)	27(2)	24(3)	25(2)	6(2)	-3(2)	0(2)
C(8)	26(2)	23(2)	27(2)	-1(2)	7(2)	6(2)
C(9)	28(2)	20(2)	20(2)	0(2)	5(2)	2(2)
C(10)	19(2)	37(3)	26(2)	0(2)	-2(2)	3(2)
C(11)	27(2)	27(3)	23(2)	-1(2)	5(2)	6(2)
C(12)	23(2)	27(3)	27(2)	-2(2)	7(2)	1(2)
C(13)	38(3)	36(3)	23(2)	4(2)	0(2)	3(2)
C(14)	51(3)	34(3)	37(3)	14(2)	8(2)	14(2)
C(15)	50(3)	23(3)	42(3)	4(2)	12(2)	5(2)
C(16)	44(3)	29(3)	31(3)	-4(2)	4(2)	2(2)
C(17)	53(3)	37(3)	27(3)	5(2)	4(2)	7(3)
C(18)	43(3)	57(4)	27(3)	-4(3)	-9(2)	0(3)
C(19)	51(3)	43(3)	34(3)	-8(2)	-7(2)	-12(2)
C(20)	46(3)	28(3)	32(3)	-5(2)	1(2)	-4(2)
C(21)	27(2)	33(3)	22(2)	-4(2)	7(2)	2(2)
C(22)	41(3)	39(3)	31(3)	-3(2)	9(2)	-6(2)
C(23)	48(3)	53(3)	41(3)	0(3)	8(3)	-21(3)
C(24)	42(3)	64(4)	48(3)	7(3)	3(3)	-18(3)
C(25)	35(3)	80(4)	36(3)	13(3)	11(2)	6(3)
C(26)	36(3)	43(3)	33(3)	4(2)	8(2)	1(2)
C(27)	25(2)	32(3)	21(2)	5(2)	3(2)	2(2)
C(28)	33(2)	33(3)	29(3)	2(2)	10(2)	8(2)
C(29)	44(3)	43(3)	26(3)	-9(2)	-2(2)	15(2)
C(30)	44(3)	32(3)	42(3)	-11(2)	-5(2)	2(2)
C(31)	43(3)	23(3)	41(3)	-2(2)	3(2)	5(2)
C(32)	34(3)	29(3)	24(2)	-2(2)	3(2)	5(2)
C(33)	26(2)	28(3)	22(2)	-4(2)	5(2)	6(2)
C(34)	36(3)	41(3)	35(3)	5(2)	11(2)	5(2)
C(35)	32(3)	59(4)	45(3)	10(3)	5(2)	-5(3)
C(36)	28(3)	87(5)	32(3)	5(3)	5(2)	11(3)
C(37)	37(3)	65(4)	47(3)	-7(3)	9(2)	14(3)
C(38)	33(3)	47(3)	41(3)	-2(2)	8(2)	3(2)
C(39)	28(2)	36(3)	17(2)	3(2)	4(2)	5(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Complex 1.

	x	y	z	U(eq)
H(1)	6394	-2026	7314	46
H(2)	8774	-2009	6837	55
H(3)	9076	-536	6448	45
H(7)	3189	1124	6746	32
H(8)	2495	1192	7759	30
H(10A)	8293	1216	8069	42
H(10B)	8307	377	7701	42
H(10C)	7865	347	8340	42
H(13)	6893	-315	9658	39
H(14)	7020	-1842	9368	48
H(15)	5680	-1971	8340	45
H(16)	5593	1906	5879	42
H(17)	3760	1969	5025	47
H(18)	2267	819	4694	53
H(19)	2628	-439	5218	53
H(20)	4526	-539	6047	43
H(22)	7314	2136	7172	44
H(23)	9359	3057	7063	57
H(24)	11116	2734	6438	63
H(25)	10802	1506	5889	60
H(26)	8730	601	5964	44
H(28)	5945	921	9890	38
H(29)	7456	1931	10450	46
H(30)	8474	3062	9994	48
H(31)	7892	3220	8987	43
H(32)	6423	2208	8427	35
H(34)	2882	-442	8890	44
H(35)	441	-353	9206	55
H(36)	-555	927	9433	58
H(37)	845	2149	9311	60
H(38)	3263	2077	8980	48

Crystallographic Data Complex 2b

Table S6. Crystal data and structure refinement for Complex 2b.

Identification code	Complex 2b
Empirical formula	C54.50 H52 Cr N5 O1.38
Formula weight	851.01
Temperature	211(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Cmc2(1)
Unit cell dimensions	a = 18.080(4) A alpha = 90 deg. b = 17.140(4) A beta = 90 deg. c = 16.732(4) A gamma = 90 deg.
Volume	5185(2) A^3
Z, Calculated density	4, 1.090 Mg/m^3
Absorption coefficient	0.261 mm^-1
F(000)	1796
Crystal size	0.30 x 0.25 x 0.20 mm
Theta range for data collection	1.64 to 23.26 deg.
Limiting indices	-19<=h<=20, -18<=k<=18, -18<=l<=18
Reflections collected / unique	15278 / 3802 [R(int) = 0.0916]
Completeness to theta = 23.26	99.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9497 and 0.9258
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3802 / 1 / 253
Goodness-of-fit on F^2	1.012
Final R indices [I>2sigma(I)]	R1 = 0.0518, wR2 = 0.1185
R indices (all data)	R1 = 0.0583, wR2 = 0.1223
Absolute structure parameter	0.09(3)
Largest diff. peak and hole	0.225 and -0.257 e.A^-3

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Complex 2b. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cr(1)	10000	8994(1)	5753(1)	27(1)
N(1)	10000	10668(2)	6177(2)	27(1)
N(2)	9160(2)	9223(2)	6582(2)	30(1)
N(3)	9185(2)	8464(2)	4983(2)	35(1)
C(1)	10000	10804(3)	7046(3)	36(1)
C(2)	9606(2)	10457(2)	4937(2)	27(1)
C(3)	9373(2)	10579(2)	5696(2)	29(1)
C(4)	8607(2)	10476(2)	6082(2)	29(1)
C(5)	8661(2)	11959(2)	6313(2)	41(1)
C(6)	8352(2)	12660(2)	6568(2)	50(1)
C(7)	7657(3)	12657(3)	6916(3)	55(1)
C(8)	7278(2)	11967(3)	7006(2)	51(1)
C(9)	7585(2)	11275(2)	6741(2)	41(1)
C(10)	8293(2)	11247(2)	6404(2)	32(1)
C(11)	7864(2)	10678(2)	4802(2)	35(1)
C(12)	7337(2)	10464(2)	4236(2)	41(1)
C(13)	6978(2)	9749(3)	4317(3)	52(1)
C(14)	7152(2)	9260(2)	4955(3)	51(1)
C(15)	7681(2)	9485(2)	5499(2)	41(1)
C(16)	8049(2)	10198(2)	5436(2)	29(1)
C(17)	8699(2)	9844(2)	6723(2)	28(1)
C(18)	8369(2)	9751(2)	7457(2)	36(1)
C(19)	8625(2)	9059(2)	7790(2)	38(1)
C(20)	9094(2)	8756(2)	7247(2)	35(1)
C(21)	9041(2)	8641(2)	4220(2)	38(1)
C(22)	8519(2)	8258(2)	3763(2)	48(1)
C(23)	8124(3)	7661(3)	4096(3)	54(1)
C(24)	8266(2)	7471(3)	4882(3)	55(1)
C(25)	8790(2)	7875(2)	5304(2)	44(1)

Table S8. Bond lengths [A] and angles [deg] for Complex 2b.

Cr(1)-N(2)#1	2.093(3)
Cr(1)-N(2)	2.093(3)
Cr(1)-N(3)	2.158(3)
Cr(1)-N(3)#1	2.158(3)
N(1)-C(3)	1.399(4)
N(1)-C(3)#1	1.399(4)
N(1)-C(1)	1.473(6)
N(2)-C(20)	1.375(5)
N(2)-C(17)	1.373(4)
N(3)-C(21)	1.338(5)
N(3)-C(25)	1.348(5)
C(2)-C(3)	1.354(5)
C(2)-C(2)#1	1.423(7)
C(3)-C(4)	1.539(5)
C(4)-C(17)	1.534(5)
C(4)-C(10)	1.536(5)
C(4)-C(16)	1.553(5)
C(5)-C(6)	1.393(5)
C(5)-C(10)	1.397(5)
C(6)-C(7)	1.385(6)
C(7)-C(8)	1.375(6)
C(8)-C(9)	1.382(6)
C(9)-C(10)	1.401(5)
C(11)-C(16)	1.384(5)
C(11)-C(12)	1.392(5)
C(12)-C(13)	1.393(6)
C(13)-C(14)	1.393(6)
C(14)-C(15)	1.376(5)
C(15)-C(16)	1.396(5)
C(17)-C(18)	1.374(5)
C(18)-C(19)	1.390(5)
C(19)-C(20)	1.347(6)
C(21)-C(22)	1.381(6)
C(22)-C(23)	1.367(6)
C(23)-C(24)	1.378(6)
C(24)-C(25)	1.370(6)
N(2)#1-Cr(1)-N(2)	92.97(15)
N(2)#1-Cr(1)-N(3)	165.85(11)
N(2)-Cr(1)-N(3)	88.80(11)
N(2)#1-Cr(1)-N(3)#1	88.80(11)
N(2)-Cr(1)-N(3)#1	165.85(11)
N(3)-Cr(1)-N(3)#1	86.15(16)
C(3)-N(1)-C(3)#1	108.2(4)
C(3)-N(1)-C(1)	125.88(19)
C(3)#1-N(1)-C(1)	125.88(19)
C(20)-N(2)-C(17)	105.0(3)
C(20)-N(2)-Cr(1)	119.4(2)
C(17)-N(2)-Cr(1)	134.4(2)
C(21)-N(3)-C(25)	116.6(3)
C(21)-N(3)-Cr(1)	127.3(3)
C(25)-N(3)-Cr(1)	116.1(2)
C(3)-C(2)-C(2)#1	108.1(2)

C(2)-C(3)-N(1)	107.8(3)
C(2)-C(3)-C(4)	131.0(3)
N(1)-C(3)-C(4)	120.0(3)
C(3)-C(4)-C(17)	106.1(3)
C(3)-C(4)-C(10)	112.4(3)
C(17)-C(4)-C(10)	113.7(3)
C(3)-C(4)-C(16)	109.2(3)
C(17)-C(4)-C(16)	109.9(3)
C(10)-C(4)-C(16)	105.6(3)
C(6)-C(5)-C(10)	121.9(4)
C(7)-C(6)-C(5)	119.3(4)
C(8)-C(7)-C(6)	120.2(4)
C(7)-C(8)-C(9)	120.2(4)
C(8)-C(9)-C(10)	121.6(4)
C(9)-C(10)-C(5)	116.8(3)
C(9)-C(10)-C(4)	120.5(3)
C(5)-C(10)-C(4)	122.5(3)
C(16)-C(11)-C(12)	122.0(3)
C(13)-C(12)-C(11)	119.0(4)
C(12)-C(13)-C(14)	119.9(4)
C(15)-C(14)-C(13)	119.7(4)
C(14)-C(15)-C(16)	121.7(4)
C(11)-C(16)-C(15)	117.7(3)
C(11)-C(16)-C(4)	120.5(3)
C(15)-C(16)-C(4)	121.7(3)
N(2)-C(17)-C(18)	109.1(3)
N(2)-C(17)-C(4)	119.5(3)
C(18)-C(17)-C(4)	131.3(3)
C(17)-C(18)-C(19)	108.2(3)
C(20)-C(19)-C(18)	105.6(3)
C(19)-C(20)-N(2)	112.1(3)
N(3)-C(21)-C(22)	123.6(4)
C(21)-C(22)-C(23)	119.1(4)
C(22)-C(23)-C(24)	118.0(4)
C(25)-C(24)-C(23)	120.1(4)
N(3)-C(25)-C(24)	122.6(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y,z

Table S9. Anisotropic displacement parameters (A^2 x 10^3) for Complex 2b. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cr(1)	28(1)	30(1)	23(1)	-4(1)	0	0
N(1)	27(2)	30(2)	23(2)	-5(2)	0	0
N(2)	28(2)	34(2)	26(2)	-4(1)	0(1)	-1(1)
N(3)	40(2)	35(2)	29(2)	-6(1)	0(1)	-5(1)
C(1)	33(3)	41(3)	35(3)	4(2)	0	0
C(2)	30(2)	29(2)	23(2)	2(2)	-3(2)	-3(1)
C(3)	31(2)	25(2)	29(2)	3(2)	-4(2)	2(1)
C(4)	23(2)	34(2)	31(2)	0(2)	5(1)	1(2)
C(5)	41(2)	37(2)	44(2)	2(2)	-2(2)	10(2)
C(6)	63(3)	31(2)	57(3)	-4(2)	-7(2)	10(2)
C(7)	63(3)	52(3)	49(3)	-7(2)	-13(2)	32(2)
C(8)	35(2)	76(3)	40(2)	-4(2)	2(2)	27(2)
C(9)	36(2)	53(2)	34(2)	-3(2)	-3(2)	6(2)
C(10)	29(2)	40(2)	26(2)	-2(2)	-4(2)	7(2)
C(11)	26(2)	40(2)	38(2)	-5(2)	2(2)	4(2)
C(12)	29(2)	53(3)	40(2)	-1(2)	-3(2)	5(2)
C(13)	31(2)	75(3)	48(3)	-19(2)	-10(2)	0(2)
C(14)	48(3)	47(2)	57(3)	5(2)	-4(2)	-9(2)
C(15)	28(2)	52(2)	42(3)	4(2)	-3(2)	-5(2)
C(16)	26(2)	35(2)	27(2)	-3(1)	5(1)	5(2)
C(17)	27(2)	35(2)	21(2)	-2(2)	-1(2)	-3(2)
C(18)	30(2)	41(2)	35(2)	-7(2)	7(2)	-4(2)
C(19)	41(2)	44(2)	29(2)	6(2)	5(2)	-1(2)
C(20)	35(2)	33(2)	38(2)	7(2)	4(2)	-1(2)
C(21)	47(2)	41(2)	27(2)	-1(2)	0(2)	-3(2)
C(22)	57(2)	55(3)	33(2)	-2(2)	-13(2)	-7(2)
C(23)	62(3)	53(3)	48(3)	-7(2)	-14(2)	-19(2)
C(24)	63(3)	49(3)	53(3)	-2(2)	4(2)	-24(2)
C(25)	52(2)	44(2)	35(2)	5(2)	-3(2)	-12(2)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Complex 2b.

	x	y	z	U(eq)
H(1A)	10506	10844	7236	54
H(1B)	9755	10372	7313	54
H(1C)	9739	11285	7163	54
H(2)	9301	10385	4488	33
H(5A)	9131	11964	6071	49
H(6A)	8613	13131	6506	60
H(7A)	7444	13127	7090	66
H(8A)	6809	11966	7248	61
H(9A)	7311	10811	6789	49
H(11A)	8100	11164	4752	42
H(12A)	7226	10796	3805	49
H(13A)	6619	9597	3941	62
H(14A)	6909	8778	5013	61
H(15A)	7797	9149	5926	49
H(18A)	8028	10096	7692	43
H(19A)	8498	8848	8290	46
H(20A)	9346	8281	7315	42
H(21A)	9310	9050	3983	46
H(22A)	8437	8406	3229	58
H(23A)	7767	7389	3799	65
H(24A)	8003	7063	5127	66
H(25A)	8877	7736	5840	53

Crystallographic Data Complex 3

Table S11. Crystal data and structure refinement for Complex 3.

Identification code	Complex 3
Empirical formula	C51 H55 Cl Cr Li N3 O3
Formula weight	852.37
Temperature	211(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pnma
Unit cell dimensions	a = 18.88(10) A alpha = 90 deg. b = 22.13(12) A beta = 90 deg. c = 11.15(6) A gamma = 90 deg.
Volume	4658(44) A^3
Z, Calculated density	4, 1.215 Mg/m^3
Absorption coefficient	0.347 mm^-1
F(000)	1800
Crystal size	0.35 x 0.10 x 0.10 mm
Theta range for data collection	1.84 to 23.25 deg.
Limiting indices	-14<=h<=20, -24<=k<=19, -12<=l<=12
Reflections collected / unique	16401 / 3428 [R(int) = 0.0946]
Completeness to theta = 23.25	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9662 and 0.8883
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3428 / 123 / 347
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0633, wR2 = 0.1279
R indices (all data)	R1 = 0.1026, wR2 = 0.1428
Largest diff. peak and hole	0.286 and -0.367 e.A^-3

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Complex 3. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cr(1)	3647(1)	2500	1058(1)	31(1)
Cl(1)	3281(1)	2500	3081(1)	43(1)
N(1)	3652(2)	2500	-950(3)	26(1)
N(2)	3897(2)	3402(1)	984(2)	33(1)
C(1)	4417(3)	2500	-1274(5)	35(1)
C(2)	2533(2)	2824(2)	-1244(3)	30(1)
C(3)	3206(2)	3024(2)	-1105(3)	25(1)
C(4)	3503(2)	3671(2)	-1131(3)	28(1)
C(5)	4536(2)	4101(2)	-2407(4)	53(1)
C(6)	4890(3)	4172(2)	-3497(4)	73(2)
C(7)	4654(3)	3891(2)	-4527(4)	61(1)
C(8)	4060(3)	3531(2)	-4451(4)	55(1)
C(9)	3705(2)	3463(2)	-3375(3)	43(1)
C(10)	3931(2)	3745(2)	-2312(3)	30(1)
C(11)	2648(2)	4458(2)	-2117(4)	43(1)
C(12)	2073(2)	4859(2)	-2050(5)	54(1)
C(13)	1690(2)	4905(2)	-1013(5)	54(1)
C(14)	1876(2)	4563(2)	-17(4)	51(1)
C(15)	2453(2)	4172(2)	-75(4)	42(1)
C(16)	2852(2)	4114(2)	-1127(3)	31(1)
C(17)	3921(2)	3807(2)	29(3)	30(1)
C(18)	4249(2)	4336(2)	385(3)	36(1)
C(19)	4448(2)	4265(2)	1603(4)	40(1)
C(20)	4232(2)	3701(2)	1927(3)	39(1)
Li(1)	2121(6)	2500	3878(10)	56(3)
O(1)	1448(3)	2520(20)	2588(6)	95(3)
C(21)	1592(6)	2732(10)	1432(10)	154(12)
C(22)	958(6)	2687(12)	718(11)	144(10)
C(23)	424(5)	2430(30)	1458(9)	105(8)
C(24)	712(5)	2594(12)	2662(10)	125(7)
O(2)	2006(12)	3215(14)	4880(20)	61(5)
C(25)	2226(5)	3788(5)	4362(9)	58(3)
C(26)	1549(9)	4158(7)	4192(11)	76(4)
C(27)	1139(13)	3938(12)	5255(17)	77(4)
C(28)	1520(8)	3397(7)	5757(11)	64(3)
O(2')	1860(30)	3220(30)	4570(50)	88(16)
C(25')	1972(15)	3741(13)	3810(20)	78(7)
C(26')	1660(20)	4229(18)	4700(30)	82(7)
C(27')	1120(30)	3980(20)	5570(40)	78(7)
C(28')	1296(19)	3290(17)	5400(30)	84(8)

Table S13. Bond lengths [A] and angles [deg] for Complex 3.

Cr(1)-N(2)	2.053(11)
Cr(1)-N(2)#1	2.053(11)
Cr(1)-N(1)	2.239(13)
Cr(1)-Cl(1)	2.359(12)
Cl(1)-Li(1)	2.363(15)
N(1)-C(3)	1.443(7)
N(1)-C(3)#1	1.443(7)
N(1)-C(1)	1.488(10)
N(2)-C(17)	1.393(7)
N(2)-C(20)	1.394(7)
C(2)-C(3)	1.354(8)
C(2)-C(2)#1	1.434(10)
C(3)-C(4)	1.538(9)
C(4)-C(17)	1.545(8)
C(4)-C(10)	1.553(8)
C(4)-C(16)	1.572(8)
C(5)-C(6)	1.396(8)
C(5)-C(10)	1.392(8)
C(6)-C(7)	1.380(8)
C(7)-C(8)	1.376(8)
C(8)-C(9)	1.383(8)
C(9)-C(10)	1.406(8)
C(11)-C(16)	1.396(7)
C(11)-C(12)	1.403(8)
C(12)-C(13)	1.367(8)
C(13)-C(14)	1.388(8)
C(14)-C(15)	1.392(8)
C(15)-C(16)	1.400(8)
C(17)-C(18)	1.383(7)
C(18)-C(19)	1.418(9)
C(19)-C(20)	1.361(8)
Li(1)-O(2')	1.84(7)
Li(1)-O(2')#1	1.84(7)
Li(1)-O(1)	1.920(15)
Li(1)-O(2)	1.95(3)
Li(1)-O(2)#1	1.95(3)
Li(1)-C(25')	2.76(3)
Li(1)-C(25')#1	2.76(3)
O(1)-C(24)	1.402(14)
O(1)-C(21)	1.396(19)
C(21)-C(22)	1.440(15)
C(22)-C(23)	1.42(3)
C(23)-C(24)	1.492(19)
O(2)-C(28)	1.40(3)
O(2)-C(25)	1.46(3)
C(25)-C(26)	1.53(2)
C(26)-C(27)	1.50(2)
C(27)-C(28)	1.50(3)
O(2')-C(28')	1.42(7)
O(2')-C(25')	1.44(7)
C(25')-C(26')	1.58(5)
C(26')-C(27')	1.51(5)

C(27')-C(28')	1.57(7)
N(2)-Cr(1)-N(2)#1	153.0(3)
N(2)-Cr(1)-N(1)	87.64(9)
N(2)#1-Cr(1)-N(1)	87.64(9)
N(2)-Cr(1)-Cl(1)	96.07(9)
N(2)#1-Cr(1)-Cl(1)	96.07(9)
N(1)-Cr(1)-Cl(1)	163.19(17)
Cr(1)-Cl(1)-Li(1)	129.1(3)
C(3)-N(1)-C(3)#1	106.9(6)
C(3)-N(1)-C(1)	122.4(3)
C(3)#1-N(1)-C(1)	122.4(3)
C(3)-N(1)-Cr(1)	96.8(2)
C(3)#1-N(1)-Cr(1)	96.8(2)
C(1)-N(1)-Cr(1)	104.3(3)
C(17)-N(2)-C(20)	104.8(5)
C(17)-N(2)-Cr(1)	131.6(3)
C(20)-N(2)-Cr(1)	122.4(3)
C(3)-C(2)-C(2)#1	109.1(2)
C(2)-C(3)-N(1)	107.4(5)
C(2)-C(3)-C(4)	130.1(3)
N(1)-C(3)-C(4)	122.6(5)
C(3)-C(4)-C(17)	110.6(3)
C(3)-C(4)-C(10)	107.7(3)
C(17)-C(4)-C(10)	115.1(5)
C(3)-C(4)-C(16)	107.2(5)
C(17)-C(4)-C(16)	105.9(4)
C(10)-C(4)-C(16)	110.1(3)
C(6)-C(5)-C(10)	121.6(4)
C(7)-C(6)-C(5)	121.2(5)
C(8)-C(7)-C(6)	118.3(5)
C(7)-C(8)-C(9)	120.7(4)
C(8)-C(9)-C(10)	122.4(5)
C(5)-C(10)-C(9)	115.8(4)
C(5)-C(10)-C(4)	123.5(4)
C(9)-C(10)-C(4)	120.6(5)
C(16)-C(11)-C(12)	121.1(4)
C(13)-C(12)-C(11)	120.1(5)
C(12)-C(13)-C(14)	120.0(5)
C(13)-C(14)-C(15)	120.0(5)
C(14)-C(15)-C(16)	121.2(4)
C(15)-C(16)-C(11)	117.6(5)
C(15)-C(16)-C(4)	118.8(4)
C(11)-C(16)-C(4)	123.6(4)
C(18)-C(17)-N(2)	109.9(4)
C(18)-C(17)-C(4)	129.4(3)
N(2)-C(17)-C(4)	119.8(4)
C(17)-C(18)-C(19)	107.4(4)
C(20)-C(19)-C(18)	106.1(4)
C(19)-C(20)-N(2)	111.8(4)
O(2')-Li(1)-O(2')#1	121(4)
O(2')-Li(1)-O(1)	97(2)
O(2')#1-Li(1)-O(1)	99.1(19)
O(2')-Li(1)-O(2)	13(2)
O(2')#1-Li(1)-O(2)	115.7(13)
O(1)-Li(1)-O(2)	109.7(15)
O(2')-Li(1)-O(2)#1	115.7(13)

O(2')#1-Li(1)-O(2)#1	13(2)
O(1)-Li(1)-O(2)#1	112.1(14)
O(2)-Li(1)-O(2)#1	108.4(18)
O(2')-Li(1)-Cl(1)	113.8(19)
O(2')#1-Li(1)-Cl(1)	113.8(19)
O(1)-Li(1)-Cl(1)	109.4(6)
O(2)-Li(1)-Cl(1)	108.6(9)
O(2)#1-Li(1)-Cl(1)	108.6(9)
O(2')-Li(1)-C(25')	28(2)
O(2')#1-Li(1)-C(25')	148(2)
O(1)-Li(1)-C(25')	83.6(15)
O(2)-Li(1)-C(25')	36.6(10)
O(2)#1-Li(1)-C(25')	144.1(11)
Cl(1)-Li(1)-C(25')	94.8(6)
O(2')-Li(1)-C(25')#1	148(2)
O(2')#1-Li(1)-C(25')#1	28(2)
O(1)-Li(1)-C(25')#1	86.3(15)
O(2)-Li(1)-C(25')#1	144.1(11)
O(2)#1-Li(1)-C(25')#1	36.6(10)
Cl(1)-Li(1)-C(25')#1	94.8(6)
C(25')-Li(1)-C(25')#1	167.9(13)
C(24)-O(1)-C(21)	102.0(13)
C(24)-O(1)-Li(1)	127.9(9)
C(21)-O(1)-Li(1)	124.8(11)
O(1)-C(21)-C(22)	109.1(11)
C(23)-C(22)-C(21)	107.1(12)
C(22)-C(23)-C(24)	100(2)
O(1)-C(24)-C(23)	106.3(11)
C(28)-O(2)-C(25)	102(2)
C(28)-O(2)-Li(1)	135.1(19)
C(25)-O(2)-Li(1)	116.5(18)
O(2)-C(25)-C(26)	106.2(14)
C(27)-C(26)-C(25)	99.1(13)
C(26)-C(27)-C(28)	107.8(14)
O(2)-C(28)-C(27)	106.6(15)
C(28')-O(2')-C(25')	114(5)
C(28')-O(2')-Li(1)	124(4)
C(25')-O(2')-Li(1)	114(4)
O(2')-C(25')-C(26')	97(3)
O(2')-C(25')-Li(1)	38(3)
C(26')-C(25')-Li(1)	134(2)
C(25')-C(26')-C(27')	114(3)
C(26')-C(27')-C(28')	98(3)
O(2')-C(28')-C(27')	110(4)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z

Table S14. Anisotropic displacement parameters (A^2 x 10^3) for Complex 3.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cr(1)	38(1)	31(1)	25(1)	0	-1(1)	0
Cl(1)	46(1)	51(1)	31(1)	0	6(1)	0
N(1)	28(2)	26(2)	24(2)	0	0(2)	0
N(2)	42(2)	30(2)	26(2)	-4(2)	-1(2)	-1(2)
C(1)	29(3)	37(4)	38(3)	0	-2(3)	0
C(2)	24(2)	29(2)	36(2)	0(2)	-5(2)	5(2)
C(3)	30(2)	24(2)	21(2)	-2(2)	-7(2)	2(2)
C(4)	31(2)	21(2)	33(2)	-2(2)	-2(2)	-2(2)
C(5)	54(3)	63(3)	43(3)	-7(2)	8(2)	-26(3)
C(6)	69(4)	90(4)	60(3)	-6(3)	15(3)	-43(3)
C(7)	68(4)	73(4)	42(3)	-5(3)	20(3)	-15(3)
C(8)	77(4)	55(3)	33(2)	-9(2)	5(2)	-13(3)
C(9)	49(3)	40(3)	40(2)	-1(2)	5(2)	-11(2)
C(10)	39(2)	26(2)	26(2)	1(2)	-2(2)	3(2)
C(11)	49(3)	37(3)	43(3)	4(2)	-10(2)	1(2)
C(12)	50(3)	40(3)	72(3)	1(2)	-21(3)	10(3)
C(13)	41(3)	32(3)	89(4)	-7(3)	-16(3)	8(2)
C(14)	41(3)	45(3)	66(3)	-17(2)	6(2)	-1(2)
C(15)	47(3)	30(2)	50(3)	-3(2)	-4(2)	6(2)
C(16)	33(2)	24(2)	37(2)	-5(2)	-1(2)	0(2)
C(17)	30(2)	29(2)	31(2)	-1(2)	-1(2)	-2(2)
C(18)	39(2)	25(2)	43(2)	-1(2)	1(2)	0(2)
C(19)	48(3)	32(3)	41(2)	-14(2)	-4(2)	-5(2)
C(20)	47(3)	44(3)	27(2)	-2(2)	-4(2)	2(2)
Li(1)	64(7)	38(6)	66(7)	0	18(6)	0
O(1)	47(3)	160(9)	79(4)	44(17)	2(3)	-10(20)
C(21)	88(7)	300(30)	77(8)	70(13)	-9(6)	-80(13)
C(22)	57(6)	250(30)	126(8)	82(13)	-10(6)	-4(10)
C(23)	60(6)	150(20)	100(7)	-28(15)	5(5)	-18(14)
C(24)	72(7)	195(18)	109(7)	-92(12)	-7(6)	62(13)
O(2)	62(4)	44(7)	78(12)	-2(7)	23(6)	7(4)
C(25)	59(6)	35(5)	82(7)	-6(5)	14(5)	-3(5)
C(26)	82(7)	47(7)	101(9)	12(7)	21(7)	12(6)
C(27)	72(6)	73(8)	86(11)	-15(7)	23(7)	28(6)
C(28)	82(9)	54(8)	56(6)	-11(5)	9(5)	-9(6)
O(2')	160(40)	26(12)	80(30)	18(16)	70(20)	20(20)
C(25')	84(17)	54(13)	96(17)	7(14)	30(12)	10(13)
C(26')	89(14)	60(11)	98(17)	-9(12)	30(14)	-2(11)
C(27')	96(15)	59(12)	78(16)	-16(13)	27(11)	-4(11)
C(28')	90(19)	61(11)	100(20)	-33(14)	52(15)	-18(13)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Complex 3.

	x	y	z	U(eq)
H(1A)	4619	2894	-1102	52
H(1B)	4468	2412	-2122	52
H(1C)	4662	2194	-809	52
H(2)	2131	3070	-1327	36
H(5A)	4711	4298	-1721	64
H(6A)	5296	4417	-3531	87
H(7A)	4892	3943	-5260	73
H(8A)	3895	3330	-5139	66
H(9A)	3297	3219	-3353	52
H(11A)	2899	4421	-2841	52
H(12A)	1951	5095	-2719	65
H(13A)	1300	5169	-974	65
H(14A)	1613	4596	695	61
H(15A)	2576	3943	603	51
H(18A)	4326	4680	-93	43
H(19A)	4683	4549	2088	48
H(20A)	4300	3534	2694	47
H(21A)	1970	2490	1069	185
H(21B)	1749	3153	1468	185
H(22A)	813	3088	438	173
H(22B)	1042	2430	17	173
H(23A)	388	1994	1352	126
H(23B)	-40	2618	1314	126
H(24A)	593	3013	2863	150
H(24B)	514	2328	3280	150
H(25A)	2462	3723	3590	70
H(25B)	2554	3999	4900	70
H(26A)	1641	4594	4234	92
H(26B)	1311	4062	3435	92
H(27A)	658	3825	5013	92
H(27B)	1107	4256	5863	92
H(28A)	1766	3505	6501	77
H(28B)	1184	3071	5929	77
H(25C)	1704	3716	3061	94
H(25D)	2475	3811	3638	94
H(26C)	1432	4550	4232	99
H(26D)	2047	4411	5156	99
H(27C)	635	4073	5340	93
H(27D)	1209	4112	6397	93
H(28C)	1430	3111	6174	101
H(28D)	876	3077	5104	101