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Supporting information

New Chromium(III)-Complexes as Highly Active Catalysts for Olefin Polymerisation

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Experimental section

All manipulations were carried out under a nitrogen atmosphere with anhydrous solvents saturated with nitrogen. Glassware was heated under vacuum prior to use. Microanalyses: Mikroanalytisches Laboratorium des Organisch-Chemischen Instituts der Universität Heidelberg. MS spectra: Jeol JMS 700. Room temperature magnetic measurements: Sherwood Scientific magnetic susceptibility balance, Mark 1. Paramagnetic ^{1}H-NMR spectra were recorded on a Bruker DRX 200 spectrometer using the following parameters: sweep width = 75 kHz; pulse length = 6.4 μs (90° flip angle); time domain = 327680 data points; 256 repetitions, acquisition rate = 0.42 sec. Assignments of NMR-signals were made by comparison of spectra of different derivatives, comparison with literature data, and to some extent by integration of the signals.

Dichloro-η^5-[1-(8-quinolyl-2,3,4,5-tetramethylcyclopentadienyl]chromium(III) (5)

A solution of 400 mg (1.6 mmol) of [1-(8-quinolyl-2,3,4,5-tetramethylcyclopentadiene in 5 ml of THF is added to a suspension of 65 mg (1.6 mmol) of potassium hydride in 20 ml of THF. The mixtures color turns intensely red violet and a red precipitate forms. After 3 h at room temperature, the reaction mixture is slowly added to a solution of 600 mg $CrCl_3(THF)_3$ in 20 ml of THF. After stirring for 16 h the solvent is evaporated in a vacuum and the residue is extracted with hot toluene. After evaporation of the toluene, the resulting green powder is washed with

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small portions of n-hexane. Yield 410 mg (70%). Mp. >250°C (dec.). ^{1}H NMR (C_6D_6): δ = -56 (CH); -1 (CH_3); -16 (CH); 15 (CH); 21 (CH_3); 51 (CH); one CH-signal in diamagnetic region, signal for CH-group adjacent to the coordinated nitrogen atom is extremely broad and lies at about -100 ppm. Magnetic moment: μ_{eff} (RT) = 3.6(1) μ_B. MS: (EI) m/z (%) = 370 (12, M^+); 334 (19, M^+-Cl); 248 (100, Cp^{*Q}). HR-EI-MS: ($C_{18}H_{18}NCl_2Cr$) 370.02213 (calcd.), 370.02203 (found). Anal. Calcd. for ($C_{18}H_{18}NCl_2Cr$): C 58.2; H 4.9; N 3.8. Found: C 57.8 H 5.1 N 3.8.

Dichloro-η^5-[1-(2-methylquinolin-8-yl-2,3,4,5-tetramethylcyclopentadienyl]chromium(III) (6)

To a solution of 300 mg (1.14 mmol) of 1-(2-methylquinolin-8-yl-2,3,4,5-tetramethylcyclopentadiene in 30 ml of THF were added 0.45 ml of a solution of n-butyllithium (2.5 M in n-hexane). After 2h, the resulting red solution was added to a solution of 420 mg (1.14 mmol) of $CrCl_3(THF)_3$ in 20 ml of THF. After 16 h the resulting green reaction mixture was worked up as described above. Yield 230 mg (53%) of a green powder. ^{1}H NMR (C_6D_6): δ = -76 (Cp-CH_3); -39 (CH), -12 (CH); 4 (CH), 13 (CH); 25 (Cp-CH_3); 48 (CH); 80 (very broad, $\nu_{1/2}$ = 2500 Hz, quinoline-CH_3). MS: (EI) m/z (%) = 384 (54, M^+); 348 (100, M^+-HCl); 263 (62, HCp^{*Qd}). HR-EI-MS: ($C_{19}H_{20}NCl_2Cr$) 384.03778 (calcd.), 384.03775 (found). Anal. Calcd. for ($C_{19}H_{20}NCl_2Cr$): C 59.2; H 5.2; N 3.6. Found: C 58.5 H 5.3 N 3.7.

Dichloro-η^5-[1-(2-N,N-dimethylaminophenyl)-2,3,4,5-tetramethylcyclopentadienyl]chromium(III) (7)

Preparation and work up analogous to **6**. From 400 mg (1.66 mmol) of (2-N,N-dimethylaminophenyl)-2,3,4,5-tetramethylcyclopentadiene, 0.65 ml (1.66 mmol) of n-BuLi (2.5 M in hexane) and 620 mg (1.66 mmol) of $CrCl_3(THF)_3$ the complex **7** was obtained as a blue

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powder. Yield: 470 mg (79%). ^{1}H NMR (C_6D_6): δ = -81 (CH_3); -1 (CH), 1 (CH); 3 (CH), 16 (CH); 27 (CH_3); 41 (CH_3). MS: (EI) m/z (%) = 362 (10, M^+); 326 (100, M^+-HCl); 241 (32, HCp^{*N}). HR-EI-MS: ($C_{17}H_{22}NCl_2Cr$) 362.0534 (calcd.) 362.0506 (found). Anal. Calcd. for($C_{17}H_{22}NCl_2Cr$): C, 56.2; H, 6.1; N, 3.9. Found: C, 55.1; H, 6.3; N, 3.7.

Dichloro-η^5-[1-(8-quinolyl-indenyl]chromium(III) (8)

Preparation and work up analogue to **5**. From 300 mg (1.23 mmol) of 1-(8-quinolyl-indene, 50 mg of KH and 460 mg of $CrCl_3(TH)_3$ the complex **8** was obtained as a green powder. Yield: 166 mg (37%). MS: (EI) m/z (%) = 364 (1, M^+); 329 (1, M^+-Cl); 242 (100, Ind^Q). HR-EI-MS: ($C_{18}H_{12}Cl_2NCr$) 363.97519 (calcd.), 363.97615 (found). Anal. Calcd. for ($C_{18}H_{12}Cl_2NCr$): C, 59.2; H, 3.3; N, 3.8. Found: C, 58.4; H, 3.6, N, 3.8.

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Details of the X-ray structural analysis of compounds 5 and 7

Table 1. Crystal data and structure refinement for 5

Identification code	pf09
Empirical formula	C18 H18 Cl2 Cr N
Formula weight	371.23
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 14.1181(2) Å α= 90°. b = 13.6030(2) Å β= 90°. c = 17.5427(2) Å γ = 90°.
Volume	3369.05(8) Å^3
Z	8
Density (calculated)	1.464 g/cm^3
Absorption coefficient	0.991 mm^{-1}
F(000)	1528
Crystal size	0.24 x 0.23 x 0.04 mm^3
Theta range for data collection	2.32 to 28.29°.
Index ranges	0<=h<=18, 0<=k<=18, 0<=l<=23
Reflections collected	33814
Independent reflections	4154 [R(int) = 0.053]
Completeness to theta = 28.29°	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.928 and 0.827
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4154 / 0 / 271
Goodness-of-fit on F^2	0.956
Final R indices [I>2sigma(I)]	R1 = 0.0305, wR2 = 0.0749
R indices (all data)	R1 = 0.0540, wR2 = 0.0823
Largest diff. peak and hole	0.339 and -0.372 e.Å^{-3}

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for pf09. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cr(1)	865(1)	7281(1)	1570(1)	22(1)
Cl(1)	906(1)	6871(1)	2836(1)	37(1)
Cl(2)	-734(1)	7518(1)	1439(1)	34(1)
N(1)	850(1)	5835(1)	1170(1)	24(1)
C(1)	2003(1)	6402(1)	274(1)	23(1)
C(2)	1433(1)	5625(1)	556(1)	23(1)
C(3)	315(2)	5119(2)	1447(1)	32(1)
C(4)	304(2)	4169(2)	1149(1)	37(1)
C(5)	863(2)	3948(2)	536(1)	34(1)
C(6)	1451(1)	4683(1)	217(1)	26(1)
C(7)	2049(2)	4533(2)	-420(1)	30(1)
C(8)	2596(2)	5280(2)	-692(1)	31(1)
C(9)	2572(2)	6212(2)	-345(1)	29(1)
C(10)	1931(1)	7355(1)	679(1)	23(1)
C(11)	1257(1)	8104(1)	520(1)	23(1)
C(12)	1282(1)	8787(1)	1139(1)	26(1)
C(13)	1980(1)	8472(1)	1667(1)	27(1)
C(14)	2383(1)	7573(1)	1391(1)	24(1)
C(15)	647(2)	8194(2)	-172(1)	29(1)
C(16)	672(2)	9689(2)	1181(1)	36(1)
C(17)	2269(2)	8980(2)	2389(1)	37(1)
C(18)	3126(2)	6959(2)	1770(1)	35(1)

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Table 3. Bond lengths [Å] and angles [°] for pf09.

Cr(1)-N(1)	2.0880(15)
Cr(1)-C(10)	2.1729(17)
Cr(1)-C(14)	2.2019(19)
Cr(1)-C(11)	2.2258(16)
Cr(1)-C(12)	2.2617(18)
Cr(1)-C(13)	2.2655(19)
Cr(1)-Cl(1)	2.2905(5)
Cr(1)-Cl(2)	2.2919(6)
N(1)-C(3)	1.326(2)
N(1)-C(2)	1.386(2)
C(1)-C(9)	1.374(3)
C(1)-C(2)	1.418(2)
C(1)-C(10)	1.482(2)
C(2)-C(6)	1.412(2)
C(3)-C(4)	1.394(3)
C(3)-H(3)	0.93(2)
C(4)-C(5)	1.368(3)
C(4)-H(4)	0.95(2)
C(5)-C(6)	1.415(3)
C(5)-H(5)	0.97(2)
C(6)-C(7)	1.415(3)
C(7)-C(8)	1.362(3)
C(7)-H(7)	0.87(2)
C(8)-C(9)	1.407(3)
C(8)-H(8)	0.98(2)
C(9)-H(9)	0.87(2)
C(10)-C(11)	1.423(3)
C(10)-C(14)	1.434(2)
C(11)-C(12)	1.430(2)
C(11)-C(15)	1.493(2)
C(12)-C(13)	1.419(3)
C(12)-C(16)	1.500(3)
C(13)-C(14)	1.431(3)
C(13)-C(17)	1.500(3)
C(14)-C(18)	1.497(3)
C(15)-H(15A)	0.95(2)
C(15)-H(15B)	0.94(2)
C(15)-H(15C)	0.98(2)
C(16)-H(16A)	1.00(2)
C(16)-H(16B)	1.00(2)
C(16)-H(16C)	0.98(2)
C(17)-H(17A)	0.89(3)
C(17)-H(17B)	0.92(3)
C(17)-H(17C)	0.95(3)
C(18)-H(18A)	0.98(3)
C(18)-H(18B)	0.92(3)
C(18)-H(18C)	0.93(4)
N(1)-Cr(1)-C(10)	78.99(6)
N(1)-Cr(1)-C(14)	97.58(6)
C(10)-Cr(1)-C(14)	38.26(7)
N(1)-Cr(1)-C(11)	101.46(6)
C(10)-Cr(1)-C(11)	37.71(7)
C(14)-Cr(1)-C(11)	63.21(7)
N(1)-Cr(1)-C(12)	138.04(6)
C(10)-Cr(1)-C(12)	62.43(7)
C(14)-Cr(1)-C(12)	62.32(7)
C(11)-Cr(1)-C(12)	37.14(6)
N(1)-Cr(1)-C(13)	134.86(7)
C(10)-Cr(1)-C(13)	62.54(7)
C(14)-Cr(1)-C(13)	37.34(7)
C(11)-Cr(1)-C(13)	61.91(6)
C(12)-Cr(1)-C(13)	36.52(7)
N(1)-Cr(1)-Cl(1)	95.54(4)
C(10)-Cr(1)-Cl(1)	133.74(5)
C(14)-Cr(1)-Cl(1)	99.06(5)
C(11)-Cr(1)-Cl(1)	156.72(5)
C(12)-Cr(1)-Cl(1)	122.54(5)
C(13)-Cr(1)-Cl(1)	94.82(5)
N(1)-Cr(1)-Cl(2)	95.14(5)
C(10)-Cr(1)-Cl(2)	127.14(5)
C(14)-Cr(1)-Cl(2)	156.73(5)
C(11)-Cr(1)-Cl(2)	95.21(5)
C(12)-Cr(1)-Cl(2)	95.45(5)

C(13)-Cr(1)-Cl(2)	126.24(5)	C(10)-C(11)-C(12)	107.47(16)
Cl(1)-Cr(1)-Cl(2)	99.01(2)	C(10)-C(11)-C(15)	127.16(17)
C(3)-N(1)-C(2)	118.15(16)	C(12)-C(11)-C(15)	125.35(18)
C(3)-N(1)-Cr(1)	125.08(13)	C(10)-C(11)-Cr(1)	69.13(9)
C(2)-N(1)-Cr(1)	116.74(12)	C(12)-C(11)-Cr(1)	72.79(10)
C(9)-C(1)-C(2)	117.86(17)	C(15)-C(11)-Cr(1)	124.78(13)
C(9)-C(1)-C(10)	125.64(17)	C(13)-C(12)-C(11)	108.43(16)
C(2)-C(1)-C(10)	116.50(15)	C(13)-C(12)-C(16)	127.90(17)
N(1)-C(2)-C(6)	121.70(17)	C(11)-C(12)-C(16)	123.65(17)
N(1)-C(2)-C(1)	117.02(16)	C(13)-C(12)-Cr(1)	71.89(10)
C(6)-C(2)-C(1)	121.27(16)	C(11)-C(12)-Cr(1)	70.07(10)
N(1)-C(3)-C(4)	123.39(19)	C(16)-C(12)-Cr(1)	125.13(14)
N(1)-C(3)-H(3)	116.7(13)	C(12)-C(13)-C(14)	108.31(16)
C(4)-C(3)-H(3)	119.9(13)	C(12)-C(13)-C(17)	126.89(18)
C(5)-C(4)-C(3)	119.47(19)	C(14)-C(13)-C(17)	124.79(18)
C(5)-C(4)-H(4)	121.5(14)	C(12)-C(13)-Cr(1)	71.59(11)
C(3)-C(4)-H(4)	119.0(14)	C(14)-C(13)-Cr(1)	68.91(10)
C(4)-C(5)-C(6)	119.62(18)	C(17)-C(13)-Cr(1)	125.58(15)
C(4)-C(5)-H(5)	122.5(13)	C(13)-C(14)-C(10)	107.12(16)
C(6)-C(5)-H(5)	117.9(13)	C(13)-C(14)-C(18)	127.20(17)
C(2)-C(6)-C(5)	117.65(18)	C(10)-C(14)-C(18)	125.67(17)
C(2)-C(6)-C(7)	118.30(18)	C(13)-C(14)-Cr(1)	73.74(11)
C(5)-C(6)-C(7)	124.06(18)	C(10)-C(14)-Cr(1)	69.78(10)
C(8)-C(7)-C(6)	120.45(18)	C(18)-C(14)-Cr(1)	121.23(14)
C(8)-C(7)-H(7)	121.5(14)	C(11)-C(15)-H(15A)	111.3(13)
C(6)-C(7)-H(7)	118.0(14)	C(11)-C(15)-H(15B)	109.7(14)
C(7)-C(8)-C(9)	120.46(18)	H(15A)-C(15)-H(15B)	108.8(18)
C(7)-C(8)-H(8)	120.3(11)	C(11)-C(15)-H(15C)	115.4(12)
C(9)-C(8)-H(8)	119.2(11)	H(15A)-C(15)-H(15C)	103.9(18)
C(1)-C(9)-C(8)	121.66(19)	H(15B)-C(15)-H(15C)	107.4(19)
C(1)-C(9)-H(9)	116.8(14)	C(12)-C(16)-H(16A)	113.2(13)
C(8)-C(9)-H(9)	121.4(14)	C(12)-C(16)-H(16B)	108.1(13)
C(11)-C(10)-C(14)	108.65(16)	H(16A)-C(16)-H(16B)	106.6(18)
C(11)-C(10)-C(1)	125.35(16)	C(12)-C(16)-H(16C)	111.9(13)
C(14)-C(10)-C(1)	124.66(16)	H(16A)-C(16)-H(16C)	103.5(18)
C(11)-C(10)-Cr(1)	73.16(10)	H(16B)-C(16)-H(16C)	113.5(18)
C(14)-C(10)-Cr(1)	71.97(10)	C(13)-C(17)-H(17A)	108.0(18)
C(1)-C(10)-Cr(1)	110.58(12)	C(13)-C(17)-H(17B)	111.6(17)

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H(17A)-C(17)-H(17B)	109(3)	C(14)-C(18)-H(18C)	114.6(19)
C(13)-C(17)-H(17C)	110.6(16)	H(18A)-C(18)-H(18C)	109(2)
H(17A)-C(17)-H(17C)	106(3)	H(18B)-C(18)-H(18C)	104(3)
H(17B)-C(17)-H(17C)	111(2)		
C(14)-C(18)-H(18A)	113.5(14)		
C(14)-C(18)-H(18B)	109.0(19)		
H(18A)-C(18)-H(18B)	106(2)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for pf09. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	21(1)	27(1)	17(1)	1(1)	0(1)	1(1)
Cl(1)	44(1)	48(1)	18(1)	4(1)	0(1)	1(1)
Cl(2)	22(1)	48(1)	33(1)	7(1)	2(1)	5(1)
N(1)	23(1)	27(1)	22(1)	2(1)	2(1)	-1(1)
C(1)	22(1)	26(1)	20(1)	1(1)	-2(1)	-1(1)
C(2)	20(1)	29(1)	20(1)	1(1)	-3(1)	0(1)
C(3)	29(1)	34(1)	33(1)	3(1)	7(1)	-6(1)
C(4)	34(1)	30(1)	45(1)	5(1)	4(1)	-10(1)
C(5)	32(1)	26(1)	42(1)	-1(1)	-4(1)	-2(1)
C(6)	24(1)	28(1)	27(1)	-1(1)	-5(1)	1(1)
C(7)	33(1)	30(1)	27(1)	-6(1)	-6(1)	7(1)
C(8)	31(1)	39(1)	23(1)	-2(1)	3(1)	7(1)
C(9)	27(1)	35(1)	26(1)	3(1)	3(1)	-3(1)
C(10)	21(1)	27(1)	21(1)	1(1)	4(1)	-5(1)
C(11)	24(1)	26(1)	21(1)	4(1)	0(1)	-5(1)
C(12)	26(1)	25(1)	26(1)	0(1)	0(1)	-4(1)
C(13)	27(1)	29(1)	26(1)	-1(1)	-2(1)	-4(1)
C(14)	21(1)	28(1)	22(1)	-1(1)	-1(1)	-2(1)
C(15)	32(1)	31(1)	24(1)	5(1)	-4(1)	-5(1)
C(16)	43(1)	24(1)	39(1)	-2(1)	-6(1)	3(1)
C(17)	40(1)	38(1)	33(1)	-10(1)	-9(1)	-1(1)
C(18)	29(1)	39(1)	36(1)	-1(1)	-9(1)	4(1)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for pf09.

	x	y	z	U(eq)
H(3)	-73(15)	5277(14)	1856(12)	31(6)
H(4)	-113(17)	3697(17)	1364(13)	43(6)
H(5)	875(15)	3303(16)	306(12)	36(6)
H(7)	2047(15)	3957(15)	-635(11)	30(6)
H(8)	3008(15)	5175(13)	-1131(11)	25(5)
H(9)	2953(17)	6680(16)	-487(12)	40(6)
H(15A)	839(15)	8733(16)	-483(12)	36(6)
H(15B)	684(15)	7616(16)	-459(13)	32(6)
H(15C)	-27(17)	8323(16)	-73(11)	37(6)
H(16A)	659(16)	9993(17)	1699(13)	46(7)
H(16B)	5(17)	9492(17)	1060(12)	45(7)
H(16C)	913(15)	10217(17)	855(12)	42(6)
H(17A)	2760(20)	9380(20)	2282(16)	80(10)
H(17B)	2450(20)	8540(20)	2757(16)	77(10)
H(17C)	1770(20)	9390(20)	2568(15)	71(9)
H(18A)	3099(18)	6260(19)	1628(12)	50(7)
H(18B)	3030(20)	6980(20)	2290(17)	78(10)
H(18C)	3740(30)	7190(20)	1706(17)	81(10)

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Table 1. Crystal data and structure refinement for 7.

Identification code	gl14	
Empirical formula	C17 H22 Cl2 Cr N	
Formula weight	363.26	
Temperature	203(2) K	
Wavelength	0.71070 Å	
Crystal system	Monoclinic	
Space group	P 2(1)/a	
Unit cell dimensions	a = 7.974(5) Å	α= 90°.
	b = 25.353(14) Å	β= 98.43(4)°.
	c = 8.563(4) Å	γ = 90°.
Volume	1712.4(16) Å^3	
Z	4	
Density (calculated)	1.409 Mg/m^3	
Absorption coefficient	0.973 mm^{-1}	
F(000)	756	
Crystal size	0.28 x 0.15 x 0.14 mm^3	
Theta range for data collection	1.61 to 25.00°.	
Index ranges	-9<=h<=9, 0<=k<=30, 0<=l<=10	
Reflections collected	3008	
Independent reflections	3008 [R(int) = 0.0000]	
Reflections with I > 2 sigma(I)	2102	
Completeness to theta = 25.00°	99.1 %	
Absorption correction	Psi-scan	
Max. and min. transmission	1.000 and 0.912	
Treatment of hydrogen atoms	difmap / refall	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3008 / 0 / 278	
Goodness-of-fit on F^2	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0441, wR2 = 0.0800	
R indices (all data)	R1 = 0.0848, wR2 = 0.0908	
Largest diff. peak and hole	0.289 and -0.364 e.Å^{-3}	

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for GL14. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cr(1)	8399(1)	3908(1)	2751(1)	24(1)
Cl(2)	9340(1)	3391(1)	4928(1)	47(1)
Cl(1)	10964(1)	4264(1)	2390(1)	37(1)
N(1)	8226(4)	3292(1)	839(4)	27(1)
C(1)	5374(4)	3671(1)	178(4)	21(1)
C(2)	6556(4)	3311(1)	-187(4)	24(1)
C(3)	6151(5)	2973(2)	-1463(5)	32(1)
C(4)	4583(5)	2995(2)	-2389(5)	34(1)
C(5)	3396(6)	3356(2)	-2029(5)	32(1)
C(6)	3785(5)	3690(2)	-763(5)	28(1)
C(7)	5854(4)	4042(1)	1511(4)	22(1)
C(8)	6806(4)	4514(1)	1408(4)	23(1)
C(9)	7218(5)	4712(1)	2977(4)	25(1)
C(10)	6548(5)	4360(2)	4032(4)	27(1)
C(11)	5702(4)	3946(2)	3121(4)	25(1)
C(12)	7238(6)	4757(2)	-75(5)	29(1)
C(13)	8138(6)	5215(2)	3417(6)	36(1)
C(14)	6682(7)	4428(2)	5792(5)	42(1)
C(15)	4790(6)	3495(2)	3754(6)	37(1)
C(16)	9579(6)	3371(2)	-176(7)	44(1)
C(17)	8469(6)	2759(2)	1568(6)	43(1)

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Table 3. Bond lengths [Å] and angles [°] for GL14.

Cr(1)-C(7)	2.175(4)
Cr(1)-C(8)	2.207(4)
Cr(1)-C(11)	2.221(4)
Cr(1)-N(1)	2.251(3)
Cr(1)-C(9)	2.267(4)
Cr(1)-C(10)	2.275(4)
Cr(1)-Cl(1)	2.2978(17)
Cr(1)-Cl(2)	2.3116(14)
N(1)-C(2)	1.484(4)
N(1)-C(17)	1.490(5)
N(1)-C(16)	1.495(5)
C(1)-C(2)	1.381(5)
C(1)-C(6)	1.399(5)
C(1)-C(7)	1.485(5)
C(2)-C(3)	1.388(5)
C(3)-C(4)	1.380(6)
C(3)-H(3)	0.86(3)
C(4)-C(5)	1.384(6)
C(4)-H(4)	1.01(4)
C(5)-C(6)	1.376(5)
C(5)-H(5)	0.92(4)
C(6)-H(6)	0.93(4)
C(7)-C(11)	1.423(5)
C(7)-C(8)	1.428(5)
C(8)-C(9)	1.427(5)
C(8)-C(12)	1.496(5)
C(9)-C(10)	1.428(5)
C(9)-C(13)	1.492(5)
C(10)-C(11)	1.420(5)
C(10)-C(14)	1.504(6)
C(11)-C(15)	1.499(6)
C(12)-H(12A)	0.97(4)
C(12)-H(12B)	0.87(5)
C(12)-H(12C)	0.93(5)
C(13)-H(13A)	0.97(5)
C(13)-H(13B)	0.90(4)
C(13)-H(13C)	0.97(5)
C(14)-H(14A)	0.88(4)
C(14)-H(14B)	0.90(6)
C(14)-H(14C)	0.90(6)
C(15)-H(15A)	0.91(5)
C(15)-H(15B)	0.96(5)
C(15)-H(15C)	0.80(5)
C(16)-H(16A)	1.04(5)
C(16)-H(16B)	0.96(4)
C(16)-H(16C)	0.92(4)
C(17)-H(17A)	1.03(4)
C(17)-H(17B)	0.97(4)
C(17)-H(17C)	0.97(5)
C(7)-Cr(1)-C(8)	38.02(12)
C(7)-Cr(1)-C(11)	37.75(13)
C(8)-Cr(1)-C(11)	63.19(13)
C(7)-Cr(1)-N(1)	78.45(12)
C(8)-Cr(1)-N(1)	97.73(13)
C(11)-Cr(1)-N(1)	100.15(13)
C(7)-Cr(1)-C(9)	62.05(13)
C(8)-Cr(1)-C(9)	37.17(13)
C(11)-Cr(1)-C(9)	61.68(14)
N(1)-Cr(1)-C(9)	134.73(12)
C(7)-Cr(1)-C(10)	62.08(13)
C(8)-Cr(1)-C(10)	62.32(13)
C(11)-Cr(1)-C(10)	36.78(13)
N(1)-Cr(1)-C(10)	136.51(13)
C(9)-Cr(1)-C(10)	36.65(13)
C(7)-Cr(1)-Cl(1)	131.14(10)
C(8)-Cr(1)-Cl(1)	96.38(11)
C(11)-Cr(1)-Cl(1)	154.34(11)
N(1)-Cr(1)-Cl(1)	97.82(9)
C(9)-Cr(1)-Cl(1)	92.67(11)

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C(10)-Cr(1)-Cl(1)	121.30(11)
C(7)-Cr(1)-Cl(2)	130.67(10)
C(8)-Cr(1)-Cl(2)	155.36(10)
C(11)-Cr(1)-Cl(2)	96.67(10)
N(1)-Cr(1)-Cl(2)	99.89(9)
C(9)-Cr(1)-Cl(2)	122.06(10)
C(10)-Cr(1)-Cl(2)	93.08(10)
Cl(1)-Cr(1)-Cl(2)	98.13(6)
C(2)-N(1)-C(17)	109.1(3)
C(2)-N(1)-C(16)	108.2(3)
C(17)-N(1)-C(16)	107.7(4)
C(2)-N(1)-Cr(1)	111.3(2)
C(17)-N(1)-Cr(1)	109.5(3)
C(16)-N(1)-Cr(1)	111.0(3)
C(2)-C(1)-C(6)	119.0(3)
C(2)-C(1)-C(7)	119.0(3)
C(6)-C(1)-C(7)	122.0(3)
C(1)-C(2)-C(3)	119.8(3)
C(1)-C(2)-N(1)	118.0(3)
C(3)-C(2)-N(1)	122.1(3)
C(4)-C(3)-C(2)	121.0(4)
C(4)-C(3)-H(3)	120(2)
C(2)-C(3)-H(3)	119(2)
C(3)-C(4)-C(5)	119.3(4)
C(3)-C(4)-H(4)	118(2)
C(5)-C(4)-H(4)	123(2)
C(6)-C(5)-C(4)	120.1(4)
C(6)-C(5)-H(5)	121(2)
C(4)-C(5)-H(5)	119(2)
C(5)-C(6)-C(1)	120.8(4)
C(5)-C(6)-H(6)	122(2)
C(1)-C(6)-H(6)	117(2)
C(11)-C(7)-C(8)	109.0(3)
C(11)-C(7)-C(1)	126.0(3)
C(8)-C(7)-C(1)	124.3(3)
C(11)-C(7)-Cr(1)	72.9(2)
C(8)-C(7)-Cr(1)	72.2(2)
C(1)-C(7)-Cr(1)	113.2(2)
C(9)-C(8)-C(7)	106.7(3)
C(9)-C(8)-C(12)	127.2(3)
C(7)-C(8)-C(12)	126.0(3)
C(9)-C(8)-Cr(1)	73.7(2)
C(7)-C(8)-Cr(1)	69.8(2)
C(12)-C(8)-Cr(1)	122.9(3)
C(8)-C(9)-C(10)	108.7(3)
C(8)-C(9)-C(13)	125.1(4)
C(10)-C(9)-C(13)	126.1(4)
C(8)-C(9)-Cr(1)	69.1(2)
C(10)-C(9)-Cr(1)	72.0(2)
C(13)-C(9)-Cr(1)	126.6(3)
C(11)-C(10)-C(9)	107.8(3)
C(11)-C(10)-C(14)	126.4(4)
C(9)-C(10)-C(14)	125.7(4)
C(11)-C(10)-Cr(1)	69.6(2)
C(9)-C(10)-Cr(1)	71.4(2)
C(14)-C(10)-Cr(1)	125.8(3)
C(10)-C(11)-C(7)	107.8(3)
C(10)-C(11)-C(15)	125.6(4)
C(7)-C(11)-C(15)	126.6(4)
C(10)-C(11)-Cr(1)	73.6(2)
C(7)-C(11)-Cr(1)	69.4(2)
C(15)-C(11)-Cr(1)	123.3(3)
C(8)-C(12)-H(12A)	110(2)
C(8)-C(12)-H(12B)	111(3)
H(12A)-C(12)-H(12B)	104(4)
C(8)-C(12)-H(12C)	110(3)
H(12A)-C(12)-H(12C)	114(4)
H(12B)-C(12)-H(12C)	107(4)
C(9)-C(13)-H(13A)	109(3)
C(9)-C(13)-H(13B)	115(3)
H(13A)-C(13)-H(13B)	100(4)
C(9)-C(13)-H(13C)	114(3)

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H(13A)-C(13)-H(13C)	113(4)
H(13B)-C(13)-H(13C)	106(4)
C(10)-C(14)-H(14A)	110(3)
C(10)-C(14)-H(14B)	106(4)
H(14A)-C(14)-H(14B)	110(4)
C(10)-C(14)-H(14C)	115(4)
H(14A)-C(14)-H(14C)	113(5)
H(14B)-C(14)-H(14C)	104(5)
C(11)-C(15)-H(15A)	110(3)
C(11)-C(15)-H(15B)	115(3)
H(15A)-C(15)-H(15B)	106(4)
C(11)-C(15)-H(15C)	112(4)
H(15A)-C(15)-H(15C)	117(5)
H(15B)-C(15)-H(15C)	97(5)
N(1)-C(16)-H(16A)	112(2)
N(1)-C(16)-H(16B)	106(2)
H(16A)-C(16)-H(16B)	108(3)
N(1)-C(16)-H(16C)	109(2)
H(16A)-C(16)-H(16C)	112(3)
H(16B)-C(16)-H(16C)	110(4)
N(1)-C(17)-H(17A)	109(2)
N(1)-C(17)-H(17B)	110(2)
H(17A)-C(17)-H(17B)	106(3)
N(1)-C(17)-H(17C)	113(3)
H(17A)-C(17)-H(17C)	103(3)
H(17B)-C(17)-H(17C)	115(4)

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for GL14. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	21(1)	27(1)	23(1)	2(1)	1(1)	2(1)
Cl(2)	50(1)	53(1)	35(1)	16(1)	-6(1)	11(1)
Cl(1)	26(1)	42(1)	44(1)	-6(1)	6(1)	-6(1)
N(1)	20(2)	29(2)	33(2)	1(2)	5(1)	2(1)
C(1)	25(2)	21(2)	17(2)	4(2)	3(2)	-3(2)
C(2)	25(2)	25(2)	23(2)	0(2)	2(2)	-5(2)
C(3)	36(2)	27(2)	34(2)	-5(2)	13(2)	0(2)
C(4)	49(3)	31(2)	21(2)	-3(2)	6(2)	-15(2)
C(5)	35(2)	33(2)	24(2)	5(2)	-3(2)	-10(2)
C(6)	27(2)	26(2)	30(2)	2(2)	-1(2)	-1(2)
C(7)	19(2)	23(2)	23(2)	0(2)	1(2)	4(2)
C(8)	19(2)	24(2)	24(2)	-1(2)	1(2)	2(2)
C(9)	23(2)	27(2)	24(2)	-4(2)	0(2)	4(2)
C(10)	29(2)	31(2)	23(2)	-1(2)	4(2)	6(2)
C(11)	23(2)	28(2)	23(2)	2(2)	3(2)	2(2)
C(12)	34(3)	27(2)	26(2)	3(2)	2(2)	0(2)
C(13)	43(3)	33(3)	29(3)	-3(2)	-1(2)	-6(2)
C(14)	44(3)	54(3)	27(2)	-3(2)	7(2)	4(3)
C(15)	42(3)	40(3)	32(3)	6(2)	12(2)	-5(2)
C(16)	31(3)	48(3)	57(3)	-20(3)	22(2)	-4(2)
C(17)	43(3)	27(2)	54(3)	-4(2)	-9(3)	8(2)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for GL14.

	x	y	z	U(eq)
H(3)	6890(4)	2748(12)	-1680(4)	10(9)
H(4)	4350(4)	2743(14)	-3320(4)	29(10)
H(5)	2360(5)	3376(15)	-2660(4)	35(11)
H(6)	3010(5)	3933(15)	-490(4)	32(11)
H(12A)	7270(5)	4486(17)	-880(5)	47(13)
H(12B)	8260(6)	4887(18)	70(5)	58(16)
H(12C)	6510(6)	5040(2)	-390(6)	66(16)
H(13A)	7380(6)	5507(19)	3110(5)	63(15)
H(13B)	8970(5)	5289(16)	2850(5)	43(13)
H(13C)	8650(5)	5231(16)	4510(6)	53(13)
H(14A)	5720(6)	4552(16)	6030(5)	43(13)
H(14B)	6880(7)	4110(2)	6220(7)	90(2)
H(14C)	7580(8)	4620(2)	6230(7)	100(2)
H(15A)	3900(6)	3618(17)	4210(5)	52(14)
H(15B)	5470(6)	3290(19)	4550(6)	64(16)
H(15C)	4600(7)	3260(2)	3110(7)	80(2)
H(16A)	9560(5)	3075(18)	-1030(5)	59(14)
H(16B)	10640(5)	3349(16)	520(5)	43(13)
H(16C)	9460(5)	3701(16)	-630(4)	32(12)
H(17A)	7490(5)	2682(15)	2200(5)	39(12)
H(17B)	8390(5)	2489(17)	750(5)	44(12)
H(17C)	9470(6)	2739(17)	2360(5)	58(14)