Molecular structure and data of $(Cy_2PC_2H_4C_5H_4)CrCl_2$ (7i)

CCDC 155398

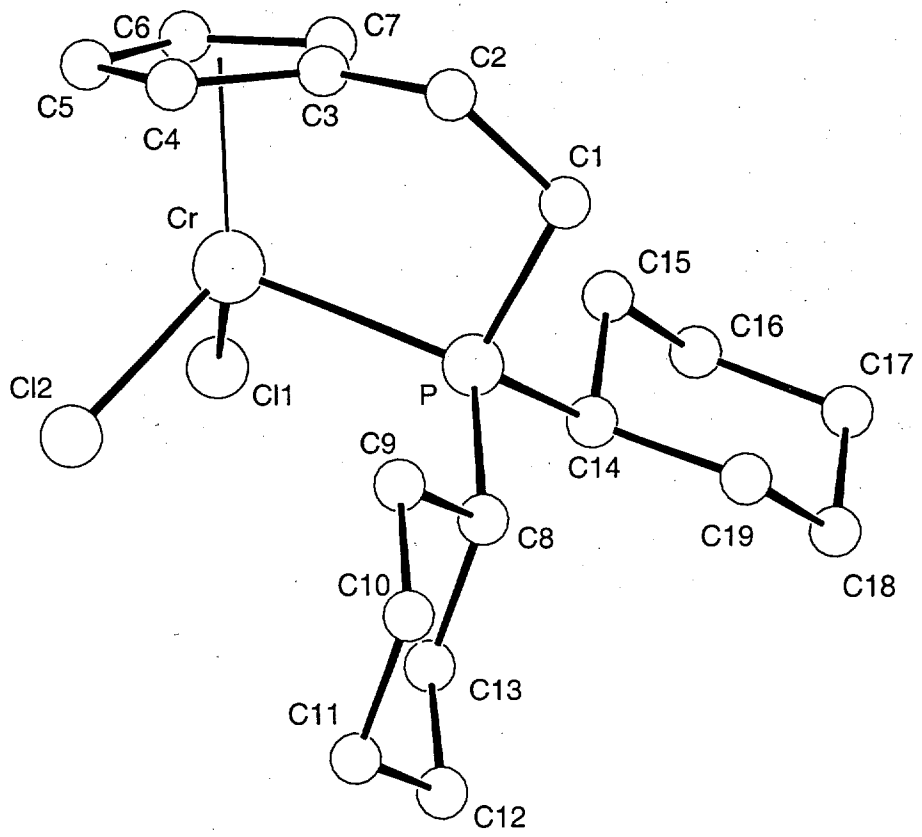

Table 1. Crystal data and structure refinement.

Identification code	2549	
Empirical formula	$C_{19}H_{30}Cl_2CrP$	
Color	dark blue	
Formula weight	412.30 $g \cdot mol^{-1}$	
Temperature	293 K	
Wavelength	0.71069 Å	
Crystal system	Monoclinic	
Space group	**$P2_1/n$, (no. 14)**	
Unit cell dimensions	a = 8.396(2) Å	α= 90°.
	b = 20.064(3) Å	β= 105.44(2)°.
	c = 12.398(3) Å	γ = 90°.
Volume	2013.0(7) $Å^3$	
Z	4	
Density (calculated)	1.360 $Mg \cdot m^{-3}$	
Absorption coefficient	0.911 mm^{-1}	
F(000)	868 e	
Crystal size	0.60 x 0.53 x 0.11 mm^3	
θ range for data collection	1.98 to 27.45°.	
Index ranges	$-10 \leq h \leq 10$, $0 \leq k \leq 26$, $0 \leq l \leq 16$	
Reflections collected	4591	
Independent reflections	4591 [R_{int} = 0.0000]	
Reflections with $I>2\sigma(I)$	3626	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4591 / 0 / 328	
Goodness-of-fit on F^2	0.905	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0434	wR^2 = 0.1197
R indices (all data)	R_1 = 0.0619	wR^2 = 0.1285
Largest diff. peak and hole	0.556 and -0.423 $e \cdot Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å^2).
U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	-0.3405(3)	0.1762(2)	0.3733(2)	0.039(1)
C(2)	-0.2596(3)	0.1206(2)	0.3218(2)	0.041(1)
C(3)	-0.0753(3)	0.1279(1)	0.3495(2)	0.034(1)
C(4)	0.0425(4)	0.0787(1)	0.3954(2)	0.041(1)
C(5)	0.2022(3)	0.1070(2)	0.4169(2)	0.044(1)
C(6)	0.1844(3)	0.1735(2)	0.3840(2)	0.042(1)
C(7)	0.0145(3)	0.1877(1)	0.3438(2)	0.035(1)
C(8)	-0.3281(3)	0.1510(1)	0.6091(2)	0.033(1)
C(9)	-0.3318(3)	0.0752(1)	0.5927(2)	0.040(1)
C(10)	-0.4211(4)	0.0410(2)	0.6699(3)	0.047(1)
C(11)	-0.3468(4)	0.0597(2)	0.7908(3)	0.055(1)
C(12)	-0.3480(5)	0.1343(2)	0.8056(3)	0.053(1)
C(13)	-0.2539(4)	0.1691(1)	0.7318(2)	0.043(1)
C(14)	-0.2435(3)	0.2837(1)	0.5418(2)	0.035(1)
C(15)	-0.1738(4)	0.3270(1)	0.4627(3)	0.045(1)
C(16)	-0.1810(4)	0.4007(2)	0.4915(3)	0.055(1)
C(17)	-0.3546(4)	0.4222(2)	0.4885(3)	0.052(1)
C(18)	-0.4286(4)	0.3791(2)	0.5629(3)	0.055(1)
C(19)	-0.4206(3)	0.3050(2)	0.5359(3)	0.046(1)
Cr	0.0634(1)	0.1590(1)	0.5229(1)	0.029(1)
Cl(1)	0.2018(1)	0.2475(1)	0.6186(1)	0.051(1)
Cl(2)	0.1249(1)	0.0870(1)	0.6703(1)	0.047(1)
P	-0.2190(1)	0.1940(1)	0.5182(1)	0.030(1)

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

C(1)-C(2)	1.531(4)	C(1)-P	1.850(3)
C(2)-C(3)	1.500(3)	C(3)-C(4)	1.406(3)
C(3)-C(7)	1.430(4)	C(3)-Cr	2.244(2)
C(4)-C(5)	1.415(4)	C(4)-Cr	2.231(2)
C(5)-C(6)	1.392(4)	C(5)-Cr	2.234(2)
C(6)-C(7)	1.410(3)	C(6)-Cr	2.240(2)
C(7)-Cr	2.224(2)	C(8)-C(13)	1.526(3)
C(8)-C(9)	1.534(3)	C(8)-P	1.845(2)
C(9)-C(10)	1.526(4)	C(10)-C(11)	1.509(5)
C(11)-C(12)	1.509(5)	C(12)-C(13)	1.528(4)
C(14)-C(19)	1.530(3)	C(14)-C(15)	1.537(4)
C(14)-P	1.843(2)	C(15)-C(16)	1.526(4)
C(16)-C(17)	1.510(5)	C(17)-C(18)	1.514(5)
C(18)-C(19)	1.528(4)	Cr-Cl(1)	2.2753(8)
Cr-Cl(2)	2.2786(8)	Cr-P	2.4588(8)
C(2)-C(1)-P	110.8(2)	C(3)-C(2)-C(1)	112.2(2)
C(4)-C(3)-C(7)	106.6(2)	C(4)-C(3)-C(2)	126.6(2)
C(7)-C(3)-C(2)	126.6(2)	C(4)-C(3)-Cr	71.19(13)
C(7)-C(3)-Cr	70.56(13)	C(2)-C(3)-Cr	119.1(2)
C(3)-C(4)-C(5)	108.9(2)	C(3)-C(4)-Cr	72.20(13)
C(5)-C(4)-Cr	71.63(15)	C(6)-C(5)-C(4)	107.9(2)
C(6)-C(5)-Cr	72.10(14)	C(4)-C(5)-Cr	71.42(14)
C(5)-C(6)-C(7)	108.5(2)	C(5)-C(6)-Cr	71.65(14)
C(7)-C(6)-Cr	70.99(14)	C(6)-C(7)-C(3)	108.0(2)
C(6)-C(7)-Cr	72.20(14)	C(3)-C(7)-Cr	72.11(13)
C(13)-C(8)-C(9)	110.9(2)	C(13)-C(8)-P	111.1(2)
C(9)-C(8)-P	112.3(2)	C(10)-C(9)-C(8)	111.0(2)
C(11)-C(10)-C(9)	111.7(2)	C(10)-C(11)-C(12)	110.7(3)
C(11)-C(12)-C(13)	111.0(3)	C(8)-C(13)-C(12)	110.5(2)
C(19)-C(14)-C(15)	110.0(2)	C(19)-C(14)-P	114.4(2)
C(15)-C(14)-P	111.9(2)	C(14)-C(15)-C(16)	110.6(2)
C(17)-C(16)-C(15)	111.6(3)	C(16)-C(17)-C(18)	111.8(3)
C(17)-C(18)-C(19)	111.9(2)	C(14)-C(19)-C(18)	111.1(2)
C(7)-Cr-C(6)	36.81(9)	C(7)-Cr-C(4)	61.40(10)
C(6)-Cr-C(4)	61.01(11)	C(7)-Cr-C(5)	61.32(9)
C(6)-Cr-C(5)	36.25(10)	C(4)-Cr-C(5)	36.95(10)

C(7)-Cr-C(3)	37.32(9)	C(6)-Cr-C(3)	61.65(9)
C(4)-Cr-C(3)	36.62(9)	C(5)-Cr-C(3)	61.65(9)
C(7)-Cr-Cl(1)	104.53(7)	C(6)-Cr-Cl(1)	91.50(8)
C(4)-Cr-Cl(1)	150.00(8)	C(5)-Cr-Cl(1)	113.41(8)
C(3)-Cr-Cl(1)	141.20(7)	C(7)-Cr-Cl(2)	155.14(7)
C(6)-Cr-Cl(2)	130.31(7)	C(4)-Cr-Cl(2)	93.91(8)
C(5)-Cr-Cl(2)	97.67(8)	C(3)-Cr-Cl(2)	122.74(7)
Cl(1)-Cr-Cl(2)	95.85(3)	C(7)-Cr-P	88.94(7)
C(6)-Cr-P	125.21(7)	C(4)-Cr-P	107.21(8)
C(5)-Cr-P	140.37(7)	C(3)-Cr-P	78.78(6)
Cl(1)-Cr-P	98.32(3)	Cl(2)-Cr-P	102.22(3)
C(8)-P-C(14)	105.39(11)	C(8)-P-C(1)	105.53(12)
C(14)-P-C(1)	106.68(12)	C(8)-P-Cr	118.96(8)
C(14)-P-Cr	115.02(8)	C(1)-P-Cr	104.28(8)

Table 4. Anisotropic displacement parameters (Å²).

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}
C(1)	0.026(1)	0.056(2)	0.034(1)	0.000(1)	0.005(1)	0.000(1)
C(2)	0.037(1)	0.049(1)	0.036(1)	-0.007(1)	0.007(1)	-0.008(1)
C(3)	0.034(1)	0.040(1)	0.029(1)	-0.005(1)	0.009(1)	0.001(1)
C(4)	0.051(1)	0.036(1)	0.038(1)	-0.005(1)	0.014(1)	0.006(1)
C(5)	0.038(1)	0.056(2)	0.040(1)	-0.002(1)	0.013(1)	0.016(1)
C(6)	0.032(1)	0.059(2)	0.038(1)	0.001(1)	0.016(1)	-0.001(1)
C(7)	0.036(1)	0.041(1)	0.030(1)	0.001(1)	0.010(1)	0.001(1)
C(8)	0.029(1)	0.040(1)	0.034(1)	0.000(1)	0.012(1)	0.000(1)
C(9)	0.039(1)	0.039(1)	0.047(1)	-0.004(1)	0.019(1)	-0.002(1)
C(10)	0.039(1)	0.043(1)	0.063(2)	0.003(1)	0.022(1)	-0.001(1)
C(11)	0.059(2)	0.057(2)	0.054(2)	0.017(1)	0.025(1)	0.004(1)
C(12)	0.064(2)	0.062(2)	0.037(1)	0.002(1)	0.022(1)	-0.002(2)
C(13)	0.052(2)	0.045(1)	0.036(1)	-0.004(1)	0.016(1)	-0.004(1)
C(14)	0.033(1)	0.037(1)	0.035(1)	0.001(1)	0.010(1)	0.002(1)
C(15)	0.044(1)	0.041(1)	0.055(2)	0.007(1)	0.022(1)	0.005(1)
C(16)	0.059(2)	0.039(1)	0.070(2)	0.005(1)	0.022(2)	-0.001(1)
C(17)	0.061(2)	0.042(1)	0.052(2)	-0.001(1)	0.010(1)	0.014(1)
C(18)	0.055(2)	0.050(2)	0.063(2)	-0.002(1)	0.023(2)	0.017(1)
C(19)	0.037(1)	0.048(2)	0.056(2)	0.001(1)	0.019(1)	0.009(1)
Cr	0.024(1)	0.035(1)	0.029(1)	-0.002(1)	0.007(1)	0.001(1)
Cl(1)	0.043(1)	0.055(1)	0.052(1)	-0.017(1)	0.007(1)	-0.013(1)
Cl(2)	0.043(1)	0.055(1)	0.040(1)	0.011(1)	0.007(1)	0.006(1)
P	0.025(1)	0.036(1)	0.031(1)	0.000(1)	0.008(1)	0.002(1)

Molecular structure and data of $(Cy_2AsC_2H_4C_5H_4)CrCl_2$ (19)

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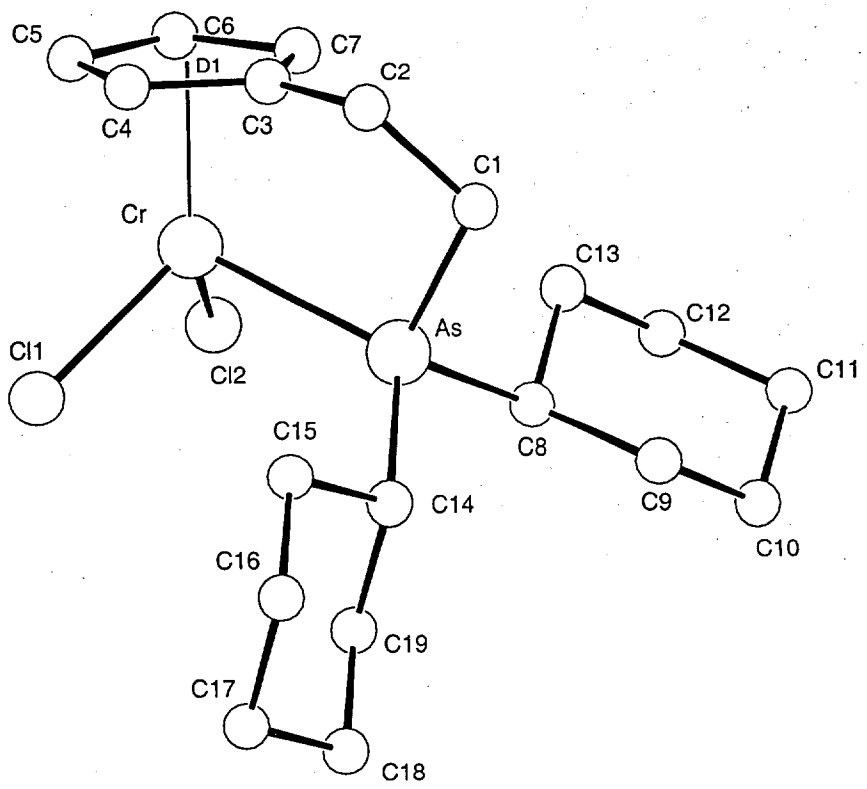

Table 1. Crystal data and structure refinement.

Identification code	2749	
Empirical formula	$C_{19}H_{30}AsCl_2Cr$	
Color	colorless	
Formula weight	456.25 $g \cdot mol^{-1}$	
Temperature	293 K	
Wavelength	0.71069 Å	
Crystal system	Monoclinic	
Space group	**$P2_1/n$, (no. 14)**	
Unit cell dimensions	a = 8.4350(10) Å	α= 90°.
	b = 20.1530(10) Å	β= 106.780(10)°.
	c = 12.3500(10) Å	γ = 90°.
Volume	2010.0(3) $Å^3$	
Z	4	
Density (calculated)	1.508 $Mg \cdot m^{-3}$	
Absorption coefficient	2.466 mm^{-1}	
F(000)	940 e	
Crystal size	0.34 x 0.19 x 0.07 mm^3	
θ range for data collection	2.00 to 34.05°.	
Index ranges	$-9 \leq h \leq 13$, $-29 \leq k \leq 31$, $-19 \leq l \leq 19$	
Reflections collected	22601	
Independent reflections	7635 [R_{int} = 0.1013]	
Reflections with $I>2\sigma(I)$	6358	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7635 / 0 / 328	
Goodness-of-fit on F^2	1.217	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0624	wR^2 = 0.1681
R indices (all data)	R_1 = 0.0779	wR^2 = 0.1875
Largest diff. peak and hole	1.869 and -1.847 $e \cdot Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å^2).
U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	0.3440(4)	0.1730(2)	0.6354(3)	0.018(1)
C(2)	0.2574(4)	0.1184(2)	0.6842(3)	0.019(1)
C(3)	0.0714(4)	0.1265(2)	0.6511(2)	0.015(1)
C(4)	-0.0471(4)	0.0763(2)	0.6058(3)	0.017(1)
C(5)	-0.2089(4)	0.1045(2)	0.5828(3)	0.019(1)
C(6)	-0.1904(4)	0.1720(2)	0.6146(3)	0.017(1)
C(7)	-0.0185(4)	0.1864(2)	0.6552(3)	0.015(1)
C(8)	0.2431(4)	0.2870(2)	0.4538(3)	0.015(1)
C(9)	0.4233(4)	0.3068(2)	0.4634(3)	0.021(1)
C(10)	0.4338(5)	0.3810(2)	0.4394(3)	0.023(1)
C(11)	0.3628(4)	0.4235(2)	0.5157(3)	0.022(1)
C(12)	0.1850(5)	0.4030(2)	0.5073(3)	0.023(1)
C(13)	0.1729(4)	0.3290(2)	0.5324(3)	0.020(1)
C(14)	0.3370(4)	0.1471(2)	0.3857(3)	0.016(1)
C(15)	0.3331(4)	0.0710(2)	0.3984(3)	0.019(1)
C(16)	0.4241(4)	0.0370(2)	0.3227(3)	0.022(1)
C(17)	0.3539(5)	0.0585(2)	0.1987(3)	0.025(1)
C(18)	0.3596(5)	0.1335(2)	0.1875(3)	0.023(1)
C(19)	0.2662(4)	0.1679(2)	0.2621(3)	0.020(1)
As(1)	0.2148(1)	0.1917(1)	0.4784(1)	0.014(1)
Cl(1)	-0.1322(1)	0.0848(1)	0.3252(1)	0.021(1)
Cl(2)	-0.2120(1)	0.2454(1)	0.3786(1)	0.022(1)
Cr(1)	-0.0750(1)	0.1559(1)	0.4747(1)	0.013(1)

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

C(1)-C(2)	1.536(5)	C(1)-As(1)	1.967(3)
C(2)-C(3)	1.511(4)	C(3)-C(4)	1.418(4)
C(3)-C(7)	1.435(4)	C(3)-Cr(1)	2.252(3)
C(4)-C(5)	1.429(5)	C(4)-Cr(1)	2.243(3)
C(5)-C(6)	1.412(5)	C(5)-Cr(1)	2.237(3)
C(6)-C(7)	1.421(4)	C(6)-Cr(1)	2.238(3)
C(7)-Cr(1)	2.227(3)	C(8)-C(13)	1.530(5)
C(8)-C(9)	1.543(4)	C(8)-As(1)	1.970(3)
C(9)-C(10)	1.532(5)	C(10)-C(11)	1.518(5)
C(11)-C(12)	1.530(5)	C(12)-C(13)	1.532(5)
C(14)-C(19)	1.528(5)	C(14)-C(15)	1.542(4)
C(14)-As(1)	1.965(3)	C(15)-C(16)	1.532(5)
C(16)-C(17)	1.536(5)	C(17)-C(18)	1.521(5)
C(18)-C(19)	1.539(5)	As(1)-Cr(1)	2.5364(6)
Cl(1)-Cr(1)	2.2768(9)	Cl(2)-Cr(1)	2.2814(9)
C(2)-C(1)-As(1)	109.4(2)	C(3)-C(2)-C(1)	113.0(3)
C(4)-C(3)-C(7)	107.1(3)	C(4)-C(3)-C(2)	126.0(3)
C(7)-C(3)-C(2)	126.8(3)	C(4)-C(3)-Cr(1)	71.3(2)
C(7)-C(3)-Cr(1)	70.4(2)	C(2)-C(3)-Cr(1)	121.8(2)
C(3)-C(4)-C(5)	108.6(3)	C(3)-C(4)-Cr(1)	72.0(2)
C(5)-C(4)-Cr(1)	71.2(2)	C(6)-C(5)-C(4)	107.8(3)
C(6)-C(5)-Cr(1)	71.7(2)	C(4)-C(5)-Cr(1)	71.6(2)
C(5)-C(6)-C(7)	108.3(3)	C(5)-C(6)-Cr(1)	71.6(2)
C(7)-C(6)-Cr(1)	71.0(2)	C(6)-C(7)-C(3)	108.1(3)
C(6)-C(7)-Cr(1)	71.9(2)	C(3)-C(7)-Cr(1)	72.3(2)
C(13)-C(8)-C(9)	111.2(3)	C(13)-C(8)-As(1)	110.8(2)
C(9)-C(8)-As(1)	113.7(2)	C(10)-C(9)-C(8)	110.4(3)
C(11)-C(10)-C(9)	112.1(3)	C(10)-C(11)-C(12)	111.1(3)
C(11)-C(12)-C(13)	111.7(3)	C(8)-C(13)-C(12)	110.4(3)
C(19)-C(14)-C(15)	111.2(3)	C(19)-C(14)-As(1)	109.7(2)
C(15)-C(14)-As(1)	111.4(2)	C(16)-C(15)-C(14)	110.7(3)
C(15)-C(16)-C(17)	111.5(3)	C(18)-C(17)-C(16)	110.9(3)
C(17)-C(18)-C(19)	111.0(3)	C(14)-C(19)-C(18)	110.8(3)
C(14)-As(1)-C(1)	104.66(13)	C(14)-As(1)-C(8)	104.40(13)
C(1)-As(1)-C(8)	106.33(14)	C(14)-As(1)-Cr(1)	121.63(9)
C(1)-As(1)-Cr(1)	102.72(9)	C(8)-As(1)-Cr(1)	115.66(9)

C(7)-Cr(1)-C(5)	61.93(12)	C(7)-Cr(1)-C(6)	37.11(11)
C(5)-Cr(1)-C(6)	36.78(12)	C(7)-Cr(1)-C(4)	61.78(12)
C(5)-Cr(1)-C(4)	37.19(12)	C(6)-Cr(1)-C(4)	61.60(12)
C(7)-Cr(1)-C(3)	37.36(11)	C(5)-Cr(1)-C(3)	62.00(12)
C(6)-Cr(1)-C(3)	61.99(11)	C(4)-Cr(1)-C(3)	36.77(11)
C(7)-Cr(1)-Cl(1)	156.82(9)	C(5)-Cr(1)-Cl(1)	99.59(9)
C(6)-Cr(1)-Cl(1)	132.79(9)	C(4)-Cr(1)-Cl(1)	95.06(9)
C(3)-Cr(1)-Cl(1)	123.16(8)	C(7)-Cr(1)-Cl(2)	103.45(8)
C(5)-Cr(1)-Cl(2)	114.21(9)	C(6)-Cr(1)-Cl(2)	91.13(9)
C(4)-Cr(1)-Cl(2)	150.81(9)	C(3)-Cr(1)-Cl(2)	139.97(8)
Cl(1)-Cr(1)-Cl(2)	96.85(4)	C(7)-Cr(1)-As(1)	88.68(8)
C(5)-Cr(1)-As(1)	140.42(9)	C(6)-Cr(1)-As(1)	125.23(9)
C(4)-Cr(1)-As(1)	106.86(8)	C(3)-Cr(1)-As(1)	78.50(8)
Cl(1)-Cr(1)-As(1)	99.85(3)	Cl(2)-Cr(1)-As(1)	97.23(3)

Table 4. Anisotropic displacement parameters (Å²).
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}
C(1)	0.014(1)	0.026(1)	0.013(1)	0.000(1)	0.002(1)	0.000(1)
C(2)	0.015(1)	0.024(1)	0.016(1)	0.005(1)	0.002(1)	0.004(1)
C(3)	0.016(1)	0.018(1)	0.012(1)	0.002(1)	0.004(1)	0.000(1)
C(4)	0.018(1)	0.019(1)	0.015(1)	0.004(1)	0.005(1)	-0.002(1)
C(5)	0.015(1)	0.025(2)	0.020(1)	0.001(1)	0.007(1)	-0.005(1)
C(6)	0.015(1)	0.023(1)	0.014(1)	0.000(1)	0.007(1)	0.002(1)
C(7)	0.014(1)	0.018(1)	0.014(1)	-0.001(1)	0.004(1)	-0.001(1)
C(8)	0.015(1)	0.017(1)	0.014(1)	-0.002(1)	0.004(1)	-0.003(1)
C(9)	0.016(1)	0.025(2)	0.024(2)	-0.002(1)	0.010(1)	-0.002(1)
C(10)	0.024(2)	0.022(2)	0.027(2)	0.000(1)	0.014(1)	-0.006(1)
C(11)	0.023(2)	0.019(1)	0.024(2)	0.000(1)	0.005(1)	-0.005(1)
C(12)	0.021(2)	0.018(1)	0.029(2)	0.000(1)	0.006(1)	-0.001(1)
C(13)	0.021(1)	0.017(1)	0.024(2)	-0.004(1)	0.010(1)	-0.003(1)
C(14)	0.015(1)	0.020(1)	0.013(1)	-0.001(1)	0.005(1)	0.000(1)
C(15)	0.018(1)	0.020(1)	0.021(1)	0.002(1)	0.009(1)	0.001(1)
C(16)	0.021(1)	0.018(1)	0.029(2)	-0.002(1)	0.013(1)	0.000(1)
C(17)	0.025(2)	0.027(2)	0.023(2)	-0.007(1)	0.010(1)	-0.002(1)
C(18)	0.027(2)	0.028(2)	0.019(2)	0.002(1)	0.010(1)	-0.001(1)
C(19)	0.022(1)	0.022(1)	0.017(1)	0.002(1)	0.006(1)	0.000(1)
As(1)	0.012(1)	0.017(1)	0.012(1)	0.000(1)	0.003(1)	-0.001(1)
Cl(1)	0.020(1)	0.026(1)	0.016(1)	-0.004(1)	0.004(1)	-0.001(1)
Cl(2)	0.019(1)	0.025(1)	0.020(1)	0.007(1)	0.004(1)	0.006(1)
Cr(1)	0.011(1)	0.017(1)	0.011(1)	0.001(1)	0.003(1)	0.000(1)

Molecular structure and data of ($Ph_2PC_3H_6C_5Me_4$)$CrCl_2$ (11)

CCDC 155400

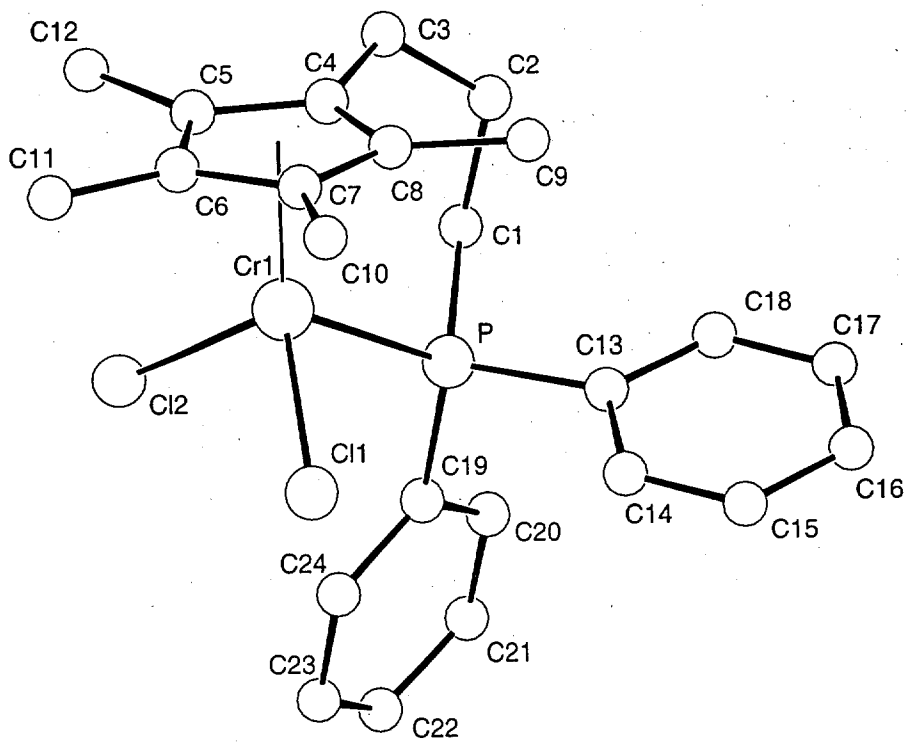

Table 1. Crystal data and structure refinement.

Identification code	2669	
Empirical formula	$C_{24}H_{28}Cl_2CrP$	
Color	black	
Formula weight	470.33 $g \cdot mol^{-1}$	
Temperature	293 K	
Wavelength	0.71069 Å	
Crystal system	Orthorhombic	
Space group	**Pbca, (no. 61)**	
Unit cell dimensions	a = 16.6206(11) Å	α= 90°.
	b = 29.5156(15) Å	β= 90°.
	c = 18.859(2) Å	γ = 90°.
Volume	9251.6(13) $Å^3$	
Z	16	
Density (calculated)	1.351 $Mg \cdot m^{-3}$	
Absorption coefficient	0.802 mm^{-1}	
F(000)	3920 e	
Crystal size	1.16 x 0.77 x 0.60 mm^3	
θ range for data collection	2.45 to 26.30°.	
Index ranges	$0 \leq h \leq 20$, $0 \leq k \leq 36$, $0 \leq l \leq 23$	
Reflections collected	9379	
Independent reflections	9379 [R_{int} = 0.0000]	
Reflections with $I>2\sigma(I)$	5204	
Completeness to θ = 0.50°	0.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9379 / 0 / 505	
Goodness-of-fit on F^2	0.921	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0469	wR^2 = 0.1155
R indices (all data)	R_1 = 0.1353	wR^2 = 0.1291
Largest diff. peak and hole	0.377 and -0.301 $e \cdot Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å^2).
U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	-0.0937(2)	0.0355(1)	0.2479(2)	0.043(1)
C(2)	-0.1279(2)	0.0200(1)	0.1772(2)	0.049(1)
C(3)	-0.0821(2)	0.0347(1)	0.1118(2)	0.049(1)
C(4)	0.0040(2)	0.0194(1)	0.1017(2)	0.041(1)
C(5)	0.0675(2)	0.0487(1)	0.0800(2)	0.046(1)
C(6)	0.1369(2)	0.0208(1)	0.0698(2)	0.048(1)
C(7)	0.1149(2)	-0.0247(1)	0.0818(2)	0.043(1)
C(8)	0.0338(2)	-0.0257(1)	0.1023(2)	0.040(1)
C(9)	-0.0139(2)	-0.0681(1)	0.1140(2)	0.051(1)
C(10)	0.1692(2)	-0.0652(1)	0.0724(2)	0.062(1)
C(11)	0.2180(2)	0.0374(2)	0.0451(2)	0.075(1)
C(12)	0.0625(3)	0.0991(1)	0.0685(2)	0.077(1)
C(13)	-0.0347(2)	-0.0518(1)	0.2982(2)	0.034(1)
C(14)	0.0230(2)	-0.0848(1)	0.3119(2)	0.049(1)
C(15)	0.0017(2)	-0.1276(1)	0.3326(2)	0.060(1)
C(16)	-0.0779(2)	-0.1396(1)	0.3387(2)	0.056(1)
C(17)	-0.1356(2)	-0.1079(1)	0.3251(2)	0.056(1)
C(18)	-0.1152(2)	-0.0644(1)	0.3053(2)	0.046(1)
C(19)	0.0193(2)	0.0292(1)	0.3636(2)	0.038(1)
C(20)	-0.0419(3)	0.0375(1)	0.4114(2)	0.053(1)
C(21)	-0.0255(3)	0.0562(2)	0.4771(2)	0.074(1)
C(22)	0.0531(4)	0.0660(2)	0.4952(2)	0.082(2)
C(23)	0.1139(3)	0.0564(2)	0.4502(2)	0.079(2)
C(24)	0.0972(2)	0.0384(1)	0.3840(2)	0.060(1)
C(101)	0.3086(2)	-0.2385(1)	0.0568(2)	0.050(1)
C(102)	0.3310(2)	-0.2770(2)	0.1076(2)	0.059(1)
C(103)	0.2844(2)	-0.2775(2)	0.1771(2)	0.058(1)
C(104)	0.1938(2)	-0.2798(1)	0.1742(2)	0.043(1)
C(105)	0.1471(2)	-0.3181(1)	0.1528(2)	0.041(1)
C(106)	0.0660(2)	-0.3093(1)	0.1705(2)	0.043(1)
C(107)	0.0617(2)	-0.2658(1)	0.2007(2)	0.050(1)
C(108)	0.1412(2)	-0.2477(1)	0.2043(2)	0.051(1)
C(109)	0.1635(3)	-0.2030(2)	0.2385(3)	0.089(2)
C(110)	-0.0129(3)	-0.2430(2)	0.2293(3)	0.080(2)

C(111)	-0.0035(2)	-0.3415(1)	0.1616(2)	0.066(1)
C(112)	0.1799(2)	-0.3619(1)	0.1242(2)	0.056(1)
C(113)	0.2476(2)	-0.3013(1)	-0.0471(2)	0.037(1)
C(114)	0.1933(2)	-0.3360(1)	-0.0593(2)	0.049(1)
C(115)	0.2133(2)	-0.3724(1)	-0.1015(2)	0.057(1)
C(116)	0.2881(3)	-0.3746(2)	-0.1320(2)	0.064(1)
C(117)	0.3426(3)	-0.3412(2)	-0.1194(3)	0.072(1)
C(118)	0.3229(2)	-0.3046(1)	-0.0771(2)	0.061(1)
C(119)	0.2095(2)	-0.2083(1)	-0.0607(2)	0.041(1)
C(120)	0.1369(2)	-0.2030(1)	-0.0960(2)	0.056(1)
C(121)	0.1290(3)	-0.1716(2)	-0.1509(2)	0.070(1)
C(122)	0.1934(3)	-0.1453(1)	-0.1694(2)	0.068(1)
C(123)	0.2646(3)	-0.1500(2)	-0.1345(3)	0.077(1)
C(124)	0.2734(2)	-0.1811(1)	-0.0807(2)	0.063(1)
Cl(1)	0.1935(1)	-0.0292(1)	0.2397(1)	0.074(1)
Cl(2)	0.1432(1)	0.0834(1)	0.2249(1)	0.086(1)
Cl(11)	0.0114(1)	-0.2840(1)	0.0104(1)	0.064(1)
Cl(12)	0.0778(1)	-0.1824(1)	0.0788(1)	0.081(1)
Cr(1)	0.1005(1)	0.0149(1)	0.1832(1)	0.040(1)
Cr(2)	0.1053(1)	-0.2577(1)	0.0900(1)	0.036(1)
P	-0.0026(1)	0.0054(1)	0.2765(1)	0.033(1)
P(2)	0.2182(1)	-0.2523(1)	0.0060(1)	0.035(1)

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

C(1)-C(2)	1.520(5)	C(1)-P	1.837(3)
C(2)-C(3)	1.513(5)	C(3)-C(4)	1.512(5)
C(4)-C(8)	1.421(5)	C(4)-C(5)	1.424(5)
C(4)-Cr(1)	2.226(3)	C(5)-C(6)	1.430(5)
C(5)-C(12)	1.506(5)	C(5)-Cr(1)	2.254(4)
C(6)-C(7)	1.412(5)	C(6)-C(11)	1.508(5)
C(6)-Cr(1)	2.230(3)	C(7)-C(8)	1.404(5)
C(7)-C(10)	1.506(5)	C(7)-Cr(1)	2.254(3)
C(8)-C(9)	1.497(4)	C(8)-Cr(1)	2.235(3)
C(13)-C(14)	1.393(4)	C(13)-C(18)	1.394(4)
C(13)-P	1.818(3)	C(14)-C(15)	1.368(5)
C(15)-C(16)	1.374(5)	C(16)-C(17)	1.365(5)
C(17)-C(18)	1.381(5)	C(19)-C(24)	1.378(5)
C(19)-C(20)	1.381(5)	C(19)-P	1.822(3)
C(20)-C(21)	1.385(5)	C(21)-C(22)	1.380(7)
C(22)-C(23)	1.350(6)	C(23)-C(24)	1.385(6)
C(101)-C(102)	1.533(5)	C(101)-P(2)	1.828(3)
C(102)-C(103)	1.523(5)	C(103)-C(104)	1.509(5)
C(104)-C(108)	1.409(5)	C(104)-C(105)	1.429(5)
C(104)-Cr(2)	2.261(3)	C(105)-C(106)	1.414(5)
C(105)-C(112)	1.504(5)	C(105)-Cr(2)	2.251(3)
C(106)-C(107)	1.407(5)	C(106)-C(111)	1.505(5)
C(106)-Cr(2)	2.246(3)	C(107)-C(108)	1.426(5)
C(107)-C(110)	1.510(5)	C(107)-Cr(2)	2.222(4)
C(108)-C(109)	1.516(5)	C(108)-Cr(2)	2.256(4)
C(113)-C(118)	1.377(5)	C(113)-C(114)	1.386(5)
C(113)-P(2)	1.825(3)	C(114)-C(115)	1.377(5)
C(115)-C(116)	1.372(5)	C(116)-C(117)	1.360(6)
C(117)-C(118)	1.382(5)	C(119)-C(124)	1.384(5)
C(119)-C(120)	1.386(5)	C(119)-P(2)	1.814(3)
C(120)-C(121)	1.395(5)	C(121)-C(122)	1.368(6)
C(122)-C(123)	1.363(6)	C(123)-C(124)	1.375(5)
Cl(1)-Cr(1)	2.2837(12)	Cl(2)-Cr(1)	2.2844(11)
Cl(11)-Cr(2)	2.3002(11)	Cl(12)-Cr(2)	2.2770(11)
Cr(1)-P	2.4722(10)	Cr(2)-P(2)	2.4621(10)
C(2)-C(1)-P	114.9(2)	C(3)-C(2)-C(1)	116.2(3)

C(4)-C(3)-C(2)	119.5(3)
C(8)-C(4)-C(3)	127.5(3)
C(8)-C(4)-Cr(1)	71.79(19)
C(3)-C(4)-Cr(1)	127.8(2)
C(4)-C(5)-C(12)	126.8(4)
C(4)-C(5)-Cr(1)	70.37(19)
C(12)-C(5)-Cr(1)	125.1(3)
C(7)-C(6)-C(11)	126.2(4)
C(7)-C(6)-Cr(1)	72.60(19)
C(11)-C(6)-Cr(1)	124.3(3)
C(8)-C(7)-C(10)	126.2(3)
C(8)-C(7)-Cr(1)	71.04(19)
C(10)-C(7)-Cr(1)	125.0(3)
C(7)-C(8)-C(9)	124.5(3)
C(7)-C(8)-Cr(1)	72.52(19)
C(9)-C(8)-Cr(1)	127.6(2)
C(14)-C(13)-P	119.3(3)
C(15)-C(14)-C(13)	121.4(3)
C(17)-C(16)-C(15)	118.9(4)
C(17)-C(18)-C(13)	120.6(3)
C(24)-C(19)-P	121.0(3)
C(19)-C(20)-C(21)	120.7(4)
C(23)-C(22)-C(21)	120.7(4)
C(19)-C(24)-C(23)	121.1(4)
C(103)-C(102)-C(101)	115.0(3)
C(108)-C(104)-C(105)	108.0(3)
C(105)-C(104)-C(103)	126.0(3)
C(105)-C(104)-Cr(2)	71.16(19)
C(106)-C(105)-C(104)	107.8(3)
C(104)-C(105)-C(112)	125.8(3)
C(104)-C(105)-Cr(2)	71.92(19)
C(107)-C(106)-C(105)	108.1(3)
C(105)-C(106)-C(111)	126.1(3)
C(105)-C(106)-Cr(2)	71.9(2)
C(106)-C(107)-C(108)	108.4(3)
C(108)-C(107)-C(110)	125.3(4)
C(108)-C(107)-Cr(2)	72.7(2)
C(104)-C(108)-C(107)	107.7(3)
C(107)-C(108)-C(109)	125.0(4)

C(8)-C(4)-C(5)	108.2(3)
C(5)-C(4)-C(3)	123.8(3)
C(5)-C(4)-Cr(1)	72.6(2)
C(4)-C(5)-C(6)	106.8(3)
C(6)-C(5)-C(12)	126.4(4)
C(6)-C(5)-Cr(1)	70.5(2)
C(7)-C(6)-C(5)	108.5(3)
C(5)-C(6)-C(11)	125.2(3)
C(5)-C(6)-Cr(1)	72.3(2)
C(8)-C(7)-C(6)	108.2(3)
C(6)-C(7)-C(10)	125.5(3)
C(6)-C(7)-Cr(1)	70.70(19)
C(7)-C(8)-C(4)	108.2(3)
C(4)-C(8)-C(9)	126.9(3)
C(4)-C(8)-Cr(1)	71.06(18)
C(14)-C(13)-C(18)	117.2(3)
C(18)-C(13)-P	123.4(3)
C(14)-C(15)-C(16)	120.7(4)
C(16)-C(17)-C(18)	121.1(4)
C(24)-C(19)-C(20)	118.3(3)
C(20)-C(19)-P	120.7(3)
C(22)-C(21)-C(20)	119.4(4)
C(22)-C(23)-C(24)	119.8(4)
C(102)-C(101)-P(2)	111.2(2)
C(104)-C(103)-C(102)	118.5(3)
C(108)-C(104)-C(103)	125.1(3)
C(108)-C(104)-Cr(2)	71.6(2)
C(103)-C(104)-Cr(2)	131.4(3)
C(106)-C(105)-C(112)	126.1(3)
C(106)-C(105)-Cr(2)	71.5(2)
C(112)-C(105)-Cr(2)	127.2(2)
C(107)-C(106)-C(111)	125.7(3)
C(107)-C(106)-Cr(2)	70.7(2)
C(111)-C(106)-Cr(2)	125.2(3)
C(106)-C(107)-C(110)	126.3(4)
C(106)-C(107)-Cr(2)	72.6(2)
C(110)-C(107)-Cr(2)	123.6(3)
C(104)-C(108)-C(109)	127.3(4)
C(104)-C(108)-Cr(2)	72.0(2)

C(107)-C(108)-Cr(2)	70.2(2)	C(109)-C(108)-Cr(2)	125.8(3)
C(118)-C(113)-C(114)	118.0(3)	C(118)-C(113)-P(2)	121.7(3)
C(114)-C(113)-P(2)	120.3(3)	C(115)-C(114)-C(113)	121.1(3)
C(116)-C(115)-C(114)	119.9(4)	C(117)-C(116)-C(115)	119.7(4)
C(116)-C(117)-C(118)	120.7(4)	C(113)-C(118)-C(117)	120.6(4)
C(124)-C(119)-C(120)	118.2(3)	C(124)-C(119)-P(2)	122.9(3)
C(120)-C(119)-P(2)	118.8(3)	C(119)-C(120)-C(121)	120.8(4)
C(122)-C(121)-C(120)	119.6(4)	C(123)-C(122)-C(121)	119.8(4)
C(122)-C(123)-C(124)	121.1(4)	C(123)-C(124)-C(119)	120.4(4)
C(4)-Cr(1)-C(6)	61.88(13)	C(4)-Cr(1)-C(8)	37.15(12)
C(6)-Cr(1)-C(8)	61.45(12)	C(4)-Cr(1)-C(5)	37.07(12)
C(6)-Cr(1)-C(5)	37.18(13)	C(8)-Cr(1)-C(5)	61.79(12)
C(4)-Cr(1)-C(7)	61.44(12)	C(6)-Cr(1)-C(7)	36.69(12)
C(8)-Cr(1)-C(7)	36.44(12)	C(5)-Cr(1)-C(7)	61.51(13)
C(4)-Cr(1)-Cl(1)	147.57(10)	C(6)-Cr(1)-Cl(1)	107.99(11)
C(8)-Cr(1)-Cl(1)	110.42(10)	C(5)-Cr(1)-Cl(1)	145.03(11)
C(7)-Cr(1)-Cl(1)	91.63(10)	C(4)-Cr(1)-Cl(2)	114.14(10)
C(6)-Cr(1)-Cl(2)	100.18(10)	C(8)-Cr(1)-Cl(2)	149.84(10)
C(5)-Cr(1)-Cl(2)	88.93(9)	C(7)-Cr(1)-Cl(2)	135.96(9)
Cl(1)-Cr(1)-Cl(2)	97.67(5)	C(4)-Cr(1)-P	89.93(9)
C(6)-Cr(1)-P	151.63(10)	C(8)-Cr(1)-P	94.67(9)
C(5)-Cr(1)-P	119.73(11)	C(7)-Cr(1)-P	128.25(9)
Cl(1)-Cr(1)-P	94.14(4)	Cl(2)-Cr(1)-P	94.01(4)
C(107)-Cr(2)-C(106)	36.69(13)	C(107)-Cr(2)-C(105)	61.39(13)
C(106)-Cr(2)-C(105)	36.64(12)	C(107)-Cr(2)-C(108)	37.13(13)
C(106)-Cr(2)-C(108)	61.35(13)	C(105)-Cr(2)-C(108)	61.26(13)
C(107)-Cr(2)-C(104)	61.39(13)	C(106)-Cr(2)-C(104)	61.27(12)
C(105)-Cr(2)-C(104)	36.92(12)	C(108)-Cr(2)-C(104)	36.36(13)
C(107)-Cr(2)-Cl(12)	97.30(10)	C(106)-Cr(2)-Cl(12)	131.73(10)
C(105)-Cr(2)-Cl(12)	152.09(10)	C(108)-Cr(2)-Cl(12)	90.83(10)
C(104)-Cr(2)-Cl(12)	118.54(10)	C(107)-Cr(2)-Cl(11)	110.88(11)
C(106)-Cr(2)-Cl(11)	90.84(10)	C(105)-Cr(2)-Cl(11)	106.56(9)
C(108)-Cr(2)-Cl(11)	147.93(10)	C(104)-Cr(2)-Cl(11)	143.30(10)
Cl(12)-Cr(2)-Cl(11)	97.65(5)	C(107)-Cr(2)-P(2)	149.30(10)
C(106)-Cr(2)-P(2)	134.46(10)	C(105)-Cr(2)-P(2)	98.88(9)
C(108)-Cr(2)-P(2)	113.87(10)	C(104)-Cr(2)-P(2)	88.53(9)
Cl(12)-Cr(2)-P(2)	91.70(4)	Cl(11)-Cr(2)-P(2)	96.81(4)
C(13)-P-C(19)	102.34(15)	C(13)-P-C(1)	105.76(16)
C(19)-P-C(1)	104.05(15)	C(13)-P-Cr(1)	117.98(11)

C(19)-P-Cr(1)	117.39(11)	C(1)-P-Cr(1)	107.96(12)
C(119)-P(2)-C(113)	101.98(15)	C(119)-P(2)-C(101)	105.63(17)
C(113)-P(2)-C(101)	104.12(16)	C(119)-P(2)-Cr(2)	115.62(12)
C(113)-P(2)-Cr(2)	120.37(11)	C(101)-P(2)-Cr(2)	107.71(13)

Table 4. Anisotropic displacement parameters (Å²).

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}
C(1)	0.042(2)	0.046(2)	0.041(2)	0.002(2)	-0.002(2)	0.009(2)
C(2)	0.032(2)	0.061(2)	0.053(2)	-0.002(2)	-0.014(2)	0.005(2)
C(3)	0.051(2)	0.054(2)	0.043(2)	0.002(2)	-0.017(2)	0.002(2)
C(4)	0.051(2)	0.044(2)	0.028(2)	-0.003(2)	-0.007(2)	-0.006(2)
C(5)	0.066(3)	0.043(2)	0.028(2)	-0.003(2)	0.002(2)	-0.014(2)
C(6)	0.055(2)	0.059(2)	0.032(2)	-0.010(2)	0.009(2)	-0.020(2)
C(7)	0.048(2)	0.047(2)	0.033(2)	-0.008(2)	0.000(2)	-0.006(2)
C(8)	0.044(2)	0.047(2)	0.029(2)	-0.004(2)	-0.005(2)	-0.012(2)
C(9)	0.059(2)	0.042(2)	0.050(2)	-0.009(2)	-0.001(2)	-0.012(2)
C(10)	0.057(3)	0.067(3)	0.060(3)	-0.012(2)	0.004(2)	0.004(2)
C(11)	0.068(3)	0.085(3)	0.072(3)	-0.010(3)	0.023(3)	-0.034(2)
C(12)	0.118(4)	0.056(3)	0.056(3)	-0.001(2)	0.007(3)	-0.016(3)
C(13)	0.031(2)	0.044(2)	0.029(2)	-0.002(2)	0.001(1)	0.002(2)
C(14)	0.033(2)	0.053(2)	0.062(3)	0.004(2)	0.008(2)	0.002(2)
C(15)	0.052(2)	0.046(2)	0.083(3)	0.003(2)	0.009(2)	0.012(2)
C(16)	0.063(3)	0.038(2)	0.068(3)	-0.005(2)	0.011(2)	-0.007(2)
C(17)	0.039(2)	0.059(3)	0.071(3)	-0.006(2)	0.002(2)	-0.014(2)
C(18)	0.030(2)	0.051(2)	0.056(2)	0.004(2)	-0.003(2)	0.002(2)
C(19)	0.044(2)	0.041(2)	0.027(2)	-0.001(2)	-0.003(2)	0.000(2)
C(20)	0.065(3)	0.053(2)	0.042(2)	-0.003(2)	0.003(2)	0.012(2)
C(21)	0.110(4)	0.068(3)	0.044(3)	-0.004(2)	0.012(3)	0.027(3)
C(22)	0.144(5)	0.068(3)	0.036(2)	-0.010(2)	-0.013(3)	-0.006(3)
C(23)	0.087(4)	0.101(4)	0.048(3)	0.001(3)	-0.026(3)	-0.028(3)
C(24)	0.055(2)	0.086(3)	0.039(2)	0.001(2)	-0.005(2)	-0.011(2)
C(101)	0.033(2)	0.065(2)	0.051(2)	0.003(2)	-0.005(2)	-0.015(2)
C(102)	0.030(2)	0.090(3)	0.057(3)	0.003(2)	-0.009(2)	-0.002(2)
C(103)	0.043(2)	0.082(3)	0.048(2)	0.005(2)	-0.008(2)	-0.008(2)
C(104)	0.036(2)	0.054(2)	0.037(2)	0.002(2)	-0.001(2)	-0.004(2)
C(105)	0.045(2)	0.040(2)	0.037(2)	0.003(2)	0.000(2)	0.001(2)
C(106)	0.040(2)	0.043(2)	0.045(2)	0.008(2)	0.001(2)	-0.003(2)
C(107)	0.050(2)	0.056(2)	0.045(2)	0.000(2)	0.013(2)	0.002(2)
C(108)	0.057(2)	0.051(2)	0.044(2)	-0.010(2)	0.005(2)	-0.007(2)
C(109)	0.104(4)	0.077(3)	0.087(4)	-0.033(3)	0.005(3)	-0.018(3)

C(110)	0.068(3)	0.083(3)	0.091(4)	-0.006(3)	0.033(3)	0.016(3)
C(111)	0.052(2)	0.059(3)	0.088(3)	0.014(2)	0.003(2)	-0.018(2)
C(112)	0.060(3)	0.045(2)	0.061(3)	0.002(2)	-0.003(2)	0.011(2)
C(113)	0.034(2)	0.038(2)	0.041(2)	0.004(2)	0.002(2)	0.005(2)
C(114)	0.041(2)	0.056(2)	0.049(2)	-0.006(2)	-0.002(2)	0.006(2)
C(115)	0.053(3)	0.057(2)	0.062(3)	-0.015(2)	-0.012(2)	0.006(2)
C(116)	0.075(3)	0.059(3)	0.058(3)	-0.010(2)	0.003(2)	0.026(2)
C(117)	0.063(3)	0.066(3)	0.086(3)	0.001(3)	0.026(3)	0.026(2)
C(118)	0.050(2)	0.054(2)	0.079(3)	-0.002(2)	0.025(2)	0.005(2)
C(119)	0.048(2)	0.039(2)	0.036(2)	0.000(2)	0.005(2)	0.006(2)
C(120)	0.053(2)	0.060(2)	0.055(3)	0.008(2)	-0.002(2)	-0.005(2)
C(121)	0.076(3)	0.079(3)	0.055(3)	0.011(2)	-0.012(2)	0.022(3)
C(122)	0.097(4)	0.050(3)	0.058(3)	0.016(2)	0.018(3)	0.015(3)
C(123)	0.074(3)	0.072(3)	0.084(3)	0.032(3)	0.021(3)	0.000(3)
C(124)	0.057(3)	0.064(3)	0.067(3)	0.024(2)	0.004(2)	-0.004(2)
Cl(1)	0.031(1)	0.133(1)	0.058(1)	-0.001(1)	-0.003(1)	0.017(1)
Cl(2)	0.124(1)	0.085(1)	0.048(1)	-0.019(1)	0.007(1)	-0.064(1)
Cl(11)	0.032(1)	0.089(1)	0.071(1)	0.002(1)	-0.011(1)	-0.007(1)
Cl(12)	0.116(1)	0.042(1)	0.086(1)	0.004(1)	0.029(1)	0.025(1)
Cr(1)	0.033(1)	0.053(1)	0.032(1)	-0.007(1)	0.001(1)	-0.013(1)
Cr(2)	0.030(1)	0.035(1)	0.043(1)	-0.001(1)	0.005(1)	0.001(1)
P	0.028(1)	0.041(1)	0.030(1)	-0.002(1)	-0.002(1)	0.000(1)
P(2)	0.027(1)	0.038(1)	0.039(1)	0.000(1)	0.001(1)	-0.002(1)

Molecular structure and data of ($Ph_2PC_2H_4C_5H_4$)$CrCl_2$.Toluene (7j')

CCDC 155401

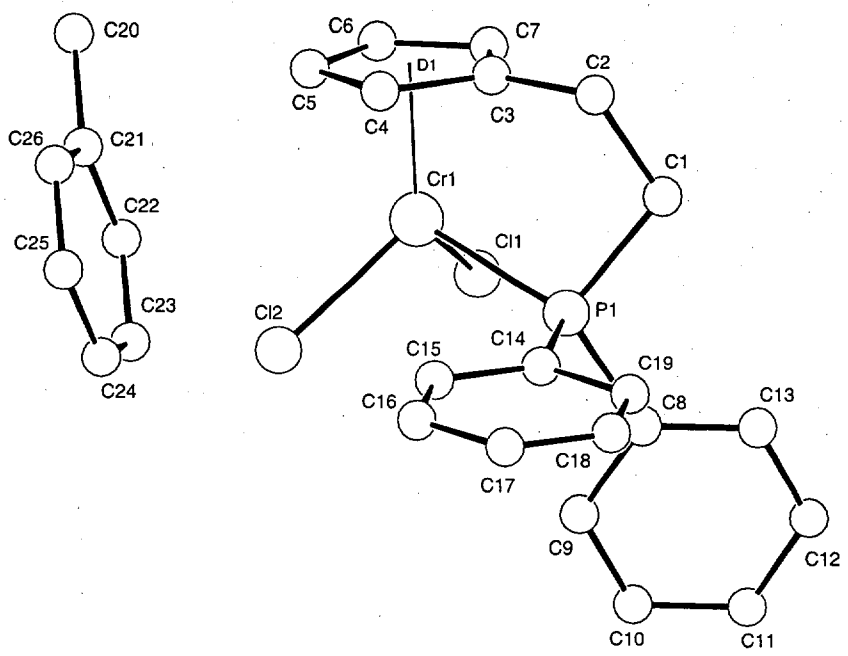

Table 1. Crystal data and structure refinement.

Identification code	2633	
Empirical formula	$C_{26}H_{26}Cl_2CrP$	
Color	dark blue	
Formula weight	492.34 $g \cdot mol^{-1}$	
Temperature	293 K	
Wavelength	0.71069 Å	
Crystal system	Triclinic	
Space group	**P1, (no. 2)**	
Unit cell dimensions	a = 9.2684(10) Å	α= 98.722(11)°.
	b = 9.7942(11) Å	β= 96.066(11)°.
	c = 14.477(3) Å	γ = 110.833(8)°.
Volume	1195.8(3) $Å^3$	
Z	2	
Density (calculated)	1.367 $Mg \cdot m^{-3}$	
Absorption coefficient	0.780 mm^{-1}	
F(000)	510 e	
Crystal size	0.63 x 0.32 x 0.14 mm^3	
θ range for data collection	2.27 to 26.31°.	
Index ranges	$-11 \leq h \leq 11$, $-12 \leq k \leq 12$, $0 \leq l \leq 18$	
Reflections collected	4854	
Independent reflections	4854 [R_{int} = 0.0000]	
Reflections with $I>2\sigma(I)$	3209	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4854 / 0 / 375	
Goodness-of-fit on F^2	0.792	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0361	wR^2 = 0.1054
R indices (all data)	R_1 = 0.0855	wR^2 = 0.1221
Largest diff. peak and hole	0.319 and -0.270 e $\cdot$ $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å^2).
U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	0.2002(3)	0.5489(3)	0.3399(2)	0.044(1)
C(2)	0.3461(3)	0.5205(4)	0.3775(2)	0.052(1)
C(3)	0.3047(3)	0.3906(3)	0.4269(2)	0.045(1)
C(4)	0.3154(3)	0.2501(4)	0.3956(2)	0.051(1)
C(5)	0.2578(4)	0.1595(4)	0.4608(3)	0.063(1)
C(6)	0.2092(4)	0.2403(4)	0.5299(2)	0.062(1)
C(7)	0.2366(4)	0.3824(4)	0.5091(2)	0.053(1)
C(8)	-0.1274(3)	0.3990(3)	0.2449(2)	0.040(1)
C(9)	-0.2640(3)	0.2718(4)	0.2137(2)	0.054(1)
C(10)	-0.4042(4)	0.2867(4)	0.1868(3)	0.064(1)
C(11)	-0.4114(4)	0.4247(4)	0.1908(2)	0.059(1)
C(12)	-0.2769(4)	0.5509(4)	0.2237(2)	0.057(1)
C(13)	-0.1356(4)	0.5385(4)	0.2510(2)	0.047(1)
C(14)	0.1173(3)	0.3367(3)	0.1631(2)	0.037(1)
C(15)	0.1346(4)	0.2045(3)	0.1304(2)	0.048(1)
C(16)	0.1848(4)	0.1813(4)	0.0449(2)	0.056(1)
C(17)	0.2170(4)	0.2893(4)	-0.0086(2)	0.056(1)
C(18)	0.2005(5)	0.4206(4)	0.0235(2)	0.066(1)
C(19)	0.1497(4)	0.4447(4)	0.1079(2)	0.056(1)
C(20)	0.4942(7)	-0.0754(7)	0.3488(4)	0.101(2)
C(21)	0.4204(4)	-0.1092(4)	0.2470(3)	0.066(1)
C(22)	0.2693(4)	-0.1157(4)	0.2235(3)	0.061(1)
C(23)	0.1994(5)	-0.1462(4)	0.1311(3)	0.074(1)
C(24)	0.2789(7)	-0.1709(5)	0.0584(4)	0.089(1)
C(25)	0.4271(6)	-0.1651(5)	0.0798(4)	0.090(1)
C(26)	0.4980(5)	-0.1344(4)	0.1725(4)	0.080(1)
Cl(1)	-0.1453(1)	0.2342(1)	0.4533(1)	0.064(1)
Cl(2)	-0.0633(1)	-0.0165(1)	0.2925(1)	0.051(1)
Cr(1)	0.0624(1)	0.2128(1)	0.3908(1)	0.039(1)
P(1)	0.0528(1)	0.3705(1)	0.2763(1)	0.035(1)

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

C(1)-C(2)	1.536(4)	C(1)-P(1)	1.821(3)
C(2)-C(3)	1.505(4)	C(3)-C(7)	1.404(4)
C(3)-C(4)	1.424(5)	C(3)-Cr(1)	2.246(3)
C(4)-C(5)	1.409(5)	C(4)-Cr(1)	2.233(3)
C(5)-C(6)	1.394(6)	C(5)-Cr(1)	2.242(3)
C(6)-C(7)	1.409(5)	C(6)-Cr(1)	2.230(3)
C(7)-Cr(1)	2.223(3)	C(8)-C(13)	1.386(4)
C(8)-C(9)	1.395(4)	C(8)-P(1)	1.812(3)
C(9)-C(10)	1.380(5)	C(10)-C(11)	1.370(5)
C(11)-C(12)	1.381(5)	C(12)-C(13)	1.380(5)
C(14)-C(15)	1.379(4)	C(14)-C(19)	1.390(4)
C(14)-P(1)	1.826(3)	C(15)-C(16)	1.384(4)
C(16)-C(17)	1.371(5)	C(17)-C(18)	1.366(5)
C(18)-C(19)	1.373(5)	C(20)-C(21)	1.492(7)
C(21)-C(22)	1.382(5)	C(21)-C(26)	1.397(6)
C(22)-C(23)	1.362(6)	C(23)-C(24)	1.386(7)
C(24)-C(25)	1.355(7)	C(25)-C(26)	1.370(7)
Cl(1)-Cr(1)	2.2720(9)	Cl(2)-Cr(1)	2.2903(9)
Cr(1)-P(1)	2.4469(8)		
C(2)-C(1)-P(1)	107.5(2)	C(3)-C(2)-C(1)	111.7(2)
C(7)-C(3)-C(4)	107.4(3)	C(7)-C(3)-C(2)	125.7(3)
C(4)-C(3)-C(2)	126.8(3)	C(7)-C(3)-Cr(1)	70.8(2)
C(4)-C(3)-Cr(1)	71.0(2)	C(2)-C(3)-Cr(1)	119.9(2)
C(5)-C(4)-C(3)	107.7(3)	C(5)-C(4)-Cr(1)	72.0(2)
C(3)-C(4)-Cr(1)	71.9(2)	C(6)-C(5)-C(4)	108.2(3)
C(6)-C(5)-Cr(1)	71.4(2)	C(4)-C(5)-Cr(1)	71.3(2)
C(5)-C(6)-C(7)	108.4(3)	C(5)-C(6)-Cr(1)	72.3(2)
C(7)-C(6)-Cr(1)	71.3(2)	C(3)-C(7)-C(6)	108.2(3)
C(3)-C(7)-Cr(1)	72.6(2)	C(6)-C(7)-Cr(1)	71.8(2)
C(13)-C(8)-C(9)	119.3(3)	C(13)-C(8)-P(1)	123.6(2)
C(9)-C(8)-P(1)	117.1(2)	C(10)-C(9)-C(8)	119.6(3)
C(11)-C(10)-C(9)	121.0(3)	C(10)-C(11)-C(12)	119.5(3)
C(13)-C(12)-C(11)	120.5(3)	C(12)-C(13)-C(8)	120.1(3)
C(15)-C(14)-C(19)	118.6(3)	C(15)-C(14)-P(1)	121.3(2)
C(19)-C(14)-P(1)	120.2(2)	C(14)-C(15)-C(16)	120.5(3)
C(17)-C(16)-C(15)	120.2(3)	C(18)-C(17)-C(16)	119.7(3)

C(17)-C(18)-C(19)	120.8(3)	C(18)-C(19)-C(14)	120.3(3)
C(22)-C(21)-C(26)	117.4(4)	C(22)-C(21)-C(20)	119.9(5)
C(26)-C(21)-C(20)	122.8(4)	C(23)-C(22)-C(21)	121.0(4)
C(22)-C(23)-C(24)	120.6(4)	C(25)-C(24)-C(23)	119.5(5)
C(24)-C(25)-C(26)	120.2(5)	C(25)-C(26)-C(21)	121.4(4)
C(7)-Cr(1)-C(6)	36.89(13)	C(7)-Cr(1)-C(4)	61.51(13)
C(6)-Cr(1)-C(4)	61.15(13)	C(7)-Cr(1)-C(5)	61.21(15)
C(6)-Cr(1)-C(5)	36.31(14)	C(4)-Cr(1)-C(5)	36.71(12)
C(7)-Cr(1)-C(3)	36.62(11)	C(6)-Cr(1)-C(3)	61.22(12)
C(4)-Cr(1)-C(3)	37.07(12)	C(5)-Cr(1)-C(3)	61.31(12)
C(7)-Cr(1)-Cl(1)	93.22(10)	C(6)-Cr(1)-Cl(1)	95.43(11)
C(4)-Cr(1)-Cl(1)	154.03(10)	C(5)-Cr(1)-Cl(1)	127.51(11)
C(3)-Cr(1)-Cl(1)	123.61(9)	C(7)-Cr(1)-Cl(2)	156.67(10)
C(6)-Cr(1)-Cl(2)	121.41(11)	C(4)-Cr(1)-Cl(2)	103.13(9)
C(5)-Cr(1)-Cl(2)	95.81(11)	C(3)-Cr(1)-Cl(2)	137.61(9)
Cl(1)-Cr(1)-Cl(2)	98.74(3)	C(7)-Cr(1)-P(1)	99.88(9)
C(6)-Cr(1)-P(1)	136.06(10)	C(4)-Cr(1)-P(1)	95.75(9)
C(5)-Cr(1)-P(1)	132.40(10)	C(3)-Cr(1)-P(1)	77.80(7)
Cl(1)-Cr(1)-P(1)	94.43(3)	Cl(2)-Cr(1)-P(1)	99.08(3)
C(8)-P(1)-C(1)	107.67(13)	C(8)-P(1)-C(14)	104.27(12)
C(1)-P(1)-C(14)	104.35(13)	C(8)-P(1)-Cr(1)	118.84(9)
C(1)-P(1)-Cr(1)	100.68(10)	C(14)-P(1)-Cr(1)	119.54(9)

Table 4. Anisotropic displacement parameters (Å²).

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}
C(1)	0.048(2)	0.032(1)	0.044(2)	0.007(1)	0.007(1)	0.007(1)
C(2)	0.039(2)	0.054(2)	0.051(2)	0.014(2)	0.002(1)	0.004(1)
C(3)	0.035(1)	0.050(2)	0.043(2)	0.013(1)	-0.002(1)	0.007(1)
C(4)	0.044(2)	0.060(2)	0.050(2)	0.014(2)	0.004(1)	0.020(1)
C(5)	0.058(2)	0.058(2)	0.069(2)	0.022(2)	-0.010(2)	0.019(2)
C(6)	0.058(2)	0.077(2)	0.043(2)	0.024(2)	-0.001(2)	0.010(2)
C(7)	0.051(2)	0.056(2)	0.040(2)	0.008(1)	-0.001(1)	0.008(2)
C(8)	0.039(1)	0.046(2)	0.037(1)	0.014(1)	0.010(1)	0.016(1)
C(9)	0.043(2)	0.047(2)	0.067(2)	0.011(2)	0.005(1)	0.014(1)
C(10)	0.041(2)	0.073(2)	0.069(2)	0.012(2)	0.003(2)	0.015(2)
C(11)	0.052(2)	0.089(3)	0.050(2)	0.018(2)	0.010(2)	0.041(2)
C(12)	0.067(2)	0.066(2)	0.054(2)	0.021(2)	0.017(2)	0.040(2)
C(13)	0.051(2)	0.046(2)	0.049(2)	0.014(1)	0.009(1)	0.020(1)
C(14)	0.037(1)	0.037(1)	0.034(1)	0.008(1)	0.006(1)	0.012(1)
C(15)	0.059(2)	0.042(2)	0.047(2)	0.014(1)	0.014(1)	0.023(1)
C(16)	0.075(2)	0.053(2)	0.053(2)	0.011(2)	0.020(2)	0.035(2)
C(17)	0.065(2)	0.067(2)	0.042(2)	0.013(2)	0.021(2)	0.028(2)
C(18)	0.100(3)	0.061(2)	0.049(2)	0.028(2)	0.029(2)	0.033(2)
C(19)	0.086(2)	0.045(2)	0.052(2)	0.021(1)	0.028(2)	0.035(2)
C(20)	0.090(4)	0.073(3)	0.111(4)	0.019(3)	-0.025(3)	0.008(3)
C(21)	0.057(2)	0.040(2)	0.093(3)	0.016(2)	-0.004(2)	0.012(2)
C(22)	0.052(2)	0.044(2)	0.085(3)	0.013(2)	0.006(2)	0.017(1)
C(23)	0.069(3)	0.053(2)	0.100(3)	0.017(2)	-0.007(2)	0.028(2)
C(24)	0.119(4)	0.063(3)	0.079(3)	0.016(2)	0.001(3)	0.032(3)
C(25)	0.100(4)	0.083(3)	0.098(4)	0.022(3)	0.024(3)	0.043(3)
C(26)	0.054(2)	0.057(2)	0.133(4)	0.022(2)	0.019(3)	0.022(2)
Cl(1)	0.055(1)	0.071(1)	0.059(1)	0.004(1)	0.023(1)	0.017(1)
Cl(2)	0.053(1)	0.041(1)	0.052(1)	0.010(1)	0.009(1)	0.009(1)
Cr(1)	0.039(1)	0.041(1)	0.036(1)	0.012(1)	0.006(1)	0.010(1)
P(1)	0.036(1)	0.034(1)	0.034(1)	0.008(1)	0.007(1)	0.011(1)

Molecular structure and data of $(Cy_2PC_2H_4C_5H_4)CrMe_2$ (15a)

CCDC 155402

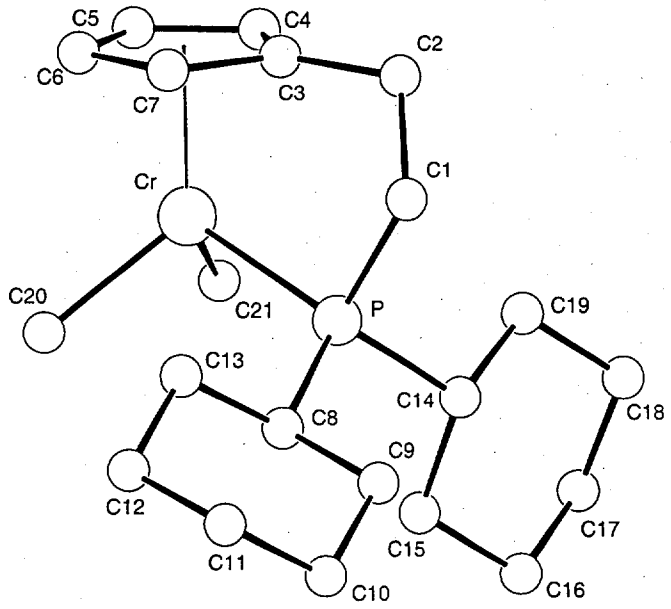

Table 1. Crystal data and structure refinement.

Identification code	2617	
Empirical formula	$C_{21}H_{36}CrP$	
Color	black	
Formula weight	371.47 $g \cdot mol^{-1}$	
Temperature	293 K	
Wavelength	0.71069 Å	
Crystal system	Monoclinic	
Space group	**$P2_1/n$, (no. 14)**	
Unit cell dimensions	a = 8.5482(9) Å	a= 90°.
	b = 19.671(3) Å	b= 104.263(8)°.
	c = 12.7262(11) Å	g = 90°.
Volume	2074.0(4) $Å^3$	
Z	4	
Density (calculated)	1.190 $Mg \cdot m^{-3}$	
Absorption coefficient	0.628 mm^{-1}	
F(000)	804 e	
Crystal size	0.35 x 0.18 x 0.11 mm^3	
q range for data collection	2.60 to 26.29°.	
Index ranges	$-10 \le h \le 10, 0 \le k \le 24, 0 \le l \le 15$	
Reflections collected	4211	
Independent reflections	4211 [R_{int} = 0.0000]	
Reflections with I>2s(I)	2649	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4211 / 0 / 208	
Goodness-of-fit on F^2	0.912	
Final R indices [I>2s(I)]	R_1 = 0.0466	wR^2 = 0.1277
R indices (all data)	R_1 = 0.1102	wR^2 = 0.1446
Largest diff. peak and hole	0.457 and -0.509 $e \cdot Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å^2).
U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	0.5490(4)	0.8219(2)	1.0257(2)	0.045(1)
C(2)	0.4780(4)	0.8791(2)	1.0811(3)	0.049(1)
C(3)	0.2952(4)	0.8753(2)	1.0551(2)	0.047(1)
C(4)	0.1876(5)	0.9274(2)	1.0088(3)	0.064(1)
C(5)	0.0283(5)	0.9009(2)	0.9898(3)	0.067(1)
C(6)	0.0391(5)	0.8342(2)	1.0244(3)	0.061(1)
C(7)	0.2020(4)	0.8174(2)	1.0645(3)	0.051(1)
C(8)	0.4619(4)	0.7157(2)	0.8609(2)	0.040(1)
C(9)	0.6371(4)	0.6937(2)	0.8717(3)	0.054(1)
C(10)	0.6476(5)	0.6185(2)	0.8450(3)	0.064(1)
C(11)	0.5667(5)	0.5741(2)	0.9125(3)	0.068(1)
C(12)	0.3930(6)	0.5954(2)	0.9018(4)	0.073(1)
C(13)	0.3822(5)	0.6701(2)	0.9306(3)	0.058(1)
C(14)	0.5458(4)	0.8516(2)	0.8001(2)	0.038(1)
C(15)	0.4799(4)	0.8349(2)	0.6801(3)	0.051(1)
C(16)	0.5672(5)	0.8749(2)	0.6091(3)	0.065(1)
C(17)	0.5615(5)	0.9496(2)	0.6279(3)	0.067(1)
C(18)	0.6319(5)	0.9666(2)	0.7462(3)	0.059(1)
C(19)	0.5461(4)	0.9281(2)	0.8198(3)	0.047(1)
C(20)	0.0276(5)	0.7659(2)	0.7976(4)	0.079(1)
C(21)	0.0991(5)	0.9070(3)	0.7498(3)	0.083(2)
Cr	0.1598(1)	0.8438(1)	0.8849(1)	0.038(1)
P	0.4333(1)	0.8066(1)	0.8850(1)	0.033(1)

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

C(1)-C(2)	1.531(5)	C(1)-P	1.844(3)
C(2)-C(3)	1.517(5)	C(3)-C(4)	1.406(5)
C(3)-C(7)	1.411(5)	C(3)-Cr	2.277(3)
C(4)-C(5)	1.422(6)	C(4)-Cr	2.250(3)
C(5)-C(6)	1.380(6)	C(5)-Cr	2.246(4)
C(6)-C(7)	1.399(5)	C(6)-Cr	2.271(3)
C(7)-Cr	2.285(3)	C(8)-C(9)	1.532(4)
C(8)-C(13)	1.534(4)	C(8)-P	1.841(3)
C(9)-C(10)	1.526(5)	C(10)-C(11)	1.507(6)
C(11)-C(12)	1.517(6)	C(12)-C(13)	1.521(5)
C(14)-C(19)	1.526(4)	C(14)-C(15)	1.527(4)
C(14)-P	1.841(3)	C(15)-C(16)	1.526(5)
C(16)-C(17)	1.492(6)	C(17)-C(18)	1.515(5)
C(18)-C(19)	1.525(4)	C(20)-Cr	2.058(4)
C(21)-Cr	2.082(4)	Cr-P	2.4493(9)
C(2)-C(1)-P	112.9(2)	C(3)-C(2)-C(1)	111.6(3)
C(4)-C(3)-C(7)	107.4(3)	C(4)-C(3)-C(2)	126.0(4)
C(7)-C(3)-C(2)	126.4(3)	C(4)-C(3)-Cr	70.9(2)
C(7)-C(3)-Cr	72.3(2)	C(2)-C(3)-Cr	118.4(2)
C(3)-C(4)-C(5)	107.7(4)	C(3)-C(4)-Cr	72.9(2)
C(5)-C(4)-Cr	71.4(2)	C(6)-C(5)-C(4)	108.0(4)
C(6)-C(5)-Cr	73.2(2)	C(4)-C(5)-Cr	71.7(2)
C(5)-C(6)-C(7)	108.8(4)	C(5)-C(6)-Cr	71.2(2)
C(7)-C(6)-Cr	72.7(2)	C(6)-C(7)-C(3)	108.1(4)
C(6)-C(7)-Cr	71.6(2)	C(3)-C(7)-Cr	71.7(2)
C(9)-C(8)-C(13)	110.3(3)	C(9)-C(8)-P	115.2(2)
C(13)-C(8)-P	112.1(2)	C(10)-C(9)-C(8)	111.3(3)
C(11)-C(10)-C(9)	112.0(3)	C(10)-C(11)-C(12)	111.4(3)
C(11)-C(12)-C(13)	111.2(3)	C(12)-C(13)-C(8)	111.3(3)
C(19)-C(14)-C(15)	111.2(3)	C(19)-C(14)-P	111.0(2)
C(15)-C(14)-P	111.4(2)	C(16)-C(15)-C(14)	111.6(3)
C(17)-C(16)-C(15)	111.9(3)	C(16)-C(17)-C(18)	110.9(3)
C(17)-C(18)-C(19)	111.5(3)	C(18)-C(19)-C(14)	111.8(3)
C(20)-Cr-C(21)	90.4(2)	C(20)-Cr-C(5)	113.8(2)
C(21)-Cr-C(5)	97.6(2)	C(20)-Cr-C(4)	150.6(2)
C(21)-Cr-C(4)	95.9(2)	C(5)-Cr-C(4)	36.86(15)

C(20)-Cr-C(6)	93.8(2)	C(21)-Cr-C(6)	128.8(2)
C(5)-Cr-C(6)	35.58(15)	C(4)-Cr-C(6)	60.2(2)
C(20)-Cr-C(3)	143.0(2)	C(21)-Cr-C(3)	126.0(2)
C(5)-Cr-C(3)	60.64(13)	C(4)-Cr-C(3)	36.17(12)
C(6)-Cr-C(3)	60.05(13)	C(20)-Cr-C(7)	107.6(2)
C(21)-Cr-C(7)	155.2(2)	C(5)-Cr-C(7)	59.83(14)
C(4)-Cr-C(7)	60.06(14)	C(6)-Cr-C(7)	35.77(13)
C(3)-Cr-C(7)	36.04(13)	C(20)-Cr-P	100.10(13)
C(21)-Cr-P	102.88(12)	C(5)-Cr-P	140.01(11)
C(4)-Cr-P	106.37(11)	C(6)-Cr-P	126.31(10)
C(3)-Cr-P	79.59(8)	C(7)-Cr-P	90.93(9)
C(8)-P-C(14)	105.04(13)	C(8)-P-C(1)	104.99(15)
C(14)-P-C(1)	104.97(15)	C(8)-P-Cr	117.12(10)
C(14)-P-Cr	119.52(10)	C(1)-P-Cr	103.62(10)

Table 4. Anisotropic displacement parameters (Å²).

The anisotropic displacement factor exponent takes the form:
$-2p^2[\, h^2 a^{*2} U_{11} + \ldots + 2\, h\, k\, a^*\, b^*\, U_{12}\,]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	0.040(2)	0.059(2)	0.034(2)	0.004(1)	0.006(1)	0.005(2)
C(2)	0.051(2)	0.053(2)	0.040(2)	-0.011(2)	0.006(2)	-0.001(2)
C(3)	0.055(2)	0.056(2)	0.029(2)	-0.013(2)	0.008(1)	0.014(2)
C(4)	0.075(3)	0.056(2)	0.059(2)	-0.022(2)	0.010(2)	0.017(2)
C(5)	0.057(2)	0.088(3)	0.053(2)	-0.019(2)	0.008(2)	0.028(2)
C(6)	0.050(2)	0.096(3)	0.043(2)	-0.003(2)	0.021(2)	0.006(2)
C(7)	0.052(2)	0.074(2)	0.031(2)	0.006(2)	0.017(1)	0.006(2)
C(8)	0.052(2)	0.034(2)	0.037(2)	0.000(1)	0.016(1)	0.001(1)
C(9)	0.061(2)	0.046(2)	0.064(2)	0.002(2)	0.029(2)	0.013(2)
C(10)	0.080(3)	0.047(2)	0.070(2)	-0.001(2)	0.028(2)	0.023(2)
C(11)	0.098(3)	0.041(2)	0.064(3)	0.000(2)	0.016(2)	0.013(2)
C(12)	0.093(3)	0.042(2)	0.090(3)	0.005(2)	0.032(2)	-0.009(2)
C(13)	0.069(2)	0.045(2)	0.067(2)	0.009(2)	0.033(2)	0.000(2)
C(14)	0.041(2)	0.042(2)	0.033(2)	0.003(1)	0.016(1)	-0.001(1)
C(15)	0.063(2)	0.057(2)	0.037(2)	-0.003(2)	0.020(2)	-0.008(2)
C(16)	0.079(3)	0.084(3)	0.038(2)	0.001(2)	0.027(2)	-0.015(2)
C(17)	0.071(3)	0.079(3)	0.052(2)	0.025(2)	0.019(2)	-0.007(2)
C(18)	0.070(2)	0.052(2)	0.060(2)	0.009(2)	0.026(2)	-0.013(2)
C(19)	0.056(2)	0.046(2)	0.042(2)	0.000(2)	0.017(2)	-0.007(2)
C(20)	0.061(3)	0.098(3)	0.074(3)	-0.039(3)	0.011(2)	-0.016(2)
C(21)	0.059(2)	0.120(4)	0.069(3)	0.047(3)	0.012(2)	0.026(3)
Cr	0.038(1)	0.046(1)	0.029(1)	-0.001(1)	0.008(1)	0.005(1)
P	0.038(1)	0.035(1)	0.029(1)	0.000(1)	0.011(1)	0.002(1)

Molecular structure and data of $(Cy_2PC_3H_6C_5H_4)CrCl_2$ (9a)

CCDC 155403

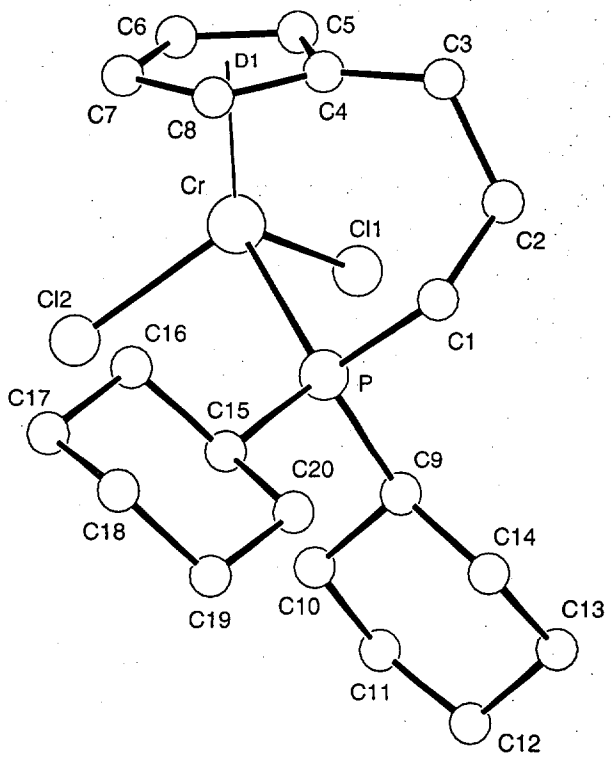

Table 1. Crystal data and structure refinement.

Identification code	2860	
Empirical formula	$C_{20}H_{32}Cl_2CrP$	
Color	blue	
Formula weight	426.33 $g \cdot mol^{-1}$	
Temperature	293 K	
Wavelength	0.71069 Å	
Crystal system	Monoclinic	
Space group	**$P2_1/c$, (no. 14)**	
Unit cell dimensions	a = 13.693(2) Å	α= 90°.
	b = 7.5311(9) Å	β= 93.662(12)°.
	c = 20.151(3) Å	γ = 90°.
Volume	2073.7(5) $Å^3$	
Z	4	
Density (calculated)	1.366 $Mg \cdot m^{-3}$	
Absorption coefficient	0.887 mm^{-1}	
F(000)	900 e	
Crystal size	0.46 x 0.32 x 0.18 mm^3	
θ range for data collection	1.49 to 24.96°.	
Index ranges	$-16 \le h \le 16$, $0 \le k \le 8$, $0 \le l \le 23$	
Reflections collected	3627	
Independent reflections	3627 [R_{int} = 0.0000]	
Reflections with $I>2\sigma(I)$	2228	
Completeness to θ = 24.96°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3627 / 0 / 217	
Goodness-of-fit on F^2	0.793	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0464	wR^2 = 0.1249
R indices (all data)	R_1 = 0.1112	wR^2 = 0.1467
Largest diff. peak and hole	0.775 and -0.365 $e \cdot Å^{-3}$	

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

C(1)-C(2)	1.514(6)	C(1)-P	1.833(4)
C(2)-C(3)	1.512(7)	C(3)-C(4)	1.505(7)
C(4)-C(8)	1.407(7)	C(4)-C(5)	1.408(7)
C(4)-Cr	2.255(4)	C(5)-C(6)	1.383(7)
C(5)-Cr	2.237(5)	C(6)-C(7)	1.393(7)
C(6)-Cr	2.210(5)	C(7)-C(8)	1.395(7)
C(7)-Cr	2.230(5)	C(8)-Cr	2.227(5)
C(9)-C(14)	1.490(7)	C(9)-C(10)	1.521(6)
C(9)-P	1.847(4)	C(10)-C(11)	1.530(7)
C(11)-C(12)	1.454(8)	C(12)-C(13)	1.507(8)
C(13)-C(14)	1.537(7)	C(15)-C(16)	1.519(6)
C(15)-C(20)	1.534(6)	C(15)-P	1.855(4)
C(16)-C(17)	1.524(6)	C(17)-C(18)	1.513(7)
C(18)-C(19)	1.503(7)	C(19)-C(20)	1.520(6)
Cl(1)-Cr	2.2930(14)	Cl(2)-Cr	2.2834(13)
Cr-P	2.4591(12)		
C(2)-C(1)-P	112.8(3)	C(1)-C(2)-C(3)	114.6(4)
C(2)-C(3)-C(4)	116.9(4)	C(8)-C(4)-C(5)	105.4(4)
C(8)-C(4)-C(3)	128.2(5)	C(5)-C(4)-C(3)	126.3(5)
C(8)-C(4)-Cr	70.6(3)	C(5)-C(4)-Cr	71.1(3)
C(3)-C(4)-Cr	124.0(3)	C(6)-C(5)-C(4)	109.5(5)
C(6)-C(5)-Cr	70.8(3)	C(4)-C(5)-Cr	72.4(2)
C(5)-C(6)-C(7)	108.2(5)	C(5)-C(6)-Cr	73.0(3)
C(7)-C(6)-Cr	72.5(3)	C(8)-C(7)-C(6)	107.3(5)
C(8)-C(7)-Cr	71.6(3)	C(6)-C(7)-Cr	71.0(3)
C(7)-C(8)-C(4)	109.5(5)	C(7)-C(8)-Cr	71.9(3)
C(4)-C(8)-Cr	72.8(3)	C(14)-C(9)-C(10)	111.3(4)
C(14)-C(9)-P	120.3(4)	C(10)-C(9)-P	111.2(3)
C(11)-C(10)-C(9)	111.1(4)	C(12)-C(11)-C(10)	113.5(5)
C(11)-C(12)-C(13)	112.3(5)	C(12)-C(13)-C(14)	110.0(4)
C(9)-C(14)-C(13)	110.4(5)	C(16)-C(15)-C(20)	109.7(4)
C(16)-C(15)-P	112.3(3)	C(20)-C(15)-P	113.1(3)
C(15)-C(16)-C(17)	111.2(4)	C(18)-C(17)-C(16)	111.6(4)
C(19)-C(18)-C(17)	109.9(4)	C(18)-C(19)-C(20)	111.4(4)
C(19)-C(20)-C(15)	111.8(4)	C(6)-Cr-C(8)	60.8(2)
C(6)-Cr-C(7)	36.56(19)	C(8)-Cr-C(7)	36.48(19)

C(6)-Cr-C(5)	36.22(18)	C(8)-Cr-C(5)	60.24(18)
C(7)-Cr-C(5)	60.4(2)	C(6)-Cr-C(4)	61.39(19)
C(8)-Cr-C(4)	36.59(17)	C(7)-Cr-C(4)	61.35(18)
C(5)-Cr-C(4)	36.54(17)	C(6)-Cr-Cl(2)	103.73(14)
C(8)-Cr-Cl(2)	116.82(13)	C(7)-Cr-Cl(2)	92.77(14)
C(5)-Cr-Cl(2)	138.88(14)	C(4)-Cr-Cl(2)	152.70(14)
C(6)-Cr-Cl(1)	105.09(17)	C(8)-Cr-Cl(1)	143.56(13)
C(7)-Cr-Cl(1)	141.64(15)	C(5)-Cr-Cl(1)	88.21(15)
C(4)-Cr-Cl(1)	107.05(14)	Cl(2)-Cr-Cl(1)	98.77(6)
C(6)-Cr-P	149.78(15)	C(8)-Cr-P	89.79(14)
C(7)-Cr-P	120.68(16)	C(5)-Cr-P	124.48(13)
C(4)-Cr-P	91.23(12)	Cl(2)-Cr-P	95.47(5)
Cl(1)-Cr-P	94.59(5)	C(1)-P-C(9)	105.8(2)
C(1)-P-C(15)	105.73(19)	C(9)-P-C(15)	107.4(2)
C(1)-P-Cr	108.24(14)	C(9)-P-Cr	110.70(16)
C(15)-P-Cr	118.25(13)		

Table 4. Anisotropic displacement parameters (Å²).

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}
C(1)	0.046(3)	0.023(2)	0.048(2)	0.001(2)	0.000(2)	-0.007(2)
C(2)	0.042(3)	0.041(3)	0.065(3)	0.000(2)	0.007(2)	-0.020(2)
C(3)	0.073(4)	0.044(3)	0.064(3)	0.004(3)	0.016(3)	-0.028(3)
C(4)	0.055(3)	0.042(3)	0.040(2)	0.006(2)	0.013(2)	-0.009(2)
C(5)	0.060(3)	0.050(3)	0.051(3)	-0.009(3)	0.024(2)	-0.005(3)
C(6)	0.087(4)	0.056(4)	0.040(3)	-0.010(3)	0.015(3)	-0.019(3)
C(7)	0.058(3)	0.073(4)	0.040(3)	0.006(3)	-0.005(2)	-0.013(3)
C(8)	0.053(3)	0.047(3)	0.046(3)	0.015(2)	0.009(2)	0.011(2)
C(9)	0.051(3)	0.034(3)	0.043(3)	0.007(2)	-0.007(2)	-0.008(2)
C(10)	0.050(3)	0.043(3)	0.041(2)	0.010(2)	-0.008(2)	-0.008(2)
C(11)	0.122(5)	0.047(3)	0.068(4)	0.026(3)	-0.037(4)	-0.021(4)
C(12)	0.102(5)	0.075(5)	0.078(4)	0.038(4)	-0.039(4)	-0.021(4)
C(13)	0.072(4)	0.074(4)	0.073(4)	0.017(3)	-0.038(3)	-0.019(3)
C(14)	0.083(4)	0.056(4)	0.070(4)	0.004(3)	-0.025(3)	-0.019(3)
C(15)	0.039(2)	0.018(2)	0.042(2)	0.001(2)	0.007(2)	-0.002(2)
C(16)	0.042(3)	0.041(3)	0.046(3)	-0.003(2)	0.002(2)	0.002(2)
C(17)	0.047(3)	0.048(3)	0.066(3)	0.006(3)	0.006(2)	0.010(2)
C(18)	0.048(3)	0.043(3)	0.074(3)	0.005(3)	0.022(3)	0.011(2)
C(19)	0.060(3)	0.049(3)	0.059(3)	-0.008(3)	0.016(3)	0.007(3)
C(20)	0.047(3)	0.044(3)	0.064(3)	-0.018(3)	-0.003(2)	0.004(2)
Cl(1)	0.059(1)	0.039(1)	0.074(1)	0.001(1)	0.010(1)	0.017(1)
Cl(2)	0.059(1)	0.055(1)	0.058(1)	0.009(1)	-0.001(1)	-0.028(1)
Cr	0.039(1)	0.025(1)	0.038(1)	-0.001(1)	0.005(1)	-0.004(1)
P	0.033(1)	0.021(1)	0.035(1)	0.002(1)	-0.001(1)	-0.003(1)