

General Remarks. All manipulations were performed under inert atmosphere using standard glovebox and Schlenk techniques.¹ $\text{CrCl}_3(\text{THF})_3$,² $\text{Ph}_3\text{Cr}(\text{THF})_3$,³ **1**,⁴ and $\text{Ph}_3\text{CB}(\text{C}_6\text{F}_5)_4$ ⁵ were prepared according to literature methods. MeMgBr , PhMgBr and trimethylphosphine were purchased from Aldrich and used as received. $\text{B}(\text{C}_6\text{F}_5)_3$ was purchased from Aldrich and sublimed just prior to use. Toluene, benzene, THF, pentane and diethyl ether were distilled from sodium benzophenone ketyl. NMR spectra were obtained using a Varian Unity 400 or 500 spectrometers. ^1H spectra were calibrated using signals from the solvent and are reported downfield from SiMe_4 . ^{11}B were calibrated and reported downfield from external BF_3OEt_2 . IR spectra were recorded using a Shimadzu FTIR-8300 Fourier Transform Infrared Spectrophotometer. DSC measurements were recorded using a Perkin-Elmer DSC Pyris 1. GPC experiments were performed with a Waters 150°C GPC at 140°C using 1,2,4-trichlorobenzene as the solvent. DSC and GPC data were recorded by Equistar Chemicals, L.P. Elemental Analyses were performed by Desert Analytics, Inc., Tucson, Arizona.

($\text{C}_5\text{H}_5\text{BPh}$) $\text{CrPh}_2(\text{PMe}_3)$ (2**). Method A:** $\text{Ph}_3\text{Cr}(\text{THF})_3$ (267.6mg, 0.5356mmol) was placed in a 20mL vial with 2mL of toluene and stir bar. While stirring, a solution of **1** (81.6mg, 0.537mmole) in 4mL of toluene was added dropwise. The solution became dark red and was stirred for 10 minutes. Volatiles were removed *in vacuo* and the product was crystallized at -35°C from a solution in 25 mL of pentane. Brown-red crystals were isolated (127.4mg, 0.2927mmol, 54.6%). **Method B:** $\text{CrCl}_3(\text{THF})_3$ (338.6mg, 0.9037mmol) was placed in a 250mL side arm flask with 15mL of THF and stir bar. The flask was fitted with an addition funnel containing 10mL of THF and PhMgBr (1.0M, 2.71mL, 2.71mmol). The flask was cooled to -45°C (dry ice/acetonitrile) under argon. The addition was performed over a 30 minute period

and the solution changed from purple to brown, then green and finally bright red. The mixture was stirred at -45°C for an additional 3 hours. A solution of **1** (137.7mg, 0.9060mmol) in 10mL of toluene was added dropwise via syringe. The solution became blood red within minutes and was held at -45°C for 30 minutes. The mixture was warmed to room temperature for an additional 30 minutes, and removed of volatiles *in vacuo*. The product was extracted with toluene, filtered and evaporated to dryness. The residue was extracted with Et_2O , filtered and cooled to -35°C , giving large, blood red cubes (235.8mg, 0.5417mmol, 59.9%). ^1H NMR (C_6D_6 , 400 MHz): δ -34.19 (br, 9H, $\text{P}(\text{CH}_3)_3$), 9.48 (br, 1H), 11.40 (br, 1H), 20.18 (br, 3H, BCH_3). ^{11}B NMR (C_6D_6 , 128 MHz): δ 370. IR (KBr plates, C_6H_6 , cm^{-1}): 3046, 1516, 1419, 1280, 1218, 954, 787, 747, 724, 699, 651. Anal. Calcd. ($\text{C}_{26}\text{H}_{29}\text{BCrP}$): C, 71.74; H, 6.72. Found: C, 71.89; H, 6.73.

($\text{C}_5\text{H}_5\text{BMe}$) $\text{CrMe}_2(\text{PMe}_3)$ (**3**). $\text{CrCl}_3(\text{THF})_3$ (1.005g, 2.683mmol) was placed in a 250mL side arm flask with 35mL of THF and stir bar. The flask was fitted with an addition funnel containing 15mL of THF and MeMgBr (3.0M, 2.69mL, 8.07mmol). The flask was cooled to -45°C (dry ice/acetonitrile) under argon. The addition was performed over a 45 minute period and the mixture was stirred at -45°C for an additional 3 hours, giving a red-brown solution. A solution of **1** (408.7mg, 2.689mmol) in 15mL of toluene was added dropwise via syringe. The solution became dark green within minutes and was held at -45°C for 30 minutes. The mixture was warmed to room temperature for an additional 30 minutes, becoming purple-black. Volatiles were removed *in vacuo* and the product was extracted with 35mL of pentane. The solution was filtered through celite and washed twice with pentane. The pentane was evaporated to dryness and the purple black crystals were recrystallized from 2mL of pentane (460.2mg,

1.848mmol, 68.9%). ^1H NMR (C_6D_6 , 400 MHz): δ -27.2 (br, 9H, $\text{P}(\text{CH}_3)_3$), 6.7 (br, 3H, BCH_3).
 ^{11}B NMR (C_6D_6 , 128 MHz): δ 219. IR (KBr plates, C_6H_6 , cm^{-1}): 2915, 1512, 1485, 1412, 1295, 1285, 1101, 945, 736, 484. Anal. Calcd. ($\text{C}_{11}\text{H}_{23}\text{BCrP}$): C, 53.04; H, 9.31. Found: C, 52.65; H, 9.47.

3/B(C_6F_5) $_3$. $\text{B}(\text{C}_6\text{F}_5)_3$ (126.7mg, 0.2475mmol) was dissolved in 6mL of pentane and placed in a 100mL round bottom flask with stir bar. While stirring, a solution of **3** (62.2mg, 0.249mmol) in 2mL of pentane was added dropwise. A dark green precipitate was formed immediately. The slurry was stirred for 20 minutes and the supernatant was decanted. The product was washed with pentane and dried *in vacuo*, giving a thermally unstable, green powder (134.6mg, 0.1769mmol, 71.5%). Nothing observed in ^1H NMR or ^{11}B NMR.

Reaction of 3/B(C_6F_5) $_3$ with PMe_3 (4). **3** (8.0mg, 32 μmol) was reacted with $\text{B}(\text{C}_6\text{F}_5)_3$ (16.6mg, 32.4 μmol) in 2mL of toluene. PMe_3 (5drops) were added and a brown-red substance phase separated out of solution. Toluene and excess PMe_3 were removed *in vacuo* and the product was extracted with 3:1 C_6D_6 :chlorobenzene. One resonances were observed at δ -14.4ppm, assigned to $[\text{MeB}(\text{C}_6\text{F}_5)_3]^-$. Volatiles were removed *in vacuo* and the oily product was extracted with diethyl ether. Slow evaporation afforded bright red crystals suitable for X-ray diffraction.

$[\text{MeB}(\text{C}_6\text{F}_5)_3]^-$. $\text{B}(\text{C}_6\text{F}_5)_3$ (4.7mg, 9.2 μmol) was reacted with MeMgBr (3.0M, 3.1 μL , 9.3 μmol) in 0.5mL of C_6D_6 , and 14 drops of $\text{THF-}d_8$ were added. A sharp resonance at δ -14.5ppm in the ^{11}B NMR spectrum was observed.

Reaction of 3/B(C₆F₅)₃ with THF. **3** (4.4mg, 18μmol) was reacted *in situ* with B(C₆F₅)₃ (9.1mg, 18μmol) in 0.5mL of C₆D₆. The solution became emerald green and 14 drops of THF-*d*₈ were added to sufficiently separate cation-anion pair. A single, sharp resonance in the ¹¹B NMR spectrum was observed at δ -14.4ppm.

Reaction of 3/B(C₆F₅)₃ with MeMgBr. [(C₅H₅BMe)CrMe(PMe₃)]⁺[MeB(C₆F₅)₃]⁻ (10.5mg, 13.8μmol) was dissolved in C₆D₆ and MeMgBr (3.0M, 4.6μL, 14μmol) was added. ¹¹B NMR reveals the clean formation of two peaks at δ -14.5ppm and 219ppm, attributed to [MeB(C₆F₅)₃]⁻ and **3** respectively.

General Polymerization Procedure. In the glovebox, 50μmol of the precatalyst was weighed to the nearest 0.1mg and dissolved in toluene. This was combined with the appropriate amount of MAO (9.6 wt. % Al, 1000 Al/M), B(C₆F₅)₃ (1 or 2 eq.) or [Ph₃C][B(C₆F₅)₄], a color change to dark green is observed. This was placed in a 100mL round bottom flask with stir bar, and enough toluene was added to bring the total volume to 50mL. The flask was fitted with a needle valve and removed from the glovebox. The mass of the apparatus was recorded to the nearest 0.001 g, and placed on a Schlenk line equipped with ethylene. Vacuum was applied for 5 seconds and the flask was maintained at room temperature with the aid of a water bath. The flask was opened to the ethylene source vented to a mercury bubbler, and polymer precipitation is immediate. After 30 minutes of reaction, the flask was cleaned and weighed again to the nearest 0.001 g for activity measurements. The reaction was quenched using 3mL of water and alumina salts were dissolved in aqueous base for the reaction using MAO activator. Reactions

using borane or borate activators were quenched with 5mL of acetone. The toluene layer was extracted to give the product and dried *in vacuo* to give the product.

Structure Determinations. Crystals were mounted onto thin glass fibers with paratone-8277 and immediately placed in a cold nitrogen stream at 150K on a Bruker SMART CCD diffractometer equipped with a normal focus, 2.4 kW sealed tube X-ray source (MoK α radiation, $\lambda = 0.71073\text{\AA}$) operating at 45kV and 40mA. The temperature control was achieved with an Oxford Cryostream that could provide a temperature range from 80 to 375K with a stability of about 0.1K. The detector to crystal distance was set to 5.10 cm and the corresponding maximum 2-theta angle was approximately 56 degrees. A full sphere of intensity data were collected in 2252 frames with ω scans (width of 0.30° and exposure time of 30 sec. per frame). The number of reflections used for the least-squares refinement of unit cell parameters (at 150K) was 8192, 7443 and 3509 for **2**, **3** and **4**, respectively. The empirical absorption corrections based on the equivalent reflections were performed using the program SADABS and other possible effects such as absorption by the glass fiber were simultaneously corrected.

The structures were solved by direct methods followed by successive difference Fourier methods. All calculations were performed using SHELXTL (version 5.0.3) running on a Silicon Graphics Indy 5000. Full-matrix refinements were against F^2 . Hydrogen atoms were calculated at idealized positions and their atomic positions were refined as riding atoms of their parent carbon atoms. The crystal data and refinement results are summarized in Table 1. Positional coordinates are listed in Table 2 while selected bond distances are given in Table 3. Table 4 lists anisotropic displacement parameters and hydrogen atom positions are tabulated in Table 5.

X-Ray report for

C₂₆H₂₉BCrP

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2. ORTEP Drawing

Table 1. Crystal data and structure refinement for **2**.

Empirical formula	C ₂₆ H ₂₉ BCrP
Formula weight	435.27
Temperature	150K
Wavelength	0.71073 Å
Crystal system	MONOCLINIC
Space group	P2(1)/n
Unit cell dimensions	a = 13.2988(9) Å α = 90deg. b = 11.7121(8) Å β = 107.7980(10)deg. c = 15.2431(11) Å γ = 90deg.
Volume, Z	2260.6(3) Å ³ ,4
Density (calculated)	1.279 Mg/m ³
Absorption coefficient	0.586 mm ⁻¹
F(000)	916
Crystal size (mm)	0.20 x 0.20 x 0.20
Theta range for data collection	1.78 to 25.00 deg.
Limiting indices	-17<=h<=17, -15<=k<=15, -19<=l<=19
Reflections collected	19667
Independent reflections	3976 [R(int)=0.0462]
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	3969/0/265
Goodness-of-fit on F ²	1.067
Final R indices [I>2sigma(I)]	R ₁ = 0.0406, wR ₂ = 0.1114

R indices (all data)

 $R_1 = 0.0508$, $wR_2 = 0.1184$

Largest diff. peak and hole

0.580 and -0.850 e.Å⁻³**Table 2.** Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å² $\times 10^3$) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cr(1)	8391(1)	7645(1)	5875(1)	18(1)
P(1)	8913(1)	7405(1)	7535(1)	19(1)
C(1)	8623(2)	6010(2)	7924(2)	31(1)
B(1)	9895(2)	6299(2)	5828(2)	24(1)
C(2)	8218(2)	8363(2)	8086(1)	26(1)
C(3)	10299(2)	7597(2)	8205(2)	30(1)
C(11)	10842(2)	5685(2)	6550(1)	25(1)
C(12)	10739(2)	4641(2)	6963(2)	30(1)
C(13)	11599(2)	4084(2)	7562(2)	37(1)
C(14)	12601(2)	4556(2)	7763(2)	38(1)
C(15)	12732(2)	5579(2)	7369(2)	37(1)
C(16)	11875(2)	6134(2)	6775(2)	31(1)
C(21)	8403(2)	9413(2)	5923(1)	22(1)
C(22)	9109(2)	10077(2)	6606(2)	27(1)
C(23)	9130(2)	11265(2)	6583(2)	30(1)
C(24)	8450(2)	11843(2)	5849(2)	29(1)
C(25)	7755(2)	11227(2)	5153(2)	30(1)
C(26)	7725(2)	10049(2)	5190(2)	27(1)
C(31)	6840(2)	7408(2)	5883(1)	22(1)
C(32)	6137(2)	8305(2)	5882(2)	28(1)
C(33)	5097(2)	8117(2)	5866(2)	34(1)
C(34)	4717(2)	7019(2)	5858(2)	31(1)
C(35)	5385(2)	6106(2)	5870(1)	29(1)
C(36)	6417(2)	6308(2)	5877(1)	25(1)
C(42)	8797(2)	5773(2)	5409(1)	25(1)
C(43)	8043(2)	6300(2)	4688(1)	29(1)
C(44)	8205(2)	7378(2)	4348(2)	28(1)
C(45)	9171(2)	7949(2)	4724(2)	29(1)
C(46)	9974(2)	7490(2)	5461(2)	25(1)

Table 3. Bond lengths [Å] and angles [deg] for **2**.

Cr(1)-C(21)	2.072(2)
Cr(1)-C(31)	2.084(2)
Cr(1)-C(44)	2.285(2)
Cr(1)-C(45)	2.322(2)
Cr(1)-C(43)	2.336(2)
Cr(1)-C(46)	2.383(2)
Cr(1)-C(42)	2.417(2)
Cr(1)-P(1)	2.4272(6)
Cr(1)-B(1)	2.565(3)
P(1)-C(2)	1.815(2)
P(1)-C(1)	1.819(2)
P(1)-C(3)	1.828(2)
C(1)-H(1A)	0.96
C(1)-H(1B)	0.96
C(1)-H(1C)	0.96
B(1)-C(46)	1.518(3)
B(1)-C(42)	1.532(3)
B(1)-C(11)	1.571(3)
C(2)-H(2A)	0.96
C(2)-H(2B)	0.96
C(2)-H(2C)	0.96
C(3)-H(3A)	0.96
C(3)-H(3B)	0.96
C(3)-H(3C)	0.96
C(11)-C(12)	1.401(3)
C(11)-C(16)	1.411(3)
C(12)-C(13)	1.389(3)
C(12)-H(12)	0.93
C(13)-C(14)	1.387(4)
C(13)-H(13)	0.93
C(14)-C(15)	1.375(4)
C(14)-H(14)	0.93
C(15)-C(16)	1.383(3)
C(15)-H(15)	0.93
C(16)-H(16)	0.93
C(21)-C(22)	1.405(3)
C(21)-C(26)	1.414(3)
C(22)-C(23)	1.391(3)
C(22)-H(22)	0.93
C(23)-C(24)	1.382(3)
C(23)-H(23)	0.93
C(24)-C(25)	1.379(3)
C(24)-H(24)	0.93

C(25)-C(26)	1.381(3)
C(25)-H(25)	0.93
C(26)-H(26)	0.93
C(31)-C(32)	1.405(3)
C(31)-C(36)	1.406(3)
C(32)-C(33)	1.394(3)
C(32)-H(32)	0.93
C(33)-C(34)	1.380(3)
C(33)-H(33)	0.93
C(34)-C(35)	1.387(3)
C(34)-H(34)	0.93
C(35)-C(36)	1.389(3)
C(35)-H(35)	0.93
C(36)-H(36)	0.93
C(42)-C(43)	1.386(3)
C(42)-H(42)	0.93
C(43)-C(44)	1.406(3)
C(43)-H(43)	0.93
C(44)-C(45)	1.406(3)
C(44)-H(44)	0.93
C(45)-C(46)	1.400(3)
C(45)-H(45)	0.93
C(46)-H(46)	0.93
C(21)-Cr(1)-C(31)	97.46(8)
C(21)-Cr(1)-C(44)	99.80(8)
C(31)-Cr(1)-C(44)	100.86(8)
C(21)-Cr(1)-C(45)	82.71(8)
C(31)-Cr(1)-C(45)	134.11(8)
C(44)-Cr(1)-C(45)	35.51(8)
C(21)-Cr(1)-C(43)	134.34(8)
C(31)-Cr(1)-C(43)	87.30(8)
C(44)-Cr(1)-C(43)	35.40(8)
C(45)-Cr(1)-C(43)	63.04(8)
C(21)-Cr(1)-C(46)	95.04(8)
C(31)-Cr(1)-C(46)	161.32(8)
C(44)-Cr(1)-C(46)	63.21(8)
C(45)-Cr(1)-C(46)	34.59(8)
C(43)-Cr(1)-C(46)	74.05(8)
C(21)-Cr(1)-C(42)	156.53(7)
C(31)-Cr(1)-C(42)	101.05(8)
C(44)-Cr(1)-C(42)	62.66(8)
C(45)-Cr(1)-C(42)	74.06(8)
C(43)-Cr(1)-C(42)	33.86(7)
C(46)-Cr(1)-C(42)	63.74(7)
C(21)-Cr(1)-P(1)	94.71(6)

C(31)-Cr(1)-P(1)	86.98(6)
C(44)-Cr(1)-P(1)	162.39(6)
C(45)-Cr(1)-P(1)	138.89(6)
C(43)-Cr(1)-P(1)	130.94(6)
C(46)-Cr(1)-P(1)	105.80(6)
C(42)-Cr(1)-P(1)	100.53(5)
C(2)-P(1)-C(1)	102.43(10)
C(2)-P(1)-C(3)	103.60(11)
C(1)-P(1)-C(3)	101.93(11)
C(2)-P(1)-Cr(1)	112.74(7)
C(1)-P(1)-Cr(1)	114.97(7)
C(3)-P(1)-Cr(1)	119.15(8)
P(1)-C(1)-H(1A)	109.47(8)
P(1)-C(1)-H(1B)	109.47(8)
H(1A)-C(1)-H(1B)	109.5
P(1)-C(1)-H(1C)	109.47(7)
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(46)-B(1)-C(42)	112.4(2)
C(46)-B(1)-C(11)	123.2(2)
C(42)-B(1)-C(11)	124.4(2)
P(1)-C(2)-H(2A)	109.47(7)
P(1)-C(2)-H(2B)	109.47(7)
H(2A)-C(2)-H(2B)	109.5
P(1)-C(2)-H(2C)	109.47(7)
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
P(1)-C(3)-H(3A)	109.47(8)
P(1)-C(3)-H(3B)	109.47(8)
H(3A)-C(3)-H(3B)	109.5
P(1)-C(3)-H(3C)	109.47(8)
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(12)-C(11)-C(16)	115.9(2)
C(12)-C(11)-B(1)	123.1(2)
C(16)-C(11)-B(1)	120.8(2)
C(13)-C(12)-C(11)	122.1(2)
C(13)-C(12)-H(12)	118.9(2)
C(11)-C(12)-H(12)	118.95(13)
C(14)-C(13)-C(12)	120.0(2)
C(14)-C(13)-H(13)	120.0(2)
C(12)-C(13)-H(13)	120.0(2)
C(15)-C(14)-C(13)	119.5(2)
C(15)-C(14)-H(14)	120.25(14)
C(13)-C(14)-H(14)	120.25(14)
C(14)-C(15)-C(16)	120.4(2)

C(14)-C(15)-H(15)	119.80(14)
C(16)-C(15)-H(15)	119.8(2)
C(15)-C(16)-C(11)	122.0(2)
C(15)-C(16)-H(16)	119.0(2)
C(11)-C(16)-H(16)	118.98(13)
C(22)-C(21)-C(26)	114.4(2)
C(22)-C(21)-Cr(1)	125.2(2)
C(26)-C(21)-Cr(1)	120.2(2)
C(23)-C(22)-C(21)	123.3(2)
C(23)-C(22)-H(22)	118.34(13)
C(21)-C(22)-H(22)	118.34(12)
C(24)-C(23)-C(22)	119.8(2)
C(24)-C(23)-H(23)	120.10(14)
C(22)-C(23)-H(23)	120.10(13)
C(25)-C(24)-C(23)	119.0(2)
C(25)-C(24)-H(24)	120.51(13)
C(23)-C(24)-H(24)	120.51(13)
C(24)-C(25)-C(26)	120.8(2)
C(24)-C(25)-H(25)	119.58(13)
C(26)-C(25)-H(25)	119.58(14)
C(25)-C(26)-C(21)	122.6(2)
C(25)-C(26)-H(26)	118.70(14)
C(21)-C(26)-H(26)	118.70(13)
C(32)-C(31)-C(36)	114.8(2)
C(32)-C(31)-Cr(1)	124.0(2)
C(36)-C(31)-Cr(1)	121.1(2)
C(33)-C(32)-C(31)	122.6(2)
C(33)-C(32)-H(32)	118.70(14)
C(31)-C(32)-H(32)	118.70(13)
C(34)-C(33)-C(32)	120.4(2)
C(34)-C(33)-H(33)	119.81(14)
C(32)-C(33)-H(33)	119.81(14)
C(33)-C(34)-C(35)	119.1(2)
C(33)-C(34)-H(34)	120.44(14)
C(35)-C(34)-H(34)	120.44(13)
C(34)-C(35)-C(36)	119.8(2)
C(34)-C(35)-H(35)	120.12(13)
C(36)-C(35)-H(35)	120.12(14)
C(35)-C(36)-C(31)	123.3(2)
C(35)-C(36)-H(36)	118.36(14)
C(31)-C(36)-H(36)	118.36(13)
C(43)-C(42)-B(1)	121.2(2)
C(43)-C(42)-Cr(1)	69.89(13)
B(1)-C(42)-Cr(1)	77.47(12)
C(43)-C(42)-H(42)	119.42(14)
B(1)-C(42)-H(42)	119.42(13)

Cr(1)-C(42)-H(42)	124.80(5)
C(42)-C(43)-C(44)	122.5(2)
C(42)-C(43)-Cr(1)	76.25(12)
C(44)-C(43)-Cr(1)	70.33(12)
C(42)-C(43)-H(43)	118.76(14)
C(44)-C(43)-H(43)	118.76(13)
Cr(1)-C(43)-H(43)	126.64(6)
C(45)-C(44)-C(43)	120.1(2)
C(45)-C(44)-Cr(1)	73.66(12)
C(43)-C(44)-Cr(1)	74.28(12)
C(45)-C(44)-H(44)	119.97(13)
C(43)-C(44)-H(44)	119.97(13)
Cr(1)-C(44)-H(44)	123.56(6)
C(46)-C(45)-C(44)	121.5(2)
C(46)-C(45)-Cr(1)	75.10(13)
C(44)-C(45)-Cr(1)	70.82(12)
C(46)-C(45)-H(45)	119.24(13)
C(44)-C(45)-H(45)	119.24(13)
Cr(1)-C(45)-H(45)	126.83(6)
C(45)-C(46)-B(1)	121.8(2)
C(45)-C(46)-Cr(1)	70.32(12)
B(1)-C(46)-Cr(1)	78.82(13)
C(45)-C(46)-H(46)	119.12(14)
B(1)-C(46)-H(46)	119.12(13)
Cr(1)-C(46)-H(46)	123.04(5)

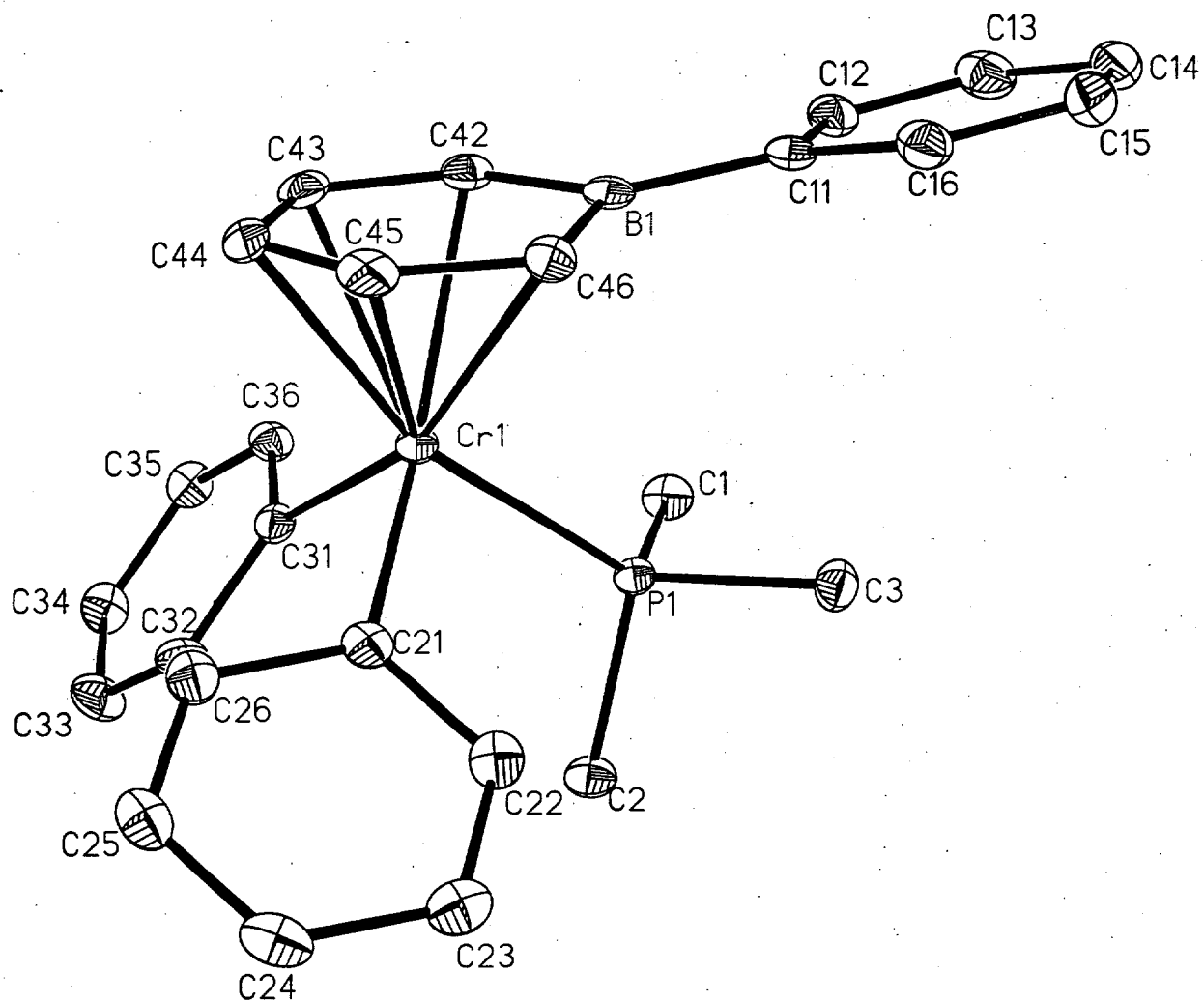
Symmetry transformations used to generate equivalent atoms:

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

	U11	U22	U33	U23	U13	U12
Cr(1)	18(1)	24(1)	16(1)	0(1)	10(1)	1(1)
P(1)	21(1)	23(1)	17(1)	0(1)	10(1)	0(1)
C(1)	41(1)	28(1)	28(1)	5(1)	17(1)	0(1)
B(1)	26(1)	31(1)	22(1)	-5(1)	17(1)	4(1)
C(2)	31(1)	29(1)	24(1)	-2(1)	17(1)	1(1)
C(3)	25(1)	40(1)	23(1)	0(1)	5(1)	1(1)
C(11)	27(1)	29(1)	23(1)	-6(1)	14(1)	4(1)
C(12)	29(1)	36(1)	29(1)	-1(1)	15(1)	4(1)
C(13)	48(2)	39(1)	31(1)	7(1)	21(1)	13(1)
C(14)	37(1)	52(2)	25(1)	0(1)	7(1)	17(1)
C(15)	27(1)	49(2)	33(1)	-6(1)	8(1)	4(1)
C(16)	29(1)	33(1)	33(1)	-3(1)	13(1)	2(1)
C(21)	21(1)	28(1)	23(1)	1(1)	15(1)	1(1)
C(22)	26(1)	32(1)	25(1)	5(1)	12(1)	-2(1)
C(23)	31(1)	32(1)	31(1)	-4(1)	17(1)	-7(1)
C(24)	35(1)	24(1)	41(1)	4(1)	28(1)	1(1)
C(25)	27(1)	35(1)	32(1)	10(1)	17(1)	6(1)
C(26)	26(1)	33(1)	26(1)	2(1)	13(1)	2(1)
C(31)	20(1)	28(1)	18(1)	-1(1)	8(1)	1(1)
C(32)	26(1)	28(1)	34(1)	-6(1)	16(1)	-3(1)
C(33)	25(1)	35(1)	47(2)	-3(1)	18(1)	5(1)
C(34)	22(1)	41(1)	34(1)	1(1)	13(1)	-4(1)
C(35)	27(1)	32(1)	29(1)	1(1)	13(1)	-6(1)
C(36)	24(1)	29(1)	26(1)	1(1)	12(1)	3(1)
C(42)	27(1)	27(1)	26(1)	-6(1)	15(1)	1(1)
C(43)	25(1)	42(1)	23(1)	-13(1)	11(1)	0(1)
C(44)	30(1)	43(1)	13(1)	0(1)	11(1)	9(1)
C(45)	34(1)	37(1)	26(1)	5(1)	23(1)	6(1)
C(46)	19(1)	37(1)	24(1)	-1(1)	14(1)	0(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2**.

	x	y	z	U(eq)
H(1A)	9017(9)	5436(2)	7721(9)	46
H(1B)	7881(3)	5856(6)	7672(9)	46
H(1C)	8817(12)	6003(5)	8585(2)	46
H(2A)	8367(9)	9139(2)	7965(8)	39
H(2B)	8447(9)	8230(9)	8738(2)	39
H(2C)	7472(2)	8227(9)	7844(7)	39
H(3A)	10540(4)	8328(5)	8065(8)	44
H(3B)	10716(2)	7005(7)	8052(8)	44
H(3C)	10370(2)	7561(13)	8851(2)	44
H(12)	10074(2)	4310(2)	6831(2)	36
H(13)	11503(2)	3395(2)	7829(2)	45
H(14)	13179(2)	4184(2)	8162(2)	46
H(15)	13402(2)	5899(2)	7503(2)	44
H(16)	11982(2)	6825(2)	6516(2)	37
H(22)	9586(2)	9705(2)	7098(2)	32
H(23)	9601(2)	11667(2)	7059(2)	36
H(24)	8460(2)	12636(2)	5825(2)	35
H(25)	7300(2)	11608(2)	4653(2)	35
H(26)	7241(2)	9659(2)	4713(2)	33
H(32)	6376(2)	9053(2)	5892(2)	34
H(33)	4656(2)	8736(2)	5860(2)	41
H(34)	4022(2)	6894(2)	5845(2)	38
H(35)	5143(2)	5362(2)	5873(1)	34
H(36)	6849(2)	5683(2)	5879(1)	30
H(42)	8634(2)	5088(2)	5643(1)	30
H(43)	7406(2)	5926(2)	4419(1)	35
H(44)	7673(2)	7713(2)	3874(2)	33
H(45)	9278(2)	8648(2)	4478(2)	35
H(46)	10573(2)	7925(2)	5734(2)	30



X-Ray report for

C₁₁H₂₃BCrP

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2. ORTEP Drawing

Table 1. Crystal data and structure refinement for **3**.

Empirical formula	$C_{11}H_{23}BCrP$
Formula weight	249.07
Temperature	150 K
Wavelength	0.71073 Å
Crystal system	MONOCLINIC
Space group	P2(1)/n
Unit cell dimensions	$a = 6.9085(3)$ Å $\alpha = 90$ deg. $b = 13.1107(6)$ Å $\beta = 100.1100(10)$ deg. $c = 15.6341(7)$ Å $\gamma = 90$ deg.
Volume, Z	$1394.08(11)$ Å ³ , 4
Density (calculated)	1.187 Mg/m ³
Absorption coefficient	0.900 mm ⁻¹
F(000)	532
Crystal size (µm)	133 x 106 x 40
Theta range for data collection	2.04 to 24.99 deg.
Limiting indices	$-9 \leq h \leq 9$, $-16 \leq k \leq 15$, $-20 \leq l \leq 20$
Reflections collected	12184
Independent reflections	2457 [R(int) = 0.0385]
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2456 / 0 / 153
Goodness-of-fit on F ²	1.065
Final R indices [I > 2σ(I)]	$R_1 = 0.0248$, $wR_2 = 0.0683$

R indices (all data)

$R_1 = 0.0301, wR_2 = 0.0707$

Largest diff. peak and hole

$0.342 \text{ and } -0.195 \text{ e.}\text{\AA}^{-3}$

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

	x	y	z	U(eq)
Cr(1)	1116(1)	4036(1)	7623(1)	22(1)
P(1)	1418(1)	3255(1)	9025(1)	32(1)
B(1)	-1430(3)	4271(2)	6306(1)	31(1)
C(2)	645(3)	4275(1)	6114(1)	32(1)
C(3)	1912(3)	3448(2)	6320(1)	36(1)
C(4)	1374(3)	2602(2)	6772(1)	39(1)
C(5)	-510(3)	2544(1)	7002(1)	36(1)
C(6)	-1865(3)	3330(1)	6812(1)	32(1)
C(7)	-2944(3)	5167(2)	6042(1)	46(1)
C(8)	-139(3)	5329(1)	8067(1)	32(1)
C(9)	3964(2)	4575(2)	7973(1)	37(1)
C(10)	2632(4)	2023(2)	9121(1)	53(1)
C(11)	-910(3)	3017(2)	9375(1)	55(1)
C(12)	2796(4)	3975(2)	9926(1)	53(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [deg] for **3**.

Cr(1)-C(9)	2.072(2)
Cr(1)-C(8)	2.078(2)
Cr(1)-C(4)	2.327(2)
Cr(1)-C(3)	2.332(2)
Cr(1)-C(2)	2.345(2)
Cr(1)-C(5)	2.376(2)
Cr(1)-P(1)	2.3953(5)
Cr(1)-C(6)	2.405(2)
Cr(1)-B(1)	2.481(2)
P(1)-C(10)	1.814(2)
P(1)-C(11)	1.815(2)
P(1)-C(12)	1.819(2)

B(1)-C(2)	1.516(3)
B(1)-C(6)	1.524(3)
B(1)-C(7)	1.579(3)
C(2)-C(3)	1.395(3)
C(2)-H(2)	0.91(2)
C(3)-C(4)	1.400(3)
C(3)-H(3)	0.95(2)
C(4)-C(5)	1.412(3)
C(4)-H(4)	0.87(2)
C(5)-C(6)	1.389(3)
C(5)-H(5)	0.96(2)
C(6)-H(6)	0.93(2)
C(7)-H(7A)	0.96
C(7)-H(7B)	0.96
C(7)-H(7C)	0.96
C(8)-H(8A)	0.96
C(8)-H(8B)	0.96
C(8)-H(8C)	0.96
C(9)-H(9A)	0.96
C(9)-H(9B)	0.96
C(9)-H(9C)	0.96
C(10)-H(10A)	0.96
C(10)-H(10B)	0.96
C(10)-H(10C)	0.96
C(11)-H(11A)	0.96
C(11)-H(11B)	0.96
C(11)-H(11C)	0.96
C(12)-H(12A)	0.96
C(12)-H(12B)	0.96
C(12)-H(12C)	0.96
C(9)-Cr(1)-C(8)	93.75(7)
C(9)-Cr(1)-C(4)	105.20(7)
C(8)-Cr(1)-C(4)	158.15(7)
C(9)-Cr(1)-C(3)	89.15(7)
C(8)-Cr(1)-C(3)	137.53(7)
C(4)-Cr(1)-C(3)	34.97(7)
C(9)-Cr(1)-C(2)	100.25(7)
C(8)-Cr(1)-C(2)	103.57(7)
C(4)-Cr(1)-C(2)	62.90(7)
C(3)-Cr(1)-C(2)	34.71(7)
C(9)-Cr(1)-C(5)	138.41(7)
C(8)-Cr(1)-C(5)	127.80(7)
C(4)-Cr(1)-C(5)	34.93(7)
C(3)-Cr(1)-C(5)	62.51(7)
C(2)-Cr(1)-C(5)	74.17(7)
C(9)-Cr(1)-P(1)	88.73(5)

C(8)-Cr(1)-P(1)	90.99(5)
C(4)-Cr(1)-P(1)	100.05(5)
C(3)-Cr(1)-P(1)	131.46(5)
C(2)-Cr(1)-P(1)	162.22(5)
C(5)-Cr(1)-P(1)	88.90(5)
C(9)-Cr(1)-C(6)	162.94(7)
C(8)-Cr(1)-C(6)	96.95(7)
C(4)-Cr(1)-C(6)	62.16(7)
C(3)-Cr(1)-C(6)	73.99(6)
C(2)-Cr(1)-C(6)	64.33(6)
C(5)-Cr(1)-C(6)	33.77(6)
P(1)-Cr(1)-C(6)	104.29(4)
C(9)-Cr(1)-B(1)	132.76(7)
C(8)-Cr(1)-B(1)	84.22(7)
C(4)-Cr(1)-B(1)	74.98(7)
C(3)-Cr(1)-B(1)	63.76(7)
C(2)-Cr(1)-B(1)	36.46(6)
C(5)-Cr(1)-B(1)	63.13(7)
P(1)-Cr(1)-B(1)	138.40(5)
C(6)-Cr(1)-B(1)	36.30(6)
C(10)-P(1)-C(11)	104.09(11)
C(10)-P(1)-C(12)	103.08(10)
C(11)-P(1)-C(12)	103.10(11)
C(10)-P(1)-Cr(1)	114.90(7)
C(11)-P(1)-Cr(1)	114.23(8)
C(12)-P(1)-Cr(1)	115.87(7)
C(2)-B(1)-C(6)	112.7(2)
C(2)-B(1)-C(7)	123.5(2)
C(6)-B(1)-C(7)	123.8(2)
C(2)-B(1)-Cr(1)	66.89(9)
C(6)-B(1)-Cr(1)	69.14(9)
C(7)-B(1)-Cr(1)	130.52(13)
C(3)-C(2)-B(1)	121.9(2)
C(3)-C(2)-Cr(1)	72.11(10)
B(1)-C(2)-Cr(1)	76.64(10)
C(3)-C(2)-H(2)	117.5(12)
B(1)-C(2)-H(2)	120.6(12)
Cr(1)-C(2)-H(2)	122.1(12)
C(2)-C(3)-C(4)	121.4(2)
C(2)-C(3)-Cr(1)	73.18(9)
C(4)-C(3)-Cr(1)	72.34(10)
C(2)-C(3)-H(3)	117.1(12)
C(4)-C(3)-H(3)	121.5(12)
Cr(1)-C(3)-H(3)	125.9(11)
C(3)-C(4)-C(5)	120.6(2)
C(3)-C(4)-Cr(1)	72.69(10)

C(5)-C(4)-Cr(1)	74.41(10)
C(3)-C(4)-H(4)	119.3(14)
C(5)-C(4)-H(4)	120.0(14)
Cr(1)-C(4)-H(4)	126.5(14)
C(6)-C(5)-C(4)	121.5(2)
C(6)-C(5)-Cr(1)	74.27(10)
C(4)-C(5)-Cr(1)	70.66(10)
C(6)-C(5)-H(5)	119.6(11)
C(4)-C(5)-H(5)	118.6(11)
Cr(1)-C(5)-H(5)	122.7(11)
C(5)-C(6)-B(1)	121.7(2)
C(5)-C(6)-Cr(1)	71.96(10)
B(1)-C(6)-Cr(1)	74.57(10)
C(5)-C(6)-H(6)	118.8(13)
B(1)-C(6)-H(6)	119.4(13)
Cr(1)-C(6)-H(6)	123.7(13)
B(1)-C(7)-H(7A)	109.47(10)
B(1)-C(7)-H(7B)	109.47(11)
H(7A)-C(7)-H(7B)	109.5
B(1)-C(7)-H(7C)	109.47(11)
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
Cr(1)-C(8)-H(8A)	109.47(5)
Cr(1)-C(8)-H(8B)	109.47(5)
H(8A)-C(8)-H(8B)	109.5
Cr(1)-C(8)-H(8C)	109.47(5)
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
Cr(1)-C(9)-H(9A)	109.47(5)
Cr(1)-C(9)-H(9B)	109.47(5)
H(9A)-C(9)-H(9B)	109.5
Cr(1)-C(9)-H(9C)	109.47(5)
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
P(1)-C(10)-H(10A)	109.47(8)
P(1)-C(10)-H(10B)	109.47(7)
H(10A)-C(10)-H(10B)	109.5
P(1)-C(10)-H(10C)	109.47(7)
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
P(1)-C(11)-H(11A)	109.47(7)
P(1)-C(11)-H(11B)	109.47(7)
H(11A)-C(11)-H(11B)	109.5
P(1)-C(11)-H(11C)	109.47(7)
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5

P(1)-C(12)-H(12A)	109.47(7)
P(1)-C(12)-H(12B)	109.47(8)
H(12A)-C(12)-H(12B)	109.5
P(1)-C(12)-H(12C)	109.47(7)
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5

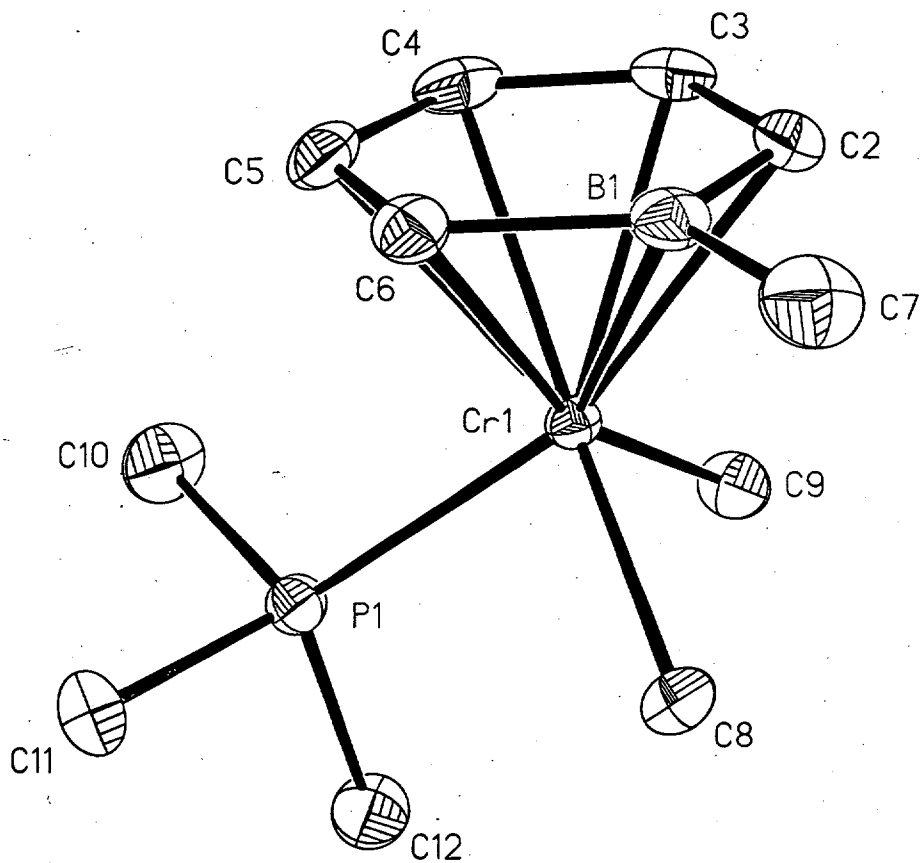
Symmetry transformations used to generate equivalent atoms:

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

	U11	U22	U33	U23	U13	U12
Cr(1)	23(1)	21(1)	21(1)	-1(1)	2(1)	0(1)
P(1)	42(1)	28(1)	24(1)	2(1)	3(1)	-2(1)
B(1)	34(1)	34(1)	22(1)	-4(1)	-3(1)	2(1)
C(2)	41(1)	35(1)	21(1)	-2(1)	6(1)	-4(1)
C(3)	35(1)	47(1)	27(1)	-14(1)	7(1)	3(1)
C(4)	46(1)	31(1)	35(1)	-13(1)	-3(1)	12(1)
C(5)	46(1)	24(1)	33(1)	-5(1)	-3(1)	-6(1)
C(6)	28(1)	36(1)	28(1)	-5(1)	0(1)	-6(1)
C(7)	48(1)	49(1)	36(1)	4(1)	-3(1)	13(1)
C(8)	32(1)	27(1)	38(1)	-7(1)	6(1)	0(1)
C(9)	28(1)	47(1)	37(1)	-5(1)	5(1)	-7(1)
C(10)	69(2)	40(1)	44(1)	10(1)	-5(1)	13(1)
C(11)	69(2)	50(1)	51(1)	4(1)	29(1)	-12(1)
C(12)	76(2)	51(1)	27(1)	-1(1)	-5(1)	-12(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3**.

	x	y	z	U(eq)
H(2)	1120(27)	4829(15)	5871(11)	37(5)
H(3)	3166(28)	3491(15)	6153(12)	36(5)
H(4)	2201(31)	2101(16)	6897(13)	45(6)
H(5)	-804(27)	1976(15)	7346(12)	39(5)
H(6)	-3042(34)	3292(15)	7022(13)	49(6)
H(7A)	-3197(17)	5504(7)	6556(1)	68
H(7B)	-4150(8)	4895(2)	5725(8)	68
H(7C)	-2404(9)	5647(6)	5684(8)	68
H(8A)	-1462(6)	5179(3)	8137(8)	49
H(8B)	-150(17)	5871(3)	7653(4)	49
H(8C)	616(11)	5533(6)	8615(4)	49
H(9A)	4332(7)	4940(9)	7494(3)	56
H(9B)	4844(4)	4011(2)	8124(8)	56
H(9C)	4035(5)	5024(8)	8463(6)	56
H(10A)	3916(9)	2089(3)	8971(10)	79
H(10B)	1870(12)	1546(3)	8735(8)	79
H(10C)	2753(21)	1782(6)	9708(3)	79
H(11A)	-1599(11)	3649(2)	9398(10)	82
H(11B)	-673(4)	2710(12)	9942(5)	82
H(11C)	-1691(11)	2564(10)	8972(6)	82
H(12A)	2279(15)	4655(4)	9922(6)	80
H(12B)	4155(5)	4002(10)	9867(6)	80
H(12C)	2681(20)	3647(7)	10464(1)	80



X-Ray report for

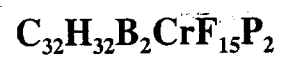


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2. ORTEP Drawing

Table 1. Crystal data and structure refinement for **4**.

Empirical formula	$C_{32}H_{32}B_2CrF_{15}P_2$
Formula weight	837.14
Temperature	150K
Wavelength	0.71073 Å
Crystal system	MONOCLINIC
Space group	P2(1)/c
Unit cell dimensions	$a=10.5916(13)$ Å $\alpha = 90\text{deg.}$ $b=19.523(2)$ Å $\beta = 97.677(2)\text{deg.}$ $c=16.929(2)$ Å $\gamma = 90\text{deg.}$
Volume, Z	$3469.3(8)$ Å ³ , 4
Density (calculated)	1.603 Mg/m ³
Absorption coefficient	0.527 mm ⁻¹
F(000)	1692
Crystal size (mm)	0.200 x 0.080 x 0.027
Theta range for data collection	1.60 to 25.00 deg.
Limiting indices	$-13 \leq h \leq 13$, $-26 \leq k \leq 25$, $-22 \leq l \leq 22$
Reflections collected	30815
Independent reflections	6125 [R(int)=0.1175]
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	6119/0/478
Goodness-of-fit on F ²	0.815
Final R indices [I>2sigma(I)]	$R_1 = 0.0415$, $wR_2 = 0.0746$

R indices (all data)

 $R_1 = 0.1032$, $wR_2 = 0.0868$

Largest diff. peak and hole

0.370 and -0.297 e.Å⁻³**Table 2.** Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å² $\times 10^3$) for 4. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cr(1)	1522(1)	264(1)	8545(1)	24(1)
P(1)	-565(1)	83(1)	7763(1)	29(1)
C(1)	2884(3)	-519(2)	7961(2)	30(1)
B(1)	3832(4)	-60(2)	8477(3)	33(1)
P(2)	2027(1)	1333(1)	7922(1)	28(1)
B(2)	2508(4)	-2067(2)	5457(2)	27(1)
C(2)	1949(3)	-879(2)	8282(2)	31(1)
C(3)	1751(3)	-787(2)	9083(2)	33(1)
C(4)	2530(4)	-345(2)	9582(2)	33(1)
C(5)	3477(3)	40(2)	9302(2)	31(1)
C(6)	5079(3)	230(2)	8194(2)	41(1)
C(7)	722(3)	832(2)	9387(2)	34(1)
C(8)	2783(3)	-2513(2)	6277(2)	39(1)
C(11)	-1334(4)	-719(2)	7962(2)	43(1)
C(12)	-528(3)	80(2)	6696(2)	38(1)
C(13)	-1792(3)	699(2)	7899(2)	38(1)
C(21)	3225(3)	1815(2)	8550(2)	41(1)
C(22)	2647(3)	1268(2)	6984(2)	39(1)
C(23)	734(3)	1941(2)	7708(2)	36(1)
C(31)	3071(3)	-1272(2)	5611(2)	26(1)
F(32)	5106(2)	-1716(1)	6129(1)	42(1)
C(32)	4344(4)	-1170(2)	5920(2)	30(1)
F(33)	6156(2)	-484(1)	6345(1)	53(1)
C(33)	4915(3)	-538(2)	6035(2)	34(1)
F(34)	4796(2)	664(1)	5897(1)	49(1)
C(34)	4247(4)	40(2)	5807(2)	35(1)
F(35)	2304(2)	541(1)	5243(1)	45(1)
C(35)	2992(4)	-25(2)	5485(2)	29(1)
F(36)	1209(2)	-667(1)	5060(1)	34(1)
C(36)	2451(3)	-666(2)	5398(2)	27(1)
C(41)	3262(3)	-2358(2)	4734(2)	25(1)
F(42)	4049(2)	-3394(1)	5362(1)	39(1)

C(42)	4010(3)	-2944(2)	4748(2)	26(1)
F(43)	5502(2)	-3684(1)	4255(1)	44(1)
C(43)	4760(3)	-3117(2)	4168(2)	31(1)
F(44)	5525(2)	-2865(1)	2960(1)	45(1)
C(44)	4780(3)	-2706(2)	3520(2)	31(1)
F(45)	4070(2)	-1703(1)	2826(1)	38(1)
C(45)	4041(3)	-2127(2)	3453(2)	28(1)
F(46)	2562(2)	-1408(1)	3915(1)	35(1)
C(46)	3308(3)	-1982(2)	4041(2)	27(1)
C(51)	935(3)	-2074(2)	5221(2)	24(1)
F(52)	827(2)	-2698(1)	4006(1)	36(1)
C(52)	238(3)	-2398(2)	4582(2)	26(1)
F(53)	-1675(2)	-2785(1)	3829(1)	39(1)
C(53)	-1081(4)	-2441(2)	4465(2)	30(1)
F(54)	-3054(2)	-2169(1)	4872(1)	42(1)
C(54)	-1781(4)	-2145(2)	4989(2)	29(1)
F(55)	-1808(2)	-1528(1)	6185(1)	41(1)
C(55)	-1142(4)	-1818(2)	5648(2)	31(1)
F(56)	710(2)	-1461(1)	6411(1)	36(1)
C(56)	171(3)	-1798(2)	5746(2)	27(1)

Table 3. Bond lengths [Å] and angles [deg] for **4**.

Cr(1)-C(7)	2.074(3)
Cr(1)-C(3)	2.245(3)
Cr(1)-C(4)	2.266(3)
Cr(1)-C(5)	2.326(3)
Cr(1)-C(2)	2.331(3)
Cr(1)-C(1)	2.403(3)
Cr(1)-P(2)	2.4295(11)
Cr(1)-P(1)	2.4466(12)
Cr(1)-B(1)	2.545(4)
P(1)-C(13)	1.808(3)
P(1)-C(12)	1.811(3)
P(1)-C(11)	1.816(4)
C(1)-C(2)	1.383(5)
C(1)-B(1)	1.529(5)
C(1)-H(1)	0.93
B(1)-C(5)	1.507(5)
B(1)-C(6)	1.570(5)
P(2)-C(22)	1.803(4)
P(2)-C(21)	1.807(3)

P(2)-C(23)	1.813(3)
B(2)-C(8)	1.631(5)
B(2)-C(41)	1.649(5)
B(2)-C(51)	1.661(5)
B(2)-C(31)	1.671(5)
C(2)-C(3)	1.411(5)
C(2)-H(2)	0.93
C(3)-C(4)	1.399(5)
C(3)-H(3)	0.93
C(4)-C(5)	1.386(5)
C(4)-H(4)	0.93
C(5)-H(5)	0.93
C(6)-H(6A)	0.96
C(6)-H(6B)	0.96
C(6)-H(6C)	0.96
C(7)-H(7A)	0.96
C(7)-H(7B)	0.96
C(7)-H(7C)	0.96
C(8)-H(8A)	0.96
C(8)-H(8B)	0.96
C(8)-H(8C)	0.96
C(11)-H(11A)	0.96
C(11)-H(11B)	0.96
C(11)-H(11C)	0.96
C(12)-H(12A)	0.96
C(12)-H(12B)	0.96
C(12)-H(12C)	0.96
C(13)-H(13A)	0.96
C(13)-H(13B)	0.96
C(13)-H(13C)	0.96
C(21)-H(21A)	0.96
C(21)-H(21B)	0.96
C(21)-H(21C)	0.96
C(22)-H(22A)	0.96
C(22)-H(22B)	0.96
C(22)-H(22C)	0.96
C(23)-H(23A)	0.96
C(23)-H(23B)	0.96
C(23)-H(23C)	0.96
C(31)-C(36)	1.377(4)
C(31)-C(32)	1.394(5)
F(32)-C(32)	1.355(4)
C(32)-C(33)	1.377(5)
F(33)-C(33)	1.353(4)
C(33)-C(34)	1.359(5)
F(34)-C(34)	1.350(4)

C(34)-C(35)	1.373(5)
F(35)-C(35)	1.357(4)
C(35)-C(36)	1.376(5)
F(36)-C(36)	1.362(4)
C(41)-C(46)	1.390(4)
C(41)-C(42)	1.390(4)
F(42)-C(42)	1.357(4)
C(42)-C(43)	1.384(5)
F(43)-C(43)	1.354(4)
C(43)-C(44)	1.361(5)
F(44)-C(44)	1.348(4)
C(44)-C(45)	1.372(5)
F(45)-C(45)	1.350(4)
C(45)-C(46)	1.372(5)
F(46)-C(46)	1.371(4)
C(51)-C(52)	1.380(4)
C(51)-C(56)	1.388(5)
F(52)-C(52)	1.358(4)
C(52)-C(53)	1.387(5)
F(53)-C(53)	1.350(4)
C(53)-C(54)	1.360(5)
F(54)-C(54)	1.338(4)
C(54)-C(55)	1.381(5)
F(55)-C(55)	1.347(4)
C(55)-C(56)	1.379(5)
F(56)-C(56)	1.361(4)
C(7)-Cr(1)-C(3)	104.07(14)
C(7)-Cr(1)-C(4)	86.69(14)
C(3)-Cr(1)-C(4)	36.13(12)
C(7)-Cr(1)-C(5)	97.90(14)
C(3)-Cr(1)-C(5)	64.20(13)
C(4)-Cr(1)-C(5)	35.09(12)
C(7)-Cr(1)-C(2)	138.70(14)
C(3)-Cr(1)-C(2)	35.86(12)
C(4)-Cr(1)-C(2)	64.10(13)
C(5)-Cr(1)-C(2)	75.20(13)
C(7)-Cr(1)-C(1)	161.03(13)
C(3)-Cr(1)-C(1)	63.06(13)
C(4)-Cr(1)-C(1)	74.83(13)
C(5)-Cr(1)-C(1)	64.41(12)
C(2)-Cr(1)-C(1)	33.92(11)
C(7)-Cr(1)-P(2)	88.40(10)
C(3)-Cr(1)-P(2)	160.55(10)
C(4)-Cr(1)-P(2)	132.71(11)
C(5)-Cr(1)-P(2)	99.74(9)

C(2)-Cr(1)-P(2)	132.79(10)
C(1)-Cr(1)-P(2)	100.88(9)
C(7)-Cr(1)-P(1)	91.53(10)
C(3)-Cr(1)-P(1)	97.38(10)
C(4)-Cr(1)-P(1)	129.97(11)
C(5)-Cr(1)-P(1)	160.84(9)
C(2)-Cr(1)-P(1)	86.69(10)
C(1)-Cr(1)-P(1)	103.53(9)
P(2)-Cr(1)-P(1)	97.14(4)
C(7)-Cr(1)-B(1)	130.4(2)
C(3)-Cr(1)-B(1)	74.83(13)
C(4)-Cr(1)-B(1)	63.12(14)
C(5)-Cr(1)-B(1)	35.69(13)
C(2)-Cr(1)-B(1)	62.68(13)
C(1)-Cr(1)-B(1)	35.86(12)
P(2)-Cr(1)-B(1)	85.72(10)
P(1)-Cr(1)-B(1)	138.09(11)
C(13)-P(1)-C(12)	103.9(2)
C(13)-P(1)-C(11)	101.7(2)
C(12)-P(1)-C(11)	104.7(2)
C(13)-P(1)-Cr(1)	116.55(13)
C(12)-P(1)-Cr(1)	113.71(13)
C(11)-P(1)-Cr(1)	114.74(13)
C(2)-C(1)-B(1)	121.6(3)
C(2)-C(1)-Cr(1)	70.2(2)
B(1)-C(1)-Cr(1)	77.1(2)
C(2)-C(1)-H(1)	119.2(2)
B(1)-C(1)-H(1)	119.2(2)
Cr(1)-C(1)-H(1)	125.15(9)
C(5)-B(1)-C(1)	112.3(3)
C(5)-B(1)-C(6)	124.1(4)
C(1)-B(1)-C(6)	123.5(4)
C(5)-B(1)-Cr(1)	64.2(2)
C(1)-B(1)-Cr(1)	67.0(2)
C(6)-B(1)-Cr(1)	141.0(3)
C(22)-P(2)-C(21)	104.1(2)
C(22)-P(2)-C(23)	102.9(2)
C(21)-P(2)-C(23)	103.2(2)
C(22)-P(2)-Cr(1)	116.70(13)
C(21)-P(2)-Cr(1)	111.73(13)
C(23)-P(2)-Cr(1)	116.48(12)
C(8)-B(2)-C(41)	113.5(3)
C(8)-B(2)-C(51)	105.1(3)
C(41)-B(2)-C(51)	112.9(3)
C(8)-B(2)-C(31)	110.1(3)
C(41)-B(2)-C(31)	103.8(3)

C(51)-B(2)-C(31)	111.7(3)
C(1)-C(2)-C(3)	121.2(4)
C(1)-C(2)-Cr(1)	75.9(2)
C(3)-C(2)-Cr(1)	68.7(2)
C(1)-C(2)-H(2)	119.4(2)
C(3)-C(2)-H(2)	119.4(2)
Cr(1)-C(2)-H(2)	128.16(9)
C(4)-C(3)-C(2)	120.5(3)
C(4)-C(3)-Cr(1)	72.7(2)
C(2)-C(3)-Cr(1)	75.4(2)
C(4)-C(3)-H(3)	119.7(2)
C(2)-C(3)-H(3)	119.7(2)
Cr(1)-C(3)-H(3)	123.56(9)
C(5)-C(4)-C(3)	121.6(3)
C(5)-C(4)-Cr(1)	74.8(2)
C(3)-C(4)-Cr(1)	71.1(2)
C(5)-C(4)-H(4)	119.2(2)
C(3)-C(4)-H(4)	119.2(2)
Cr(1)-C(4)-H(4)	126.82(9)
C(4)-C(5)-B(1)	121.9(3)
C(4)-C(5)-Cr(1)	70.1(2)
B(1)-C(5)-Cr(1)	80.1(2)
C(4)-C(5)-H(5)	119.1(2)
B(1)-C(5)-H(5)	119.1(2)
Cr(1)-C(5)-H(5)	121.86(9)
B(1)-C(6)-H(6A)	109.5(2)
B(1)-C(6)-H(6B)	109.5(2)
H(6A)-C(6)-H(6B)	109.5
B(1)-C(6)-H(6C)	109.5(2)
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
Cr(1)-C(7)-H(7A)	109.47(10)
Cr(1)-C(7)-H(7B)	109.47(10)
H(7A)-C(7)-H(7B)	109.5
Cr(1)-C(7)-H(7C)	109.47(10)
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
B(2)-C(8)-H(8A)	109.5(2)
B(2)-C(8)-H(8B)	109.5(2)
H(8A)-C(8)-H(8B)	109.5
B(2)-C(8)-H(8C)	109.5(2)
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
P(1)-C(11)-H(11A)	109.47(13)
P(1)-C(11)-H(11B)	109.47(13)
H(11A)-C(11)-H(11B)	109.5

P(1)-C(11)-H(11C)	109.47(13)
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
P(1)-C(12)-H(12A)	109.47(12)
P(1)-C(12)-H(12B)	109.47(12)
H(12A)-C(12)-H(12B)	109.5
P(1)-C(12)-H(12C)	109.47(12)
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
P(1)-C(13)-H(13A)	109.47(12)
P(1)-C(13)-H(13B)	109.47(12)
H(13A)-C(13)-H(13B)	109.5
P(1)-C(13)-H(13C)	109.47(12)
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
P(2)-C(21)-H(21A)	109.47(12)
P(2)-C(21)-H(21B)	109.47(12)
H(21A)-C(21)-H(21B)	109.5
P(2)-C(21)-H(21C)	109.47(12)
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
P(2)-C(22)-H(22A)	109.47(12)
P(2)-C(22)-H(22B)	109.47(12)
H(22A)-C(22)-H(22B)	109.5
P(2)-C(22)-H(22C)	109.47(12)
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
P(2)-C(23)-H(23A)	109.47(12)
P(2)-C(23)-H(23B)	109.47(12)
H(23A)-C(23)-H(23B)	109.5
P(2)-C(23)-H(23C)	109.47(12)
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(36)-C(31)-C(32)	112.3(3)
C(36)-C(31)-B(2)	127.5(3)
C(32)-C(31)-B(2)	119.8(3)
F(32)-C(32)-C(33)	115.7(3)
F(32)-C(32)-C(31)	119.9(3)
C(33)-C(32)-C(31)	124.4(4)
F(33)-C(33)-C(34)	119.2(4)
F(33)-C(33)-C(32)	120.7(4)
C(34)-C(33)-C(32)	120.1(4)
F(34)-C(34)-C(33)	121.1(4)
F(34)-C(34)-C(35)	120.5(4)
C(33)-C(34)-C(35)	118.4(3)
F(35)-C(35)-C(34)	119.8(3)

F(35)-C(35)-C(36)	120.6(3)
C(34)-C(35)-C(36)	119.6(3)
F(36)-C(36)-C(31)	120.6(3)
F(36)-C(36)-C(35)	114.2(3)
C(31)-C(36)-C(35)	125.1(3)
C(46)-C(41)-C(42)	111.5(3)
C(46)-C(41)-B(2)	121.3(3)
C(42)-C(41)-B(2)	127.0(3)
F(42)-C(42)-C(43)	115.1(3)
F(42)-C(42)-C(41)	120.4(3)
C(43)-C(42)-C(41)	124.5(3)
F(43)-C(43)-C(44)	119.8(4)
F(43)-C(43)-C(42)	120.1(3)
C(44)-C(43)-C(42)	120.1(3)
F(44)-C(44)-C(43)	120.4(3)
F(44)-C(44)-C(45)	120.8(4)
C(43)-C(44)-C(45)	118.8(4)
F(45)-C(45)-C(46)	121.3(3)
F(45)-C(45)-C(44)	119.9(3)
C(46)-C(45)-C(44)	118.8(3)
F(46)-C(46)-C(45)	115.2(3)
F(46)-C(46)-C(41)	118.6(3)
C(45)-C(46)-C(41)	126.2(3)
C(52)-C(51)-C(56)	112.6(3)
C(52)-C(51)-B(2)	127.3(3)
C(56)-C(51)-B(2)	119.7(3)
F(52)-C(52)-C(51)	120.8(3)
F(52)-C(52)-C(53)	114.9(3)
C(51)-C(52)-C(53)	124.3(3)
F(53)-C(53)-C(54)	119.7(3)
F(53)-C(53)-C(52)	119.8(3)
C(54)-C(53)-C(52)	120.5(3)
F(54)-C(54)-C(53)	121.0(3)
F(54)-C(54)-C(55)	120.8(3)
C(53)-C(54)-C(55)	118.3(4)
F(55)-C(55)-C(56)	121.1(3)
F(55)-C(55)-C(54)	119.7(3)
C(56)-C(55)-C(54)	119.2(3)
F(56)-C(56)-C(55)	114.7(3)
F(56)-C(56)-C(51)	120.0(3)
C(55)-C(56)-C(51)	125.2(3)

Symmetry transformations used to generate equivalent atoms:

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

	U11	U22	U33	U23	U13	U12
Cr(1)	24(1)	24(1)	25(1)	0(1)	5(1)	2(1)
P(1)	27(1)	28(1)	32(1)	2(1)	3(1)	-1(1)
C(1)	27(2)	32(2)	31(2)	0(2)	9(2)	9(2)
B(1)	29(3)	33(3)	36(3)	3(2)	2(2)	10(2)
P(2)	28(1)	25(1)	30(1)	0(1)	6(1)	0(1)
B(2)	26(3)	28(3)	25(2)	0(2)	1(2)	0(2)
C(2)	31(2)	19(2)	43(3)	-3(2)	5(2)	5(2)
C(3)	33(2)	24(2)	45(3)	11(2)	13(2)	6(2)
C(4)	40(3)	33(2)	25(2)	8(2)	4(2)	15(2)
C(5)	27(2)	31(2)	33(2)	-1(2)	-3(2)	5(2)
C(6)	29(2)	39(2)	56(3)	1(2)	5(2)	5(2)
C(7)	42(3)	33(2)	29(2)	3(2)	11(2)	3(2)
C(8)	38(3)	40(3)	37(2)	8(2)	3(2)	5(2)
C(11)	37(3)	43(3)	49(3)	7(2)	4(2)	-9(2)
C(12)	38(3)	40(3)	34(2)	1(2)	-3(2)	-2(2)
C(13)	31(2)	37(2)	47(3)	2(2)	7(2)	7(2)
C(21)	40(3)	31(2)	50(3)	-7(2)	2(2)	-6(2)
C(22)	40(3)	41(2)	38(2)	6(2)	10(2)	2(2)
C(23)	33(3)	33(2)	43(2)	4(2)	10(2)	0(2)
C(31)	29(2)	29(2)	20(2)	0(2)	3(2)	1(2)
F(32)	27(1)	45(1)	52(1)	-3(1)	-1(1)	6(1)
C(32)	33(3)	30(2)	26(2)	-2(2)	3(2)	4(2)
F(33)	29(1)	65(2)	64(2)	-21(1)	6(1)	-12(1)
C(33)	20(2)	48(3)	35(2)	-13(2)	7(2)	-7(2)
F(34)	58(2)	38(1)	55(2)	-16(1)	21(1)	-22(1)
C(34)	42(3)	26(2)	39(3)	-13(2)	16(2)	-15(2)
F(35)	66(2)	24(1)	43(1)	4(1)	3(1)	2(1)
C(35)	38(3)	24(2)	26(2)	-2(2)	8(2)	3(2)
F(36)	35(1)	27(1)	37(1)	3(1)	-5(1)	4(1)
C(36)	28(2)	30(2)	22(2)	-1(2)	1(2)	-3(2)
C(41)	22(2)	22(2)	28(2)	2(2)	-4(2)	-2(2)
F(42)	45(1)	27(1)	42(1)	9(1)	-2(1)	4(1)
C(42)	25(2)	19(2)	31(2)	3(2)	-7(2)	-8(2)
F(43)	40(1)	34(1)	56(2)	-3(1)	1(1)	13(1)
C(43)	25(2)	21(2)	43(3)	-6(2)	-5(2)	1(2)
F(44)	39(1)	49(2)	48(2)	-11(1)	12(1)	5(1)
C(44)	27(2)	34(2)	32(2)	-9(2)	1(2)	0(2)
F(45)	47(1)	37(1)	30(1)	0(1)	7(1)	2(1)

C(45)	34(2)	24(2)	25(2)	-2(2)	-2(2)	-5(2)
F(46)	48(1)	29(1)	29(1)	5(1)	7(1)	14(1)
C(46)	28(2)	19(2)	32(2)	-2(2)	-2(2)	6(2)
C(51)	29(2)	15(2)	28(2)	4(2)	2(2)	0(2)
F(52)	37(1)	33(1)	37(1)	-8(1)	-1(1)	4(1)
C(52)	31(2)	17(2)	29(2)	3(2)	3(2)	4(2)
F(53)	39(1)	35(1)	40(1)	-6(1)	-9(1)	-7(1)
C(53)	35(3)	22(2)	30(2)	3(2)	-5(2)	-7(2)
F(54)	24(1)	51(1)	50(1)	5(1)	0(1)	-5(1)
C(54)	22(2)	28(2)	37(2)	8(2)	2(2)	-4(2)
F(55)	33(1)	49(1)	44(1)	-6(1)	12(1)	-2(1)
C(55)	34(3)	31(2)	29(2)	0(2)	12(2)	1(2)
F(56)	37(1)	43(1)	28(1)	-9(1)	3(1)	-5(1)
C(56)	30(2)	25(2)	25(2)	-1(2)	-2(2)	-3(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4.

	x	y	z	U(eq)
H(1)	2938(3)	-557(2)	7419(2)	36
H(2)	1440(3)	-1187(2)	7963(2)	37
H(3)	1098(3)	-1023(2)	9280(2)	40
H(4)	2411(4)	-308(2)	10115(2)	39
H(5)	3904(3)	370(2)	9633(2)	37
H(6A)	4932(7)	313(10)	7631(3)	62
H(6B)	5756(6)	-96(5)	8310(12)	62
H(6C)	5311(12)	651(6)	8469(10)	62
H(7A)	178(15)	1179(7)	9123(2)	51
H(7B)	1386(3)	1045(8)	9745(8)	51
H(7C)	231(16)	536(2)	9681(8)	51
H(8A)	2389(18)	-2955(4)	6196(4)	58
H(8B)	2436(18)	-2278(6)	6697(4)	58
H(8C)	3685(4)	-2569(10)	6420(7)	58
H(11A)	-1378(19)	-757(6)	8523(3)	64
H(11B)	-850(12)	-1095(2)	7794(12)	64
H(11C)	-2179(8)	-729(5)	7675(11)	64
H(12A)	101(14)	-240(8)	6569(2)	57
H(12B)	-317(20)	530(3)	6526(3)	57
H(12C)	-1349(7)	-50(11)	6428(2)	57
H(13A)	-1929(15)	703(8)	8448(3)	57