Coordinating Anions: (Phosphino)tetraphenylborate Ligands as New **Reagents for Synthesis**

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Experimental Section.

All syntheses reported were carried out using standard glovebox and Schlenk techniques in the absence of water and dioxygen, unless otherwise noted. Acetonitrile, benzene, dichloromethane, diethyl ether, petroleum ether, tetrahydrofuran, and toluene were dried by sparging with N_2 gas followed by passage through an activated alumina column. Ethanol was deoxygenated via sparging with N2 drying over CaH, and distilling prior to use. All solvents were stored over 3-Å molecular sieves. Deuterated benzene, chloroform, acetonitrile, and acetone, were purchased from Cambridge Isotope Laboratories, Inc., degassed via repeated freeze-pump-thaw cycles, and dried over 3-Å molecular sieves. Nonhalogenated solvents were frequently tested using a standard solution of sodium benzophenone ketyl in tetrahydrofuran to confirm the absence of oxygen and moisture. (COD)PtMe₂¹ (TMEDA)LiCH₂PPh₂² and ASNBr³ were prepared using literature methods. $P(i-Pr)_2Ph$ was prepared by reaction of $(i-Pr)_2PCl$ with PhMgBr in THF at -90 °C. (Bromophenyl)diphenylphosphine was prepared using a modification of the literature procedure as described below.⁴ $B(C_6F_5)_3$ was purchased from Strem and recrystallized from pentane at -35 °C prior to use. All other chemicals were purchased from Aldrich, Strem, Alfa Aesar, or Lancaster and used without further purification. NMR spectra were recorded at ambient temperature on Varian Mercury 300 MHz, Inova 500 MHz, and Joel 400 MHz spectrometers. ¹H and ¹³C NMR chemical shifts were referenced to residual solvent. ³¹P NMR shifts were referenced to 85 % H₃PO₄. IR spectra were recorded on a Bio-Rad Excalibur FTS 3000 spectrometer controlled by Win-IR Pro software. Elemental Analyses were performed by Desert Analytics, Tuscon, AZ. X-ray diffraction experiments were carried out by the Beckman Institute Crystallographic Facility on a Bruker Smart 1000 CCD diffractometer.

[(TMEDA)Li][Ph₂PCH₂BPh₃] (1). [Li(TMEDA)][CH₂PPh₂] (1.0364 g, 3.215 mmol) was dissolved in toluene (18 mL) and placed under and N₂ atmosphere. To this solution was added BPh₃ (0.778 g, 3.21 mmol) in toluene (10 mL) at -78 °C. Mixture was stirred and allowed to warm to room temperature slowly over a period of 2.5 hours. Volatiles were then removed in vacuo. Solids were re-dissolved in toluene (30 mL) followed by filtration through a Celite plug. Volatiles was removed from the filtrate in vacuo (~ 90 % crude yield by ³¹P NMR). The product was recrystallized via vapor diffusion of petroleum ether into THF (~ 50 %). ¹H NMR (300 MHz, d₆-acetone): δ = 7.38 (m, 6H), δ = 7.17 (m, 4H), δ = 7.02 (m, 4H), δ = 7.00 (m, 2H), δ = 6.83 (m, 6H), δ = 6.69 (m, 3H), δ = 3.63 (m, 8H, THF), δ = 1.89 (m, 2H, CH₂), δ = 1.79 (m, 8H, THF). ¹³C NMR (75.397 MHz, CH₃CN): δ = 135.13, 132.99, 132.78, 127.71, 126.62, 125.91, 122.18, 67.83, 25.80. ³¹P NMR (121.475 MHz, d₆-acetone): -10.34 (s).

(3-Bromophenyl)diphenylphosphine (2a). 1,3-dibromobenzene (11.0 g, 47.01 mmol) was dissolved in 150 mL dry, degassed THF and cooled to -95 °C under nitrogen using an acetone/liquid nitrogen bath. ⁿBuLi (1.6 M in hexane, 29.4 mL, 47.04 mmol) was added dropwise and the resulting cloudy solution was stirred at -95 °C. After 1 hour,

¹ Costa, E.; Pringle, P.G.; Ravetz, M.; Inorg. Synth. 1995, 31, 284-286.

² Schore, N.E.; Benner, L.S.; Labelle, B.E. Inorg. Chem. 1981, 20, 3200-3208.

³ Blicke, F.F.; Hotelling, E.B. J. Am. Chem. Soc. 1954, 76, 5099-5103.

⁴ Lustenberger, P.; Diederich, F. Helv. Chim. Acta 2000, 83, 2865-2883.

chlorodiphenylphosphine (8.43 mL, 46.98 mmol) was added dropwise. The solution was allowed to warm to room temperature over the course of 2 hours, and was then filtered through Celite in air. The resulting filtrate was dried in vacuo. The solids were then extracted with hexanes followed by filtration through a silica plug. Volatiles were removed in vacuo to afford a spectroscopically pure, moderately air-stable viscous oil (11.70 g, 74.0 %). ¹H NMR (300 MHz, d₆-acetone): δ = 7.56 (m, 1H), δ = 7.41 (m, 4H), δ = 7.25-7.40 (m, 9H), 7.35. ¹³C NMR (75.397 MHz, CH₃CN): δ = 137.45, 136.55, 134.74, 133.25, 132.78, 131.61, 130.37, 129.92, 123.87. ³¹P NMR (121.475 MHz, d₆-acetone): δ = -4.22 (s).

(4-Bromophenyl)diphenylphosphine (2b). 1,4-dibromobenzene (3.05 g, 13.0 mmol) was dissolved in 75 mL dry, degassed THF and cooled to -95 °C under nitrogen using an acetone/liquid nitrogen bath. ⁿBuLi (1.6 M in hexane, 8.2 mL, 13.0 mmol) was added dropwise and the resulting cloudy solution was stirred at -95 °C. After 1 hour, chlorodiphenylphosphine (2.88 g, 13.0 mmol) was added dropwise. The solution was allowed to warm to room temperature over the course of 2 hours, and was then filtered through Celite under air. The filtrate was then dried in vacuo. The resulting solids were extracted with hexanes followed by filtration through a silica plug. Volatiles were then removed in vacuo to afford a spectroscopically pure, moderately air-stable viscous oil (3.060 g, 69 %). ¹H NMR (300 MHz, d₆-acetone): $\delta = 7.52$ (m, 2H), $\delta = 7.33-7.37$ (m, 6H), $\delta = 7.26$ (m, 4H), 7.16 (m, 2H). ¹³C NMR (75.397 MHz, THF): $\delta = 137.28$, 137.04, 135.38, 133.72, 131.67, 128.66, 128.94, 123.26. ³¹P NMR (121.475 MHz, d₆-acetone): $\delta = -5.70$ (s).

(3-Bromophenyl)diisopropylphosphine (2c). 1,3-dibromobenzene (4.2 g, 17.95 mmol) was dissolved in 150 mL dry, degassed THF and cooled to -95 °C under nitrogen using an acetone/liquid nitrogen bath. ⁿBuLi (1.6 M in hexane, 11.2 mL, 17.95 mmol) was added dropwise and the resulting cloudy solution was stirred at -95 °C. After 1 hour, chlorodiisopropylphosphine (2.8 mL, 17.7 mmol) was added dropwise. The solution was allowed to warm to room temperature over the course of 2 hours, and was then filtered through Celite under a nitrogen atmosphere. The resulting filtrate was dried in vacuo and the remaining solids were extracted with petroleum ether followed by filtration through a silica plug. The volatiles were then removed in vacuo to afford the spectroscopically pure product as a viscous oil (2.95 g, 60.6 %). ¹H NMR (300 MHz, d₆-acetone): δ = 7.63 (m, 1H), δ = 7.57 (m, 1H), δ = 7.50 (m, 1H), 7.35 (t, 1H, J = 7.6Hz), δ = 2.15 (m, 2H), δ = 1.07 (m, 6H), 0.90 (m, 6H). ¹³C NMR (75.397 MHz, THF): δ = 137.31, 134.95, 133.55, 132.24, 129.98, 122.87, 23.55, 20.20, 19.17. ³¹P NMR (121.475 MHz, d₆-acetone): δ = 13.54 (s).

(4-Bromophenyl)diisopropylphosphine (2d). 1,4-dibromobenzene (12.5 g, 53.42 mmol) was dissolved in 150 mL dry, degassed THF and cooled to -95 °C under nitrogen using an acetone/liquid nitrogen bath. ⁿBuLi (1.6 M in hexane, 33.3 mL, 53.28 mmol) was added dropwise and the resulting cloudy solution was stirred at -95 °C. After 1 hour, chlorodiisopropylphosphine (8.5 mL, 53.45 mmol) was added dropwise. The solution was allowed to warm to room temperature over the course of 2 hours and was then filtered through Celite under a nitrogen atmosphere. The remaining filtrate was dried in

vacuo and the solids were extracted with petroleum ether followed by filtration through a silica plug. Solvent was removed in vacuo yielding the spectroscopically pure product as a viscous oil (12.03 g, 83.0 %). ¹H NMR (300 MHz, d₆-acetone): δ = 7.51 (m, 2H), δ = 7.36 (m, 2H), δ =2.07 (m, 2H), δ = 1.02 (m, 6H), 0.84 (m, 6H). ¹³C NMR (75.397 MHz, THF): δ = 136.63, 134.92, 134.19, 131.42, 24.45, 20.23, 19.12. ³¹P NMR (121.475 MHz, d₆-acetonitrile): δ = 15.75 (s).

[ASN][Ph₃BP^{*m*-Ph²}] (3). *m*-BrC₆H₄PPh₂ (2a) (0.734 g, 2.15 mmol) was dissolved in 75 mL of dry, degassed THF and the stirring solution was cooled to -90 °C. To this solution was added tert-BuLi (1.50 M in pentane, 1.43 mL, 2.15 mmol) and the resulting yellow solution was stirred for 1 hour at -90 °C. Triphenylborane (0.520 g, 2.15 mmol) was then added to the reaction pot as a THF solution. The mixture was then stirred and allowed to warm to room temperature. Volatiles were then removed in vacuo and the remaining solids were taken up in CH₂Cl₂. A solution of [ASN][Br] (0.443 g, 2.15 mmol) in CH₂Cl₂ was added dropwise. After stirring for 1 hour, copious amounts of Et₂O were added to precipitate the product. The resulting solids were collected on a sintered glass frit and washed with Et₂O and dried thoroughly to afford analytically pure **3** (1.175 g, 87 %). Crystals suitable for an X-ray diffraction study were grown by vapor diffusion of Et₂O into acetonitrile. ¹H NMR (300 MHz, d₃-acetonitrile): $\delta = 7.50$ (m, 1H), $\delta = 7.20$ -7.32 (m, 19H), $\delta = 6.98$ (m, 6H), $\delta = 6.83$ (m, 3H), $\delta = 3.83$ (m, 8H), $\delta = 2.10$ (m, 8H). ¹³C NMR (75.396 MHz, CH₃CN): δ = 163, 142.51, 139.36, 136.96, 135.94, 133.62, 132.38, 128.68, 128.55, 127.98, 126.04, 122.24, 65.10, 22.19. ³¹P NMR (121.475 MHz, d₃-acetonitrile): $\delta = \delta = -0.829$ (s). ¹¹B NMR (400 MHz, d₃-acetonitrile): $\delta = -10.99$ (s). Anal. Calcd. for C₄₄H₄₅BNP: C, 83.93; H, 6.84; N, 2.61. Found: C, 83.64; H, 7.03; N, 2.41.

[NBu₄][Ph₃BP^{*p*-Ph²}] (4). *p*-BrC₆H₄PPh₂ (2b) (1.254 g, 3.68 mmol) was dissolved in 75 mL of dry, degassed THF and the stirring solution was then cooled to -90 °C. To this solution was added tert-BuLi (1.50 M in pentane, 2.45 mL, 3.68 mmol) to form a yellow solution that was stirred for 1 hour at -90 °C. Triphenylborane (0.890 g, 3.68 mmol) was added as a THF solution after 1 hour and the resulting solution was stirred while warming gradually to room temperature. The reaction volatiles were then removed in vacuo and the remaining solids were taken up in CH_2Cl_2 A solution of [NBu₄][Br] (1.186 g, 3.68 mmol) in CH₂Cl₂ was added dropwise. After 1 hour, copious amounts of Et₂O were added and the solution was cooled to -35 °C to precipitate the product, which was isolated and dried to afford spectroscopically pure 4 (1.584 g, 57.8 %). ¹H NMR (300 MHz, d₃acetonitrile): $\delta = 7.37$ (m, 4H), $\delta = 7.20-7.33$ (m, 12H), $\delta = 7.04$ (m, 2H), $\delta = 7.00$ (m. 6H), $\delta = 6.85$ (m, 3H) $\delta = 3.07$ (m, 8H, NBu₄), $\delta = 1.56$ (m, 8H, NBu₄), $\delta = 1.33$ (m, 8H, NBu₄), $\delta = 0.96$ (m, 12H, NBu₄). ¹³C NMR (75.397 MHz, CH₃CN): $\delta = 162, 139.30,$ 136.52, 135.95, 133.49, 131.72, 128.69, 128.58, 126.01, 125.97, 122.23, 58.69, 23.79, 19.81, 13.36. ³¹P NMR (121.475 MHz, d₃-acetonitrile): $\delta = -3.23$ (s). ¹¹B NMR (400 MHz, d₃-acetonitrile): $\delta = -11.08$. Anal. Calcd. for C₅₂H₆₅BNP: C, 83.74; H, 8.78; N, 1.88. Found: C, 83.52; H, 8.01; N, 2.32.

 $[NBu_4][Ph_3BP^{m-iPr2}]$ (5). *m*-BrC₆H₄PⁱPr₂ (2c) (0.671 g, 2.46 mmol) was dissolved in 75 mL dry, degassed THF and stirring solution was cooled to -90 °C. To this solution was

added tert-BuLi (1.50 M in pentane, 1.64 mL, 2.46 mmol) and vellow solution was stirred for 1 hour at -90 °C. Triphenylborane (0.595 g, 2.46 mmol) was added as a THF solution and the solution was allowed to stir and warm to room temperature. Volatiles were removed in vacuo and remaining solids were taken up in CH₂Cl₂ A solution of NBu₄Br (0.793 g, 2.46 mmol) in CH₂Cl₂ was added. Solution was allowed to stir for 3 hours, then filtered through Celite. Solvent was removed in vacuo and solids were washed with copious amounts of petroleum ether and diethyl ether to afford 5 (0.802 g)48 %). This borate ligand is more difficult to crystallize than the others described, and its combustion analysis proved consequently high in carbon and low in nitrogen (two attempts). Crystals suitable for an X-ray diffraction study were grown via vapor diffusion of Et₂O into THF. ¹H NMR (300 MHz, d₃-acetonitrile): $\delta = 7.51(m, 3H)$, $\delta = 7.37(m, 3H)$ 6H), $\delta = 7.01$ (m, 1H), $\delta = 6.94$ (m, 6H), $\delta = 6.81$ (m, 3H) $\delta = 3.43$ (m, 8H, NBu₄), $\delta =$ 1.95 (m, 2H), $\delta = 1.82$ (m, 8H, NBu₄), $\delta = 1.45$ (m, 8H), $\delta = 1.12$ (m, 6H), $\delta = 0.99$ (m, 12H, NBu₄), $\delta = 0.84$ (m, 6H). ¹³C NMR (75.397 MHz, acetonitrile): $\delta = 162, 136.40,$ 135.96, 133.70, 128.77, 126.45, 125.85, 125.46, 122.08, 58.70, 23.80, 22.85, 20.06, 19.81, 18.76, 13.33. ³¹P NMR (121.475 MHz, d₃-acetonitrile): $\delta = 13.99$ (s). ¹¹B NMR (400 MHz, d₃-acetonitrile): $\delta = -11.02$ (s). Anal. Calcd. for C₄₆H₆₉BNP: C, 81.51; H, 10.26; N, 2.07. Found: C, 83.07; H, 11.26; N, 1.32.

 $[NBu_4][Ph_3BP^{p-iPr^2}]$ (6). p-BrC₆H₄PⁱPr₂ (2d) (1.391 g, 5.11 mmol) was dissolved in 75 mL dry, degassed THF and stirring solution was cooled to -90 °C. To this solution was added *tert*-BuLi (1.50 M in pentane, 3.41 mL, 5.11 mmol), providing a yellow solution that was stirred for 1 hour at -90 °C. Triphenylborane (1.235 g, 5.11 mmol) was added as a THF solution and the solution was stirred and allowed to warm to room temperature. Volatiles were removed in vacuo and the remaining solids were taken up in CH_2Cl_2 . A solution of [NBu₄][Br] (1.647 g, 5.11 mmol) in CH₂Cl₂ was then added. The resulting solution was then allowed to stir for 3 hours, followed by filtration through Celite. Solvent was removed in vacuo and the solids were washed with copious amounts of petroleum ether and ether to afford 6 (2.895 g, 84 %). ¹H NMR (300 MHz, d_3 acetonitrile): $\delta = 7.26$ (m, 8H), $\delta = 7.13$ (m, 2H), $\delta = 7.00$ (m, 6H), $\delta = 6.85$ (m, 3H) $\delta =$ 3.07 (m, 8H, NBu₄), $\delta = 2.05$ (m, 2H), $\delta = 1.59$ (m, 8H, NBu₄), $\delta = 1.34$ (m, 8H), $\delta = 1.03$ (m, 6H), $\delta = 0.96$ (m, 12H, NBu₄), $\delta = 0.88$ (m, 6H). ¹³C NMR (75.397 MHz, acetonitrile): $\delta = 162, 135.98, 135.69, 132.36, 126.45, 125.89, 122.16, 58.70, 23.80,$ 22.90, 20.13, 19.81, 18.91, 13.33. ³¹P NMR (121.475 MHz, d₃-acetonitrile): $\delta = 12.42$ (s). ¹¹B NMR (400 MHz, d_3 -acetonitrile): -11.13 (s). Anal. Calcd. for C₄₆H₆₉BNP: C, 81.51; H, 10.26; N, 2.07. Found: C, 81.71; H, 10.58; N, 2.26.

(**Ph**₃**SiP**^{*m*-Ph2}) (7). *m*-BrC₆H₄PⁱPr₂ (2a) (1.391 g, 5.11 mmol) was dissolved in 75 mL of dry, degassed Et₂O and stirred at -90 °C. To this solution was added *tert*-BuLi (1.50 M in pentane, 3.41 mL, 5.11 mmol) to form a yellow solution that was stirred for 1 hour at -90 °C. Triphenylsilylchloride (1.235 g, 5.11 mmol) was then added as an Et₂O solution, and the reaction mixture was stirred while allowing it to warm to room temperature. The final solution was filtered through Celite to remove LiCl, and the volatiles were removed from the filtrate in vacuo. The remaining oil was taken up in toluene and refluxed for 6 hours to precipitate the remaining LiCl salts. The supernatant was filtered through a pad of Celite and the volatiles were again removed to yield the product 7 (70 %). ¹H NMR

(300 MHz, d₆-benzene): δ = 7.96 (m, 1H), δ = 7.64-7.77 (m, 2H), δ = 7.58 (m, 6H), δ = 7.49 (m, 1H), δ = 7.35 (m, 4H), δ = 7.20 (m, 4H), δ = 7.11 (m, 6H), δ = 7.04 (m, 2H), δ = 7.00 (m, 3H). ³¹P NMR (121.475 MHz, d₆-benzene): δ = -7.29 (s). ES-MS⁺ (m/z) = 521.2

(**Ph**₃**SiP**^{*p*-Ph2}) (8). *m*-BrC₆H₄PⁱPr₂ (**2b**) (1.391 g, 5.11 mmol) was dissolved in 75 mL of dry, degassed Et₂O and stirred at -90 °C. To this solution was added *tert*-BuLi (1.50 M in pentane, 3.41 mL, 5.11 mmol) to form a yellow solution that was stirred for 1 hour at -90 °C. Triphenylsilylchloride (1.235 g, 5.11 mmol) was then added as an Et₂O solution, and the reaction mixture was then stirred while being allowed to warm to room temperature. The resulting suspension was filtered through Celite to remove LiCl and the volatiles were removed from the filtrate in vacuo. The remaining oil was then extracted into toluene and refluxed for 6 hours to further precipitate the remaining LiCl salts. The supernatant was filtered through a pad of Celite and the volatiles were again removed to afford product **8** (68 %). ¹H NMR (300 MHz, d₆-benzene): δ = 7.46 (m, 8H), δ = 7.34 (m, 4H), δ = 7.30 (m, 6H), δ = 7.26 (m, 6H), δ = 7.19 (m, 3H). ³¹P NMR (121.475 MHz, d₆-benzene): δ = -9.21 (s). ES-MS⁺ (m/z) = 521.2

(**Ph**₃**SiP**^{*m*-i**P**r²}) (9). *m*-BrC₆H₄PⁱPr₂ (**2c**) (1.391 g, 5.11 mmol) was dissolved in 75 mL of dry, degassed Et₂O and stirred at -90 °C. To this solution was added *tert*-BuLi (1.50 M in pentane, 3.41 mL, 5.11 mmol) to form a yellow solution that was stirred for 1 hour at -90 °C. Triphenylsilylchloride (1.235 g, 5.11 mmol) was added as an Et₂O solution, and the resulting suspension was allowed to warm to room temperature while stirring. The mixture was filtered through Celite to remove LiCl and the volatiles were then removed in vacuo from the filtrate. The remaining oil was taken up in toluene and refluxed for 6 hours to further precipitate the remaining LiCl salts. The solution was then filtered through a pad of Celite and the solvent was removed to afford product 9 (51 %). ¹H NMR (300 MHz, d₆-benzene): δ = 7.98 (m, 1H), δ = 7.69 (m, 6H), δ = 7.65 (m, 1H), δ = 7.57 (m, 1H), δ = 7.17 (m, 9H), δ = 7.10 (m, 1H), δ = 1.88 (m, 2H), δ = 0.99 (m, 6H), δ = 0.87 (m, 6H). ¹³C NMR (75.397 MHz, acetonitrile): ³¹P NMR (121.475 MHz, d₆-benzene): δ = 8.41 (s). ES-MS⁺ (m/z) = 453.1

(**Ph₃SiP**^{*p*-i**P**r²}) (10). *m*-BrC₆H₄PⁱPr₂ (2d) (1.391 g, 5.11 mmol) was dissolved in 75 mL of dry, degassed Et₂O and stirred at -90 °C. To this solution was added *tert*-BuLi (1.50 M in pentane, 3.41 mL, 5.11 mmol) to form a yellow solution that was stirred for 1 hour at -90 °C. Triphenylsilylchloride (1.235 g, 5.11 mmol) was added as an Et₂O solution, and the mixture was stirred and warmed gradually to room temperature. The resulting suspension was filtered through Celite to remove LiCl and the volatiles were then removed from the filtrate in vacuo. The remaining oil was extracted into toluene and refluxed for 6 hours to further precipitate the remaining LiCl salts. The solution was then filtered through a pad of Celite and the filtrate dried in vacuo to provide product **10** (56 %). ¹H NMR (300 MHz, d₆-benzene): δ = 7.71 (m, 2H), δ = 7.67 (m, 6H), δ = 7.47 (m, 2H), δ = 7.16 (m, 6H), δ = 7.11 (m, 3H), δ = 1.95 (m, 2H), δ = 1.02 (m, 6H), δ = 0.90 (m, 6H). ³¹P NMR (121.475 MHz, d₆-benzene): δ = 11.36 (s). ES-MS⁺ (m/z) = 453.1

{(NBD)RhCl][Ph₃BP^{*m*-iPr²}]}{NBu₄} (11). Solid [(NBD)RhCl]₂ (0.0144 g, 0.0224 mmol) was dissolved in THF. To this solution was added 6 (0.0302 g, 0.0461 mmol) as a THF solution. The reaction solution immediately changed from yellow to orange. Volatiles were removed in vacuo to yield product that was spectroscopically pure (yield ~ guantitative). ¹H NMR (300 MHz, d₆-acetone): $\delta = 7.33$ (m, 8H, o-BPh₃), $\delta = 7.04$ (m, 2H), $\delta = 6.96$ (m, 6H, *m*-BPh₃), $\delta = 6.82$ (m, 3H, *p*-BPh₃), $\delta = 3.62$ (m, 4H, NBD), $\delta =$ 3.52 (br, 2H, NBD), $\delta = 3.42$ (m, 8H, NBu₄), $\delta = 2.43$ (m, 2H, ¹Pr), $\delta = 1.82$ (m, 8H, NBu₄), $\delta = 1.44$ (m, 8H, NBu₄), $\delta = 1.22$ (m, 6H, ¹Pr), $\delta = 1.08$ (m, 6H, ¹Pr), $\delta = 0.99$ (m, 12H, NBu₄), $\delta = 0.85$ (m, 2H, NBD). ¹³C NMR (75.397 MHz, acetonitrile): $\delta = 163.6$, 138.25, 136.07, 135.72, 130.89, 128.60, 126.06, 122.35, 67.78, 58.86, 51.63, 50.98, 50.00, 23.91, 23.02, 19.11, 19.94, 18.91, 13.45. ³¹P NMR (121.475 MHz, d₆-acetone): 44.88 (d, ${}^{1}J_{Rh-P} = 166.4$ Hz). Anal. Calcd. for C₅₃H₇₇BClNPRh: C, 70.08; H, 8.54; N, 1.54. Found: C, 69.76; H, 8.49; N, 1.72. Note: A crystallographic study was performed on crystals of 11 generated from a separate experiment that showed significant bromide incorporation at the halide site. The batch of ligand 6 used in that preparation had not been thoroughly freed of [NBu₄][Br].

{ASN}₂{[Ph₃BP^{*m*-Ph²}]₂PtMe₂} (12). Solid (COD)PtMe₂ (0.0276 g, 0.083 mmol) and **3** (0.1024 g, 0.169 mmol) were dissolved and stirred in THF at room temperature for one hour. White precipitate was collected on a fine frit and washed first with petroleum ether (2 x 2 mL) and then with copious amounts of Et₂O. Thorough drying provided the desired white product **12** (isolated yield = 80 %). Crystals suitable for an X-ray diffraction study were grown from a crude product sample by vapor diffusion of Et₂O into acetonitrile. ¹H NMR (300 MHz, d₆-acetone): δ = 8.03 (m, 1H), δ = 7.66 (m, 1H), δ = 7.38 (m, 1H), δ = 7.30 (m, 6H, *o*-BPh₃), δ = 7.22 (m, 1H), δ = 7.15 (m, 4H, PPh₂), δ = 7.00 (m, 4H, PPh₂), δ = 6.86-6.96 (m, 8H, PPh₂, *m*-BPh₃), δ = 6.80 (m, 3H, *p*-BPh₃), δ = 3.48 (m, 16H, ASN), δ = 2.09 (m, 16H, ASN), δ = 0.32 (m, 6H, Pt-Me, ²J_{Pt-H} = 72.0 Hz). ¹³C NMR (75.396 MHz, acetonitrile): δ = 163, 138.8, 136.94, 134.64, 133.4, 129.28, 128.32, 127.05, 123.19, 65.10, 23.30, -19.5. ³¹P NMR (121.475 MHz, d₆-acetone): 28.63 (s, ¹J_{Pt-P} = 1947 Hz). Anal. Calcd. for C₉₀H₉₆B₂N₂P₂Pt: C, 72.82; H, 6.52; N, 1.89. Found: C, 72.45; H, 6.75; N, 2.20.

{NBu₄}₂{[Ph₃BP^{*p***-Ph²}]₂PtMe₂} (13).** Solid (COD)PtMe₂ (0.0756 g, 0.226 mmol) and 4 (0.3372 g, 0.453 mmol) were stirred in THF at room temperature for one hour. Volatiles were then removed in vacuo and the remaining solids were washed first with petroleum ether (2 x 2 mL) and then with a copious amount of Et₂O to provide, after drying, the desired product 13 (yield ~ quantitative). The product was readily recrystallized from THF/Et₂O. ¹H NMR (300 MHz, d₆-acetone): δ = 7.43 (m, 2H), δ = 7.38 (m, 4H, PPh₂), δ = 7.36 (m, 6H, *o*-BPh₃), δ = 7.28 (m, 4H, PPh₂), δ = 7.08 (m, 2H), δ = 6.94-7.01 (m, 8H, PPh₂, *m*-BPh₃), δ = 6.81 (m, 3H, *p*-BPh₃), δ = 3.38 (m, 16H, NBu₄), δ = 1.78 (m, 16H, NBu₄), δ = 1.40 (m, 16H, NBu₄), δ = 0.96 (m, 24H, NBu₄), δ = 0.33 (m, 6H, Pt-Me, ²*J*_{Pt-H} = 69.5 Hz). ¹³C NMR (75.397 MHz, acetonitrile): δ = 164, 136.30, 135.68, 134.32, 133.66, 129.08, 128.91, 127.60, 126.20, 122.50, 122.23, 58.87, 23.87, 19.91, 13.44. ³¹P NMR (121.475 MHz, d₆-acetone): 27.47 (s, ¹*J*_{Pt-P} = 1935 Hz). Anal. Calcd. for C₁₀₆H₁₃₆B₂N₂P₂Pt: C, 74.15; H, 7.56; N, 1.63. Found: C, 73.77; H, 8.18; N, 1.90.

{**NEt**₄}₂{(**Ph**₃**BP**^{*m*-i**P**r²})₂**PtMe**₂} (14). (COD)PtMe₂ (0.0840 g, 0.252 mmol) and **5** (0.1681 g, 0.298 mmol) were stirred in THF at room temperature for one hour. The reaction volatiles were then removed in vacuo and the resulting solids were washed with petroleum ether (2 x 2 mL) and then copious amounts of Et₂O to yield, after drying, the desired product **14** (yield ~ quantitative). The product was easily recrystallized from THF/Et₂O. ¹H NMR (300 MHz, d₆-acetone): δ = 7.51 (m, 1H), δ = 7.44(m, 1H), δ = 7.31 (m, 6H, *o*-BPh₃), δ = 7.23 (m, 1H), δ = 7.14 (m, 1H), δ = 7.02 (m, 6H, *m*-BPh₃), δ = 6.88 (m, 3H, *p*-BPh₃), δ = 3.05 (m, 16H, NEt₄),), δ = 0.17 (m, 6H, Pt-Me, ²J_{Pt-H} = 67.5 Hz). ¹³C NMR (75.396 MHz, acetonitrile): δ = 165 (*ipso*-B), 140.33, 137.17, 136.36, 133.65, 128.86, 126.48, 126.11, 123.48, 122.32, 52.61, 23.91, 20.70, 18.73, 7.27, -10.93. ³¹P NMR (121.475 MHz, d₆-acetone): 38.11 (s, ¹J_{Pt-P} = 1910 Hz). Anal. Calcd. For C₇₈H₁₁₂B₂N₂P₂Pt: C, 69.07; H, 8.32; N, 2.07. Found: C, 69.29; H, 8.17; N, 1.36.

[NBu₄]₂[(Ph₃BP^{*p*-iPr²})₂PtMe₂] (15). (COD)PtMe₂ (0.0840 g, 0.252 mmol) and **6** (0.1681 g, 0.298 mmol) were stirred in THF at room temperature for one hour. The reaction volatiles were then removed in vacuo and the resulting solids were washed with petroleum ether (2 x 2 mL) and then copious amounts of Et₂O to provide the desired white product (yield ~ quantitative). Product was recrystallized from THF/Et₂O. ¹H NMR (300 MHz, d₆-acetone): $\delta = 7.25-7.34$ (m, 12H), $\delta = 7.18-7.24$ (m, 4H), $\delta = 7.07$ (m, 4H), $\delta = 6.93$ (m, 12H), $\delta = 6.79$ (m, 6H), $\delta = 3.41$ (m, 16H, NBu₄), $\delta = 2.20$ (m, 4H, ⁱPr), $\delta = 1.78$ (m, 16H, NBu₄), $\delta = 1.41$ (m, 16H, NBu₄), $\delta = 1.14$ (m, 12H, ⁱPr), $\delta = 1.04$ (m, 12H, ⁱPr), $\delta = 0.97$ (m, 24H, NBu₄), $\delta = 0.30$ (m, 6H, Pt-Me, ²*J*_{Pt-H} = 66.0 Hz). ¹³C NMR (75.396 MHz, acetonitrile): $\delta = 164$ (*ipso*-B), 138.17, 136.05, 134.86, 131.13, 125.93, 122.19, 67.75, 58.78, 23.85, 20.58, 19.88, 18.92, 13.41, -9.8. ³¹P NMR (121.475 MHz, d₆-acetone): 31.53 (s, ¹*J*_{Pt-P} = 1907 Hz). Anal. Calcd. For C₉₄H₁₄₄B₂N₂P₂Pt: C, 71.42; H, 9.18; N, 1.77. Found: C, 71.29; H, 9.21; N, 2.25.

(**Ph₃SiP**^{*p*-i**P**r²})₂**PtMe₂** (16). (COD)PtMe₂ (0.0840 g, 0.252 mmol) was stirred in the presence of 10 (0.1681 g, 0.298 mmol) in THF at room temperature for one hour. The reaction volatiles were then removed in vacuo and the remaining solids were washed with petroleum ether (2 x 2 mL) and Et₂O (2 x 2 mL) to provide the desired white product quantitatively. ¹H NMR (300 MHz, d₆-acetone): δ = 7.34-7.64 (m, 38H), δ = 2.42 (m, 4H, ⁱPr), δ = 1.13 (m, 12H, ⁱPr), δ = 1.01 (m, 12H, ⁱPr), δ = 0.30 (m, 6H, Pt-Me, ²*J*_{Pt-H} = 63.0 Hz). ³¹P NMR (121.475 MHz, d₆-acetone): 36.94 (s, ¹*J*_{Pt-P} = 1883 Hz).

 $(Ph_3SiP^{p-Ph})_2PtMe_2$ (17). Prepared as for the case of 16. ¹H NMR (300 MHz, d₆-acetone): $\delta = 7.45$ (m, 12H), $\delta = 7.16-7.45$ (m, 46H), $\delta = 0.39$ (m, 6H, Pt-Me, ² $J_{Pt-H} = 60.0$ Hz). ³¹P NMR (121.475 MHz, d₆-acetone): 30.45 (s, ¹ $J_{Pt-P} = 1900$ Hz).

[*cis*-(Ph₃SiP^{*p*-Ph²})₂PtMe(solv)][Me(B(C₆F₅)₃] (18). Complex 17 (0.0195 g, 0.0154 mmol) was stirred in a THF solution containing B(C₆F₅)₃ (0.0079 g, 0.0154 mmol) for 12 hours. The ³¹P NMR spectrum verified clean generation of a single *cis* mono-solvento, mono-methyl species (18). ¹H NMR (300 MHz, d₆-acetone): $\delta = 6.98-8.02$ (m, 58H), $\delta = 0.52$ (br s, 3H, Me(B(C₆F₅)₃), $\delta = 0.61$ (m, 3H, Pt-Me, ²*J*_{Pt-H} = 54.0 Hz). ³¹P NMR (121.475 MHz, d₆-acetone): 24.4 (d, ¹*J*_{Pt-P} = 1942 Hz, ²*J*_{P-P} = 396 Hz).

{**NBu**₄}{**Mo**(**CO**)₅[**Ph**₃**BP**^{*m*-i**P**r²}]} (19). Solid Mo(CO₆) (0.0078 g, 0.030 mmol) and solid 5 (0.0204 g, 0.0301 mmol) were combined in THF and refluxed for 12 hours to provide a yellow solution. Volatiles were then removed in vacuo. The solid product was recrystallized from THF/Et₂O to provide **19**. ¹H NMR (300 MHz, d₆-acetonitrile): δ = 7.42 (m, 3H), δ = 7.34 (m, 6H), δ = 7.11 (m, 1H), δ = 6.95 (m, 6H), δ = 6.80 (m, 3H) δ = 3.43 (m, 8H, NBu₄), δ = 2.32 (m, 2H), δ = 1.81 (m, 8H, NBu₄), δ = 1.42 (m, 8H), δ = 1.07 (m, 6H, ⁱPr), δ = 0.97 (m, 12H, NBu₄), δ = 0.91 (m, 6H, ⁱPr). ³¹P NMR (121.475 MHz, d₆-acetone): δ = 52.33 (s). IR: (KBr/CH₂Cl₂): 2065, 1925 cm⁻¹. ES-MS⁻ (m/z) = 671, 643, 615.

[NBu₄][Mo(CO)₅(Ph₃SiP^{*m*-iPr²})] (20). Solid Mo(CO₆) (0.0078 g, 0.030 mmol) and solid 9 (0.0204 g, 0.0301 mmol) were combined in THF and refluxed for 12 hours to provide a yellow solution. The reactions volatiles were removed in vacuo and the remaining solid product was recrystallized from THF/Et₂O. ¹H NMR (300 MHz, d₆-benzene): δ = 7.68 (m, 1H), δ = 7.59 (m, 6H), δ = 7.47 (m, 1H), δ = 7.29 (m, 1H), δ = 7.16 (m, 9H), δ = 7.10 (m, 1H), δ = 2.03 (m, 2H), δ = 1.04 (m, 6H), δ = 0.89 (m, 6H). ³¹P NMR (121.475 MHz, d₆-benzene): δ = 51.86 (s). IR: (KBr/CH₂Cl₂): 2070, 1942 cm⁻¹.

General Procedure for Suzuki coupling reactions. $Pd_2(dba)_3$ (0.0046 g, 1.5 mol %), **5** (0.0135 g, 6.0 mol %), PhB(OH)₂ (0.0446 g, 0.367 mmol), and Cs₂CO₃ (0.2606 g, 0.800 mmol) were combined under air in a 5 mL screw-cap vial equipped with a stir bar. The vial was then sealed with a septum and flushed thoroughly with nitrogen, after which time one equivalent of the appropriate aryl halide was added as a THF solution (dry, 1.5 mL). While under nitrogen, the septum was quickly replaced with a Teflon-lined cap. The reaction mixture was then refluxed with stirring for 24 hours. The mixture was then diluted with copious amounts of ether and filtered through a silica plug. Volatiles were removed in vacuo, and the product was purified by flash chromatography.

4-chlorobiphenyl. Aryl halide: 1,4-dichlorobenzene (0.0489 g, 0.333 mmol). Product was isolated via column chromatography (hexanes). ¹H NMR (300 MHz, CDCl₃): $\delta = 7.37-7.58$ (m, 9H).

4-methylbiphenyl. Aryl halide: 4-chlorotoluene (39.4 µL, 0.333 mmol). Product was isolated via column chromatography (hexanes). ¹H (NMR (300 MHz, CDCl₃): δ = 7.57 (m, 2H), δ = 7.49 (m, 2H), δ = 7.42 (m, 2H), δ = 7.32 (m, 1H), δ = 7.35 (m, 2H), δ = 2.39 (s, 3H).

4-phenylacetophenone. Aryl halide: 4-chloroacetophenone (43.2 µL, 0.333 mmol). Product was isolated via column chromatography (1% EtOAc/hexanes). ¹H NMR (300 MHz, CDCl₃): $\delta = 8.03$ (m, 2H), $\delta = 7.69$ (m, 2H), $\delta = 7.63$ (m, 2H), $\delta = 7.47$ (m, 2H), 7.40 (m, 1H), $\delta = 2.64$ (s, 3H). Note on Suzuki coupling reactions: A point of concern pertains to whether the tetraarylborate unit of ligand **5** is transferred during the cross-coupling reactions. While we cannot rule-out this possibility altogether, we note that (i) tolylboronic acids were also screened and found to give comparable yields of cross-coupled products. Also, the yield of cross-coupled product far exceeds the molar ratio of the (phosphino)borate ligand, which was used in catalytic quantity. Thus, aryl transfer from the ligand is not critical to cross-coupling of the chloride substrates shown in Table 1 in the main text.

Additional Suzuki Coupling Data using *o*-tolylboronic acid:

The following data were obtained as non-optimized yields by crude GC-MS analysis.

1.5 mol % Pd ₂ (dba) ₃ B(OH) ₂ X 6 0 mol % INBu JIPb ₂ BP ^{m-jPr2} 1 /				
+	1.1 equiv. Cs	2 ^{CO3}	R	
1.1 equiv R	toluene, 18	3 hrs, 100°C		
Substrate	Yield (%) ^a	Substrate	Yield (%) ^a	
	99 %	0 Br	59 %	
H ₂ N	46 %	MeO	54 %	
0	99 %	O ₂ N Br	53 %	
OH	47 %	O CI	23 %	
Br	71 %	O CI	25 %	
^a Unoptimized GC yields.				

Figure 1: Fully labeled drawing of $\{[NEt_4][Ph_3BP^{m-Ph_2}]\}_2$. Hydrogens have been omitted for clarity. One of the two cations in the unit cell was found to be disordered over two positions, contributing to the high GOF value for this structure. Only one of these positions is modeled in the following representation.



Figure 2: Fully labeled drawing of $\{[NEt_4][Ph_3BP^{m-iPr2}]\}_2$. Hydrogens have been omitted for clarity.



Figure 3: Fully labeled drawing of $\{NBu_4\} \{[Ph_3BP^{p-iPr2}]RhX(NBD)\}$ (X modeled as Br (60%), Cl (40%)). Hydrogens have been omitted for clarity. Bromide contamination in this crystal likely resulted from the presence of $[NBu_4][Br]$ in the batch of ligand used to prepare the rhodium sample. This crystal structure was obtained prior to optimization of the ligand purifaction procedure, and serves to establish the proposed connectivity. Pure

 ${NBu_4} {[Ph_3BP^{p-iPr2}]RhCl(NBD)}$ can be obtained by the procedure outlined in the experimental section above using $[NBu_4][Ph_3BP^{p-iPr2}]$ free of $[NBu_4][Br]$ contaminant.



Figure 4: Fully labeled drawing of $\{ASN\}_2\{[Ph_3BP^{m-Ph_2}]_2PtMe_2\}$. Hydrogens have been omitted for clarity. This crystal co-crystallized with one equiv of an [ASN][Br] salt, and one solvent molecule (Et₂O). These have been omitted for clarity. The [ASN][Br]

contamination arises from its presence in the sample of [ASN][Ph₃BP^{*m*-Ph²}] used to prepare this sample. This sample that afforded this crystal structure was obtained prior to the optimization of the preparation of [ASN][Ph₃BP^{*m*-Ph²}], which frees the ligand from [ASN][Br].



Empirical formula	C44H49BNP
Formula weight	633.62
Crystal Habit	plate
Crystal Color	colorless
Crystal size	0.581 x 0.24 x 0.085 mm ³

Table 1. Crystal data and structure refinement for $\{[NEt_4][Ph_3BP^{m-Ph_2}]\}_2$

Data Collection

Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Data collection temperature	98(2) K	
Unit cell dimensions	a = 18.0519(13) Å b = 10.4941(8) Å c = 38.060(3) Å	$\alpha = 90^{\circ}$ $\beta = 90.4990(10)^{\circ}$ $\gamma = 90^{\circ}$
Volume	7209.7(9) Å ³	
Ζ	8	
Crystal system	Monoclinic	
Space group	P2 ₁	
Density (calculated)	1.167 Mg/m ³	
F(000)	2720	
θ range for data collection	1.55 to 28.58°	
Completeness to $\theta = 28.58^{\circ}$	$\theta = 28.58^{\circ} \qquad 93.1 \%$	
Index ranges	$-24 \le h \le 23, -13 \le k \le 14, -49$	$\leq l \leq 50$
Reflections collected	122531	
Independent reflections	17132 [R(int) = 0.1101]	
Absorption coefficient	0.108 mm ⁻¹	
Absorption correction	None	
Structure solut	ion and refinement	
Structure solution program	SHELXS-97 (Sheldrick (1990)	1
Primary solution method	direct methods	
Secondary solution method	Difference Fourier Map	
Hydrogen placement	calculated positions	
Structure refinement program	SHELXL-97 (Sheldrick (1997)	

Structure refinement program

Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	17132 / 0 / 856		
Goodness-of-fit on F ²	2.159		
Final R indices [I>2sigma(I)]	R1 = 0.0903, wR2 = 0.1242		
R indices (all data)	R1 = 0.1742, wR2 = 0.1309		
Largest diff. peak and hole	1.538 and -1.535 e.Å ⁻³		

Special Refinement Details: One of the cations in the unit cell is disordered. Attempts to model the disorder were unsuccessful.

	X	У	Z	U(eq)
B(1)	1098(2)	8608(3)	935(1)	18(1)
P(1)	1611(1)	12247(1)	1886(1)	30(1)
C(1)	1144(2)	7051(3)	877(1)	23(1)
C(2)	1278(2)	6206(3)	1148(1)	41(1)
C(3)	1278(2)	4853(4)	1090(1)	49(1)
C(4)	1139(2)	4418(4)	756(1)	49(1)
C(5)	981(2)	5205(4)	484(1)	49(1)
C(6)	995(2)	6508(3)	550(1)	36(1)
C(7)	1398(2)	9370(3)	587(1)	20(1)
C(8)	1982(2)	8909(3)	385(1)	27(1)
C(9)	2290(2)	9589(4)	111(1)	35(1)
C(10)	2028(2)	10781(4)	31(1)	43(1)
C(11)	1451(2)	11277(4)	217(1)	42(1)
C(12)	1150(2)	10577(3)	492(1)	36(1)
C(12)	226(2)	8857(3)	1019(1)	20(1)
C(14)	-318(2)	9025(3)	758(1)	$\frac{23(1)}{33(1)}$
C(15)	-1077(2)	9079(3)	833(1)	38(1)
C(16)	-1305(2)	8973(3)	1170(1)	43(1)
C(17)	-800(2)	8807(4)	1434(1)	52(1)
C(18)	-53(2)	8760(3)	1355(1)	37(1)
C(19)	1653(2)	9127(3)	1249(1)	19(1)
C(20)	2335(2)	8574(3)	1333(1)	23(1)
C(21)	2819(2)	9093(3)	1581(1)	26(1)
C(22)	2630(2)	10193(3)	1752(1)	27(1)
C(23)	1963(2)	10803(3)	1676(1)	23(1)
C(24)	1501(2)	10253(3)	1424(1)	23(1)
C(25)	2431(2)	12950(3)	2098(1)	29(1)
C(26)	2769(2)	13968(3)	1930(1)	33(1)
C(27)	3404(2)	14506(3)	2070(1)	38(1)
C(28)	3696(2)	14054(3)	2382(1)	36(1)
C(29)	3362(2)	13063(3)	2553(1)	35(1)
C(30)	2736(2)	12507(3)	2412(1)	30(1)
C(31)	1135(2)	11585(3)	2266(1)	30(1)
C(32)	1134(2)	10302(3)	2360(1)	34(1)
C(33)	743(2)	9858(4)	2645(1)	40(1)
C(34)	342(2)	10689(4)	2852(1)	43(1)
C(35)	331(2)	11968(4)	2761(1)	44(1)
C(36)	718(2)	12402(4)	2474(1)	36(1)
B(2)	6141(2)	6265(3)	959(1)	17(1)
P(2)	6254(1)	2867(1)	2049(1)	30(1)
C(37)	5248(2)	5948(3)	910(1)	18(1)
C(38)	4744(2)	6059(3)	1186(1)	24(1)
C(39)	3972(2)	5980(3)	1133(1)	27(1)
C(40)	3694(2)	5779(3)	799(1)	28(1)
C(41)	4168(2)	5642(3)	520(1)	29(1)
C(42)	4927(2)	5720(3)	577(1)	23(1)

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters $(Å^2x \ 10^3)$ for $\{[NEt_4][Ph_3BP^{m-Ph_2}]\}_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

C(43)	6189(2)	7822(3)	926(1)	18(1)
C(44)	6193(2)	8638(3)	1216(1)	23(1)
C(45)	6232(2)	9962(3)	1180(1)	27(1)
C(46)	6257(2)	10508(3)	851(1)	29(1)
C(47)	6234(2)	9737(3)	560(1)	31(1)
C(48)	6193(2)	8432(3)	601(1)	27(1)
C(49)	6617(2)	5539(3)	650(1)	19(1)
C(50)	7205(2)	6095(3)	470(1)	30(1)
C(51)	7589(2)	5458(4)	211(1)	39(1)
C(52)	7415(2)	4219(4)	124(1)	34(1)
C(53)	6868(2)	3619(3)	310(1)	31(1)
C(54)	6483(2)	4264(3)	565(1)	26(1)
C(55)	6513(2)	5764(3)	1328(1)	18(1)
C(56)	6264(2)	4731(3)	1526(1)	25(1)
C(57)	6646(2)	4263(3)	1823(1)	23(1)
C(58)	7299(2)	4846(3)	1927(1)	27(1)
C(59)	7564(2)	5872(3)	1738(1)	27(1)
C(60)	7178(2)	6308(3)	1447(1)	22(1)
C(61)	5830(2)	3578(3)	2439(1)	28(1)
C(62)	5517(2)	2766(4)	2687(1)	33(1)
C(63)	5181(2)	3239(4)	2981(1)	40(1)
C(64)	5145(2)	4533(4)	3039(1)	37(1)
C(65)	5456(2)	5350(4)	2799(1)	33(1)
C(66)	5789(2)	4884(3)	2501(1)	30(1)
C(67)	7076(2)	2135(3)	2257(1)	28(1)
C(68)	7382(2)	1069(3)	2100(1)	36(1)
C(69)	8009(2)	494(4)	2240(1)	47(1)
C(70)	8335(2)	970(4)	2545(1)	47(1)
C(71)	8027(2)	2010(3)	2705(1)	40(1)
C(72)	7414(2)	2584(3)	2564(1)	33(1)
N(1)	3943(1)	1514(2)	792(1)	21(1)
C(73)	4004(2)	1917(3)	412(1)	28(1)
C(74)	4782(2)	1974(3)	268(1)	35(1)
C(75)	4305(2)	222(3)	861(1)	28(1)
C(76)	4047(2)	-851(3)	626(1)	36(1)
C(77)	3129(2)	1413(3)	884(1)	24(1)
C(78)	2704(2)	2663(3)	886(1)	34(1)
C(79)	4339(2)	2500(3)	1015(1)	25(1)
C(80)	4261(2)	2347(3)	1405(1)	36(1)
N(2)	8900(2)	3264(3)	1049(1)	41(1)
C(81)	9184(3)	3230(6)	1419(2)	117(2)
C(82)	9501(4)	2307(6)	1593(1)	146(3)
C(87)	9393(3)	2548(6)	831(2)	176(4)
C(88)	9187(4)	2556(5)	438(1)	127(3)
C(84)	7648(2)	2473(5)	1225(2)	103(2)
C(86)	9161(3)	5576(5)	919(2)	173(4)
C(83)	8172(3)	2824(12)	1062(2)	333(9)
C(85)	8925(7)	4523(5)	940(2)	325(9)

B(1)-C(13)	1.629(4)	C(26)-C(27)	1.382(5)
B(1)-C(7)	1.643(5)	C(26)-H(26)	0.9500
B(1)-C(19)	1.644(5)	C(27)-C(28)	1.379(5)
B(1)-C(1)	1.651(5)	C(27)-H(27)	0.9500
P(1)-C(31)	1.823(4)	C(28)-C(29)	1.370(4)
P(1)-C(23)	1.829(3)	C(28)-H(28)	0.9500
P(1)-C(25)	1.834(3)	C(29)-C(30)	1.376(4)
C(1)-C(2)	1.379(4)	C(29)-H(29)	0.9500
C(1)-C(6)	1.395(4)	C(30)-H(30)	0.9500
C(2)-C(3)	1.437(5)	C(31)-C(36)	1.393(4)
C(2)-H(2)	0.9500	C(31)-C(32)	1.394(5)
C(3)-C(4)	1 372(5)	C(32)-C(33)	1 379(4)
C(3)-H(3)	0.9500	C(32)-H(32)	0.9500
C(4)-C(5)	1 351(5)	C(32) - C(34)	1.383(5)
C(4)-H(4)	0.9500	C(33)-H(33)	0.9500
C(5) - C(6)	1 390(5)	C(34) - C(35)	1.386(5)
C(5)-U(5)	0.9500	C(34)-C(35)	0.0500
C(5) - H(5) C(6) + H(6)	0.9500	C(35) C(36)	1.381(5)
$C(0) - \Pi(0)$	0.3300 1.201(4)	C(35)-C(30)	1.361(3)
C(7) - C(12)	1.391(4) 1.207(4)	$C(33) - \Pi(33)$	0.9300
C(7) - C(8)	1.39/(4) 1.29((4)	$C(50)-\Pi(50)$	0.9300
C(8) - C(9)	1.380(4)	B(2) - C(33)	1.030(4)
C(8) - H(8)	0.9500	B(2)-C(43)	1.641(5)
C(9) - C(10)	1.3/1(5)	B(2) - C(49)	1.031(3)
C(9)-H(9)	0.9500	B(2)-C(37)	1.054(4)
C(10) - C(11)	1.369(5)	P(2) - C(61)	1.834(4)
C(10)-H(10)	0.9500	P(2)-C(6/)	1.843(3)
C(11)-C(12)	1.393(4)	P(2)-C(57)	1.843(3)
C(11)-H(11)	0.9500	C(37)-C(38)	1.400(4)
C(12)-H(12)	0.9500	C(37)-C(42)	1.409(4)
C(13)-C(18)	1.381(4)	C(38)-C(39)	1.409(4)
C(13)-C(14)	1.403(4)	C(38)-H(38)	0.9500
C(14)-C(15)	1.405(4)	C(39)-C(40)	1.377(4)
C(14)-H(14)	0.9500	C(39)-H(39)	0.9500
C(15)-C(16)	1.354(5)	C(40)-C(41)	1.376(4)
C(15)-H(15)	0.9500	C(40)-H(40)	0.9500
C(16)-C(17)	1.363(5)	C(41)-C(42)	1.388(4)
C(16)-H(16)	0.9500	C(41)-H(41)	0.9500
C(17)-C(18)	1.386(5)	C(42)-H(42)	0.9500
C(17)-H(17)	0.9500	C(43)-C(48)	1.394(4)
C(18)-H(18)	0.9500	C(43)-C(44)	1.396(4)
C(19)-C(24)	1.384(4)	C(44)-C(45)	1.398(4)
C(19)-C(20)	1.396(4)	C(44)-H(44)	0.9500
C(20)-C(21)	1.389(4)	C(45)-C(46)	1.379(4)
C(20)-H(20)	0.9500	C(45)-H(45)	0.9500
C(21)-C(22)	1.370(4)	C(46)-C(47)	1.372(4)
C(21)-H(21)	0.9500	C(46)-H(46)	0.9500
C(22) - C(23)	1.392(4)	C(47) - C(48)	1.381(4)
C(22)-H(22)	0.9500	C(47)-H(47)	0.9500
C(23)-C(24)	1.392(4)	C(48)-H(48)	0.9500
C(24)-H(24)	0.9500	C(49)-C(50)	1.395(4)
C(25) - C(26)	1.390(4)	C(49)-C(54)	1.397(4)
C(25)-C(30)	1.392(4)	C(50)-C(51)	1.384(4)

Table 3. Bond lengths [Å] and angles [°] for $\{[NEt_4][Ph_3BP^{m-Ph_2}]\}_2$.

C(50)-H(50)	0.9500	C(77)-C(78)	1.519(4)
C(51)-C(52)	1.377(5)	C(77)-H(77A)	0.9900
C(51)-H(51)	0.9500	C(77)-H(77B)	0.9900
C(52)-C(53)	1.373(4)	C(78)-H(78A)	0.9800
C(52)-H(52)	0.9500	C(78)-H(78B)	0.9800
C(53)-C(54)	1.376(4)	C(78)-H(78C)	0.9800
C(53)-H(53)	0.9500	C(79)-C(80)	1.502(4)
C(54)-H(54)	0.9500	C(79)-H(79A)	0.9900
C(55)- $C(56)$	1 397(4)	C(79)-H(79B)	0 9900
C(55)- $C(60)$	1 401(4)	C(80)-H(80A)	0.9800
C(56)- $C(57)$	1 408(4)	C(80)-H(80B)	0.9800
C(56)-H(56)	0.9500	C(80)-H(80C)	0.9800
C(57)- $C(58)$	1384(4)	N(2)-C(85)	1 387(6)
C(58)- $C(59)$	1 383(4)	N(2) - C(83)	1 393(6)
C(58)-H(58)	0.9500	N(2) - C(87)	1.335(0) 1.434(6)
C(59)- $C(60)$	1.382(4)	N(2) - C(81)	1 495(6)
C(59)- $H(59)$	0.9500	C(81)- $C(82)$	1 303(6)
C(60)-H(60)	0.9500	C(81) - H(81A)	0.9900
C(61)- $C(66)$	1.393(4)	C(81)-H(81B)	0.9900
C(61)-C(62)	1.393(4) 1.304(4)	C(82) - H(82A)	0.9900
C(62)-C(63)	1.371(5)	C(82)-H(82R)	0.9800
C(62)-C(03)	0.9500	C(82)-H(82C)	0.9800
$C(62)-\Gamma(62)$	1 378(5)	C(82)-T(62C)	1 539(8)
C(63)-U(63)	0.9500	C(87) - H(87A)	0.0000
C(64)-C(65)	1.374(4)	C(87)-H(87B)	0.9900
C(64)-H(64)	0.9500	C(88)-H(88A)	0.9900
C(65)-C(66)	1.378(4)	C(88)-H(88B)	0.9800
C(65)- $H(65)$	0.9500	C(88)-H(88C)	0.9800
C(66)-H(66)	0.9500	C(84)-C(83)	1 195(6)
C(67)- $C(68)$	1 386(4)	C(84)-H(84A)	0.9800
C(67)- $C(72)$	1 394(4)	C(84)-H(84B)	0.9800
C(68)-C(69)	1 384(5)	C(84)-H(84C)	0.9800
C(68)-H(68)	0.9500	C(86)-C(85)	1 187(8)
C(69)- $C(70)$	1 390(5)	C(86) - H(86A)	0 9800
C(69)-H(69)	0.9500	C(86)-H(86B)	0 9800
C(70)- $C(71)$	1 371(5)	C(86)-H(86C)	0.9800
C(70)-H(70)	0.9500	C(83)-H(83A)	0 9900
C(71)- $C(72)$	1 366(4)	C(83)-H(83B)	0 9900
C(71)-H(71)	0.9500	C(85)-H(85A)	0 9900
C(72)-H(72)	0.9500	C(85)-H(85B)	0.9900
N(1)-C(79)	1.513(4)		
N(1)-C(73)	1 514(4)	C(13)-B(1)-C(7)	113 9(3)
N(1)-C(77)	1 517(4)	C(13)-B(1)-C(19)	112.8(3)
N(1)-C(75)	1 526(4)	C(7)-B(1)-C(19)	102.8(2)
C(73)-C(74)	1 514(4)	C(13)-B(1)-C(1)	102.6(2) 103 6(2)
C(73)-H(73A)	0.9900	C(7)-B(1)-C(1)	100.0(2) 110.9(3)
C(73)-H(73B)	0.9900	C(19)-B(1)-C(1)	113.2(3)
C(74)-H(74A)	0.9800	C(31)-P(1)-C(23)	101.2(3)
C(74)-H(74B)	0.9800	C(31)-P(1)-C(25)	100 88(16)
C(74)-H(74C)	0.9800	C(23)-P(1)-C(25)	104 07(15)
C(75)-C(76)	1.508(4)	C(2)-C(1)-C(6)	115.9(3)
C(75)-H(75A)	0.9900	C(2)-C(1)-B(1)	123.0(3)
C(75)-H(75B)	0.9900	C(6)-C(1)-B(1)	120.9(3)
C(76)-H(76A)	0.9800	C(1)-C(2)-C(3)	121.3(4)
C(76)-H(76B)	0.9800	C(1)-C(2)-H(2)	119.3
C(76)-H(76C)	0.9800	C(3)-C(2)-H(2)	119.3

C(4)-C(3)-C(2)	118.2(4)	C(20)-C(21)-H(21)	120.1
C(4)-C(3)-H(3)	120.9	C(21)-C(22)-C(23)	120.4(3)
С(2)-С(3)-Н(3)	120.9	C(21)-C(22)-H(22)	119.8
C(5)-C(4)-C(3)	122.8(4)	C(23)-C(22)-H(22)	119.8
C(5)-C(4)-H(4)	118.6	C(22)-C(23)-C(24)	117.7(3)
C(3)-C(4)-H(4)	118.6	C(22)-C(23)-P(1)	126.4(3)
C(4)-C(5)-C(6)	117.4(4)	C(24)-C(23)-P(1)	115.9(2)
C(4)-C(5)-H(5)	121.3	C(19)-C(24)-C(23)	124.5(3)
C(6)-C(5)-H(5)	121.3	C(19)-C(24)-H(24)	117.8
C(5)-C(6)-C(1)	124.4(4)	C(23)-C(24)-H(24)	117.8
C(5)-C(6)-H(6)	117.8	C(26)-C(25)-C(30)	118.7(3)
C(1)-C(6)-H(6)	117.8	C(26)-C(25)-P(1)	117.5(3)
C(12)-C(7)-C(8)	114.5(3)	C(30)-C(25)-P(1)	123.7(3)
C(12)-C(7)-B(1)	123.1(3)	C(27)-C(26)-C(25)	120.1(3)
C(8)-C(7)-B(1)	122.1(3)	С(27)-С(26)-Н(26)	119.9
C(9)-C(8)-C(7)	123.2(3)	C(25)-C(26)-H(26)	119.9
C(9)-C(8)-H(8)	118.4	C(28)-C(27)-C(26)	120.1(4)
C(7)-C(8)-H(8)	118.4	С(28)-С(27)-Н(27)	119.9
C(10)-C(9)-C(8)	119.8(4)	С(26)-С(27)-Н(27)	119.9
C(10)-C(9)-H(9)	120.1	C(29)-C(28)-C(27)	120.3(4)
C(8)-C(9)-H(9)	120.1	C(29)-C(28)-H(28)	119.9
C(11)-C(10)-C(9)	119.6(4)	C(27)-C(28)-H(28)	119.9
С(11)-С(10)-Н(10)	120.2	C(28)-C(29)-C(30)	120.0(4)
C(9)-C(10)-H(10)	120.2	C(28)-C(29)-H(29)	120.0
C(10)-C(11)-C(12)	119.6(4)	С(30)-С(29)-Н(29)	120.0
С(10)-С(11)-Н(11)	120.2	C(29)-C(30)-C(25)	120.7(3)
С(12)-С(11)-Н(11)	120.2	С(29)-С(30)-Н(30)	119.6
C(7)-C(12)-C(11)	123.3(4)	С(25)-С(30)-Н(30)	119.6
C(7)-C(12)-H(12)	118.3	C(36)-C(31)-C(32)	116.4(4)
C(11)-C(12)-H(12)	118.3	C(36)-C(31)-P(1)	118.5(3)
C(18)-C(13)-C(14)	114.0(3)	C(32)-C(31)-P(1)	125.1(3)
C(18)-C(13)-B(1)	122.0(3)	C(33)-C(32)-C(31)	122.1(4)
C(14)-C(13)-B(1)	123.6(3)	C(33)-C(32)-H(32)	118.9
C(13)-C(14)-C(15)	122.5(4)	C(31)-C(32)-H(32)	118.9
C(13)-C(14)-H(14)	118.7	C(32)-C(33)-C(34)	120.5(4)
C(15)-C(14)-H(14)	118.7	C(32)-C(33)-H(33)	119.7
C(16)-C(15)-C(14)	119.7(4)	C(34)-C(33)-H(33)	119.7
C(16)-C(15)-H(15)	120.1	C(33)-C(34)-C(35)	118.4(4)
C(14)-C(15)-H(15)	120.1	C(33)-C(34)-H(34)	120.8
C(15)-C(16)-C(17)	120.2(4)	C(35)-C(34)-H(34)	120.8
C(15)-C(16)-H(16)	119.9	C(36)-C(35)-C(34)	120.6(4)
C(17)-C(16)-H(16)	119.9	C(36)-C(35)-H(35)	119.7
C(16)-C(17)-C(18)	119.2(4)	C(34)-C(35)-H(35)	119.7
C(16)-C(17)-H(17)	120.4	C(35)-C(36)-C(31)	121.9(4)
C(18)-C(17)-H(17)	120.4	C(35)-C(36)-H(36)	119.1
C(13)-C(18)-C(17)	124.3(4)	C(31)-C(36)-H(36)	119.1
C(13)-C(18)-H(18)	117.8	C(55)-B(2)-C(43)	111.4(3)
C(17)-C(18)-H(18)	117.8	C(55)-B(2)-C(49)	104.5(2)
C(24)-C(19)-C(20)	115.0(3)	C(43)-B(2)-C(49)	112.1(3)
C(24)-C(19)-B(1)	120.7(3)	C(55)-B(2)-C(37)	115.1(3)
C(20)-C(19)-B(1)	124.0(3)	C(43)-B(2)-C(37)	104.1(3)
C(21)-C(20)-C(19)	122.7(3)	C(49)-B(2)-C(37)	109.8(3)
С(21)-С(20)-Н(20)	118.6	C(61)-P(2)-C(67)	99.36(15)
C(19)-C(20)-H(20)	118.6	C(61)-P(2)-C(57)	102.65(16)
C(22)-C(21)-C(20)	119.7(3)	C(67)-P(2)-C(57)	102.81(15)
C(22)-C(21)-H(21)	120.1	C(38)-C(37)-C(42)	114.9(3)

C(38)-C(37)-B(2)	122.6(3)	C(55)-C(56)-C(57)	123.1(3)
C(42)-C(37)-B(2)	121.9(3)	C(55)-C(56)-H(56)	118.5
C(37)-C(38)-C(39)	122.6(3)	C(57)-C(56)-H(56)	118.5
C(37)-C(38)-H(38)	118.7	C(58)-C(57)-C(56)	119.2(3)
C(39)-C(38)-H(38)	118.7	C(58)-C(57)-P(2)	123.1(3)
C(40)-C(39)-C(38)	119.4(3)	C(56)-C(57)-P(2)	117.7(3)
C(40)-C(39)-H(39)	120.3	C(59)-C(58)-C(57)	119.5(3)
С(38)-С(39)-Н(39)	120.3	C(59)-C(58)-H(58)	120.3
C(41)-C(40)-C(39)	120.3(3)	C(57)-C(58)-H(58)	120.3
C(41)-C(40)-H(40)	119.9	C(60)-C(59)-C(58)	120.1(3)
C(39)-C(40)-H(40)	119.9	C(60)-C(59)-H(59)	119.9
C(40)-C(41)-C(42)	119.5(3)	C(58)-C(59)-H(59)	119.9
C(40)-C(41)-H(41)	120.3	C(59)-C(60)-C(55)	123.3(3)
C(42)-C(41)-H(41)	120.3	C(59)-C(60)-H(60)	118.4
C(41)-C(42)-C(37)	123.3(3)	C(55)-C(60)-H(60)	118.4
C(41)-C(42)-H(42)	118.4	C(66)-C(61)-C(62)	117.7(3)
C(37)-C(42)-H(42)	118.4	C(66)-C(61)-P(2)	124.1(3)
C(48)-C(43)-C(44)	114.8(3)	C(62)-C(61)-P(2)	118.2(3)
C(48)-C(43)-B(2)	121.7(3)	C(63)-C(62)-C(61)	121.0(4)
C(44)-C(43)-B(2)	123.4(3)	C(63)-C(62)-H(62)	119.5
C(43)-C(44)-C(45)	122.3(3)	C(61)-C(62)-H(62)	119.5
C(43)-C(44)-H(44)	118.9	C(62)-C(63)-C(64)	120.6(4)
C(45)-C(44)-H(44)	118.9	C(62)-C(63)-H(63)	119.7
C(46)-C(45)-C(44)	120.2(3)	C(64)-C(63)-H(63)	119.7
C(46)-C(45)-H(45)	119.9	C(65)-C(64)-C(63)	119.3(4)
C(44)-C(45)-H(45)	119.9	C(65)-C(64)-H(64)	120.3
C(47)-C(46)-C(45)	119.1(3)	C(63)-C(64)-H(64)	120.3
C(47)-C(46)-H(46)	120.4	C(64)-C(65)-C(66)	120.5(4)
C(45)-C(46)-H(46)	120.4	C(64)-C(65)-H(65)	119.7
C(46)-C(47)-C(48)	119.8(3)	C(66)-C(65)-H(65)	119.7
C(46)-C(47)-H(47)	120.1	C(65)-C(66)-C(61)	120.9(3)
C(48)-C(47)-H(47)	120.1	C(65)-C(66)-H(66)	119.6
C(47)-C(48)-C(43)	123.7(3)	C(61)-C(66)-H(66)	119.6
C(47)-C(48)-H(48)	118.1	C(68)-C(67)-C(72)	117.4(3)
C(43)-C(48)-H(48)	118.1	C(68)-C(67)-P(2)	118.3(3)
C(50)-C(49)-C(54)	114.7(3)	C(72)-C(67)-P(2)	124.3(3)
C(50)-C(49)-B(2)	124.0(3)	C(69)-C(68)-C(67)	120.9(4)
C(54)-C(49)-B(2)	121.1(3)	C(69)-C(68)-H(68)	119.5
C(51)-C(50)-C(49)	122.4(3)	C(67)-C(68)-H(68)	119.5
C(51)-C(50)-H(50)	118.8	C(68)-C(69)-C(70)	120.2(4)
C(49)-C(50)-H(50)	118.8	C(68)-C(69)-H(69)	119.9
C(52)-C(51)-C(50)	120.8(3)	C(70)-C(69)-H(69)	119.9
C(52)-C(51)-H(51)	119.6	C(71)-C(70)-C(69)	119.2(4)
C(50)-C(51)-H(51)	119.6	C(71)-C(70)-H(70)	120.4
C(53)-C(52)-C(51)	118.3(3)	C(69)-C(70)-H(70)	120.4
C(53)-C(52)-H(52)	120.9	C(72)-C(71)-C(70)	120.4(4)
C(51)-C(52)-H(52)	120.9	C(72)-C(71)-H(71)	119.8
C(52)-C(53)-C(54)	120.5(3)	C(70)-C(71)-H(71)	119.8
C(52)-C(53)-H(53)	119.8	C(71)-C(72)-C(67)	121.9(4)
C(54)-C(53)-H(53)	119.8	C(71)-C(72)-H(72)	119.1
C(53)-C(54)-C(49)	123.2(3)	C(67)-C(72)-H(72)	119.1
C(53)-C(54)-H(54)	118.4	C(79)-N(1)-C(73)	107.9(2)
C(49)-C(54)-H(54)	118.4	C(79)-N(1)-C(77)	111.9(2)
C(56)-C(55)-C(60)	114.9(3)	C(73)-N(1)-C(77)	108.6(2)
C(56)-C(55)-B(2)	125.4(3)	C(79)-N(1)-C(75)	108.2(2)
C(60)-C(55)-B(2)	119.4(3)	C(73)-N(1)-C(75)	112.2(2)

C(77)-N(1)-C(75)	108.2(2)	C(85)-N(2)-C(81)	107.1(5)
N(1)-C(73)-C(74)	115.7(3)	C(83)-N(2)-C(81)	106.0(4)
N(1)-C(73)-H(73A)	108.4	C(87)-N(2)-C(81)	108.9(5)
C(74)-C(73)-H(73A)	108.4	C(82)-C(81)-N(2)	129.9(5)
N(1)-C(73)-H(73B)	108.4	C(82)-C(81)-H(81A)	104.8
C(74)-C(73)-H(73B)	108.4	N(2)-C(81)-H(81A)	104.8
H(73A)-C(73)-H(73B)	107.4	C(82)-C(81)-H(81B)	104.8
C(73)-C(74)-H(74A)	109.5	N(2)-C(81)-H(81B)	104.8
C(73)-C(74)-H(74B)	109.5	H(2) = C(01) H(012) H(81A) - C(81) - H(81B)	105.8
H(74A)-C(74)-H(74B)	109.5	C(81)-C(82)-H(82A)	109.5
C(73)-C(74)-H(74C)	109.5	C(81)-C(82)-H(82B)	109.5
H(74A)-C(74)-H(74C)	109.5	$H(82\Delta) - C(82) - H(82B)$	109.5
H(74R) - C(74) - H(74C)	109.5	C(81)-C(82)-H(82C)	109.5
C(76)-C(75)-N(1)	115 7(3)	H(82A) - C(82) - H(82C)	109.5
C(76) C(75) H(75A)	108.7(5)	H(82R) - C(82) - H(82C)	109.5
N(1) C(75) H(75A)	108.4	N(2) C(87) C(88)	109.3 114.4(5)
C(76) C(75) H(75P)	108.4	N(2) - C(87) - C(88) N(2) - C(87) - H(87A)	109.6
N(1) C(75) H(75D)	100.4	$N(2)-C(07)-\Pi(07A)$	108.0
N(1)-C(75)-H(75B)	108.4	V(88)-V(87)-H(87A)	108.0
H(75A)-C(75)-H(75B)	107.4	N(2)-C(87)-H(87B)	108.0
C(75)-C(76)-H(76A)	109.5	C(88)-C(87)-H(87B)	108.6
U(75)-U(76)-H(76B)	109.5	H(8/A)-C(8/)-H(8/B)	107.6
H(76A)-C(76)-H(76B)	109.5	C(87)-C(88)-H(88A)	109.5
C(75)-C(76)-H(76C)	109.5	C(87)-C(88)-H(88B)	109.5
H(/6A)-C(/6)-H(/6C)	109.5	H(88A)-C(88)-H(88B)	109.5
H(/6B)-C(/6)-H(/6C)	109.5	C(87)-C(88)-H(88C)	109.5
N(1)-C(7)-C(78)	115.6(3)	H(88A)-C(88)-H(88C)	109.5
N(1)-C(77)-H(77A)	108.4	H(88B)-C(88)-H(88C)	109.5
C(78)-C(77)-H(77A)	108.4	C(83)-C(84)-H(84A)	109.5
N(1)-C(77)-H(77B)	108.4	C(83)-C(84)-H(84B)	109.5
С(78)-С(77)-Н(77В)	108.4	H(84A)-C(84)-H(84B)	109.5
H(//A)-C(//)-H(//B)	107.5	C(83)-C(84)-H(84C)	109.5
C(77)-C(78)-H(78A)	109.5	H(84A)-C(84)-H(84C)	109.5
C(77)-C(78)-H(78B)	109.5	H(84B)-C(84)-H(84C)	109.5
H(78A)-C(78)-H(78B)	109.5	C(85)-C(86)-H(86A)	109.5
C(77)-C(78)-H(78C)	109.5	C(85)-C(86)-H(86B)	109.5
H(78A)-C(78)-H(78C)	109.5	H(86A)-C(86)-H(86B)	109.5
H(78B)-C(78)-H(78C)	109.5	C(85)-C(86)-H(86C)	109.5
C(80)-C(79)-N(1)	115.7(3)	H(86A)-C(86)-H(86C)	109.5
C(80)-C(79)-H(79A)	108.4	H(86B)-C(86)-H(86C)	109.5
N(1)-C(79)-H(79A)	108.4	C(84)-C(83)-N(2)	150.6(6)
C(80)-C(79)-H(79B)	108.4	C(84)-C(83)-H(83A)	99.0
N(1)-C(79)-H(79B)	108.4	N(2)-C(83)-H(83A)	99.0
H(79A)-C(79)-H(79B)	107.4	C(84)-C(83)-H(83B)	99.0
C(79)-C(80)-H(80A)	109.5	N(2)-C(83)-H(83B)	99.0
C(79)-C(80)-H(80B)	109.5	H(83A)-C(83)-H(83B)	103.9
H(80A)-C(80)-H(80B)	109.5	C(86)-C(85)-N(2)	156.9(12)
C(79)-C(80)-H(80C)	109.5	C(86)-C(85)-H(85A)	97.1
H(80A)-C(80)-H(80C)	109.5	N(2)-C(85)-H(85A)	97.1
H(80B)-C(80)-H(80C)	109.5	C(86)-C(85)-H(85B)	97.1
C(85)-N(2)-C(83)	111.0(7)	N(2)-C(85)-H(85B)	97.1
C(85)-N(2)-C(87)	107.7(5)	H(85A)-C(85)-H(85B)	103.5
C(83)-N(2)-C(87)	115.8(6)		

Table 4. Anisotropic displacement parameters $(Å^2x \ 10^3)$ for $\{[NEt_4][Ph_3BP^{m-Ph_2}]\}_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 \ a^{*2}U^{11} + ... + 2h \ a^{*}b^{*}U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
B(1)	18(2)	18(2)	17(2)	-2(2)	2(2)	-2(2)
P(1)	37(1)	24(1)	29(1)	-2(1)	-7(1)	3(1)
$\dot{C(1)}$	11(2)	20(2)	37(2)	4(2)	2(2)	-2(2)
C(2)	32(2)	29(2)	62(3)	10(2)	-17(2)	-10(2)
C(3)	31(2)	32(3)	83(4)	20(2)	-15(2)	-1(2)
C(4)	18(2)	29(3)	98(4)	-3(3)	2(2)	2(2)
C(5)	39(3)	35(3)	72(3)	-19(2)	25(2)	-10(2)
C(6)	40(2)	22(2)	46(3)	-6(2)	20(2)	-9(2)
C(7)	24(2)	17(2)	19(2)	-6(2)	-2(2)	-5(2)
C(8)	33(2)	20(2)	29(2)	-2(2)	$\frac{2(2)}{4(2)}$	-8(2)
C(9)	46(2)	35(2)	25(2)	-11(2)	14(2)	-18(2)
C(10)	62(3)	41(3)	25(2) 26(2)	6(2)	7(2)	-25(2)
C(10)	61(3)	31(2)	35(2)	12(2)	2(2)	-4(2)
C(12)	54(3)	26(2)	29(2)	2(2)	9(2)	3(2)
C(12) C(13)	23(2)	$\frac{20(2)}{8(2)}$	29(2) 28(2)	-2(2)	-3(2)	$\frac{3(2)}{2(1)}$
C(13)	$\frac{23(2)}{38(2)}$	10(2)	$\frac{20(2)}{41(2)}$	-2(2)	-3(2)	$\frac{2(1)}{1(2)}$
C(14)	25(2)	$\frac{19(2)}{23(2)}$	41(2)	-10(2)	-17(2)	1(2) 1(2)
C(15)	23(2)	$\frac{23(2)}{10(2)}$	87(4)	-11(2)	-17(2)	$\frac{1(2)}{4(2)}$
C(10) C(17)	22(2) 37(3)	19(2)	67(4)	4(2) 10(3)	$\frac{3(2)}{10(2)}$	-4(2)
C(17)	$\frac{37(3)}{24(2)}$	51(3)	36(3)	19(3) 11(2)	$\frac{19(2)}{7(2)}$	$\frac{2(2)}{4(2)}$
C(10)	24(2)	$\frac{31(3)}{17(2)}$	30(2)	$\frac{11(2)}{6(2)}$	7(2)	-4(2)
C(19)	20(2)	$\frac{1}{(2)}$	20(2)	0(2)	5(2)	-3(2)
C(20)	30(2)	10(2)	22(2)	1(2)	-1(2)	-2(2)
C(21)	23(2)	$\frac{2}{2}$	29(2)	7(2)	-3(2)	1(2)
C(22)	28(2)	52(2)	22(2)	2(2)	-7(2)	-4(2)
C(23)	29(2)	10(2)	22(2)	-1(2)	-3(2)	0(2)
C(24)	24(2)	$\frac{2}{2}$	19(2)	2(2)	-3(2)	4(2)
C(25)	50(2)	20(2)	31(2)	-4(2)	-4(2)	1(2)
C(26)	44(2)	29(2)	$\frac{2}{2}$	-4(2)	-3(2)	0(2)
C(27)	48(3)	29(2)	38(2)	0(2)	3(2)	-9(2)
C(28)	35(2)	28(2)	44(3)	-5(2)	I(2)	-4(2)
C(29)	36(2)	27(2)	40(2)	1(2)	-6(2)	-2(2)
C(30)	33(2)	23(2)	35(2)	-1(2)	-6(2)	-4(2)
C(31)	29(2)	26(2)	35(2)	-12(2)	-14(2)	/(2)
C(32)	29(2)	35(2)	38(2)	-3(2)	-2(2)	-1(2)
C(33)	35(2)	35(2)	50(3)	6(2)	-6(2)	-5(2)
C(34)	27(2)	67(3)	33(2)	2(2)	0(2)	-6(2)
C(35)	35(3)	49(3)	48(3)	-22(2)	-1(2)	2(2)
C(36)	31(2)	39(3)	38(2)	-7(2)	2(2)	-1(2)
B(2)	23(2)	18(2)	11(2)	0(2)	4(2)	-2(2)
P(2)	33(1)	23(1)	32(1)	4(1)	-9(1)	-5(1)
C(37)	23(2)	10(2)	22(2)	3(2)	2(2)	0(1)
C(38)	26(2)	18(2)	28(2)	-2(2)	2(2)	-1(2)
C(39)	24(2)	20(2)	38(2)	1(2)	12(2)	3(2)
C(40)	18(2)	18(2)	49(3)	6(2)	-3(2)	-4(2)
C(41)	36(2)	15(2)	35(2)	6(2)	-9(2)	2(2)
C(42)	23(2)	21(2)	24(2)	4(2)	2(2)	3(2)

C(43)	13(2)	22(2)	18(2)	-2(2)	5(1)	-3(2)
C(44)	22(2)	21(2)	24(2)	2(2)	1(2)	-1(2)
C(45)	20(2)	25(2)	36(2)	-11(2)	4(2)	-3(2)
C(46)	24(2)	20(2)	44(2)	6(2)	9(2)	-1(2)
C(47)	26(2)	34(2)	34(2)	15(2)	14(2)	7(2)
C(48)	33(2)	24(2)	24(2)	2(2)	6(2)	2(2)
C(49)	23(2)	20(2)	14(2)	4(2)	-3(2)	2(2)
C(50)	35(2)	17(2)	38(2)	0(2)	13(2)	3(2)
C(51)	43(3)	33(2)	43(3)	9(2)	26(2)	4(2)
C(52)	47(3)	38(2)	18(2)	-3(2)	7(2)	13(2)
C(53)	31(2)	27(2)	36(2)	-11(2)	-4(2)	5(2)
C(54)	29(2)	24(2)	26(2)	-2(2)	3(2)	3(2)
C(55)	22(2)	17(2)	16(2)	-5(2)	8(2)	0(2)
C(56)	32(2)	20(2)	24(2)	-1(2)	-2(2)	-3(2)
C(57)	33(2)	19(2)	19(2)	3(2)	1(2)	-4(2)
C(58)	33(2)	21(2)	28(2)	5(2)	-6(2)	1(2)
C(59)	26(2)	27(2)	27(2)	1(2)	0(2)	-6(2)
C(60)	23(2)	19(2)	24(2)	3(2)	2(2)	-2(2)
C(61)	26(2)	30(2)	27(2)	7(2)	-3(2)	0(2)
C(62)	33(2)	24(2)	43(2)	7(2)	-4(2)	1(2)
C(63)	36(2)	43(3)	41(3)	20(2)	2(2)	1(2)
C(64)	33(2)	44(3)	35(2)	5(2)	1(2)	-3(2)
C(65)	35(2)	33(2)	31(2)	0(2)	-3(2)	-5(2)
C(66)	29(2)	27(2)	32(2)	5(2)	-6(2)	-7(2)
C(67)	34(2)	19(2)	32(2)	6(2)	-4(2)	-2(2)
C(68)	45(2)	24(2)	37(2)	3(2)	-2(2)	4(2)
C(69)	45(3)	33(3)	62(3)	-1(2)	9(2)	12(2)
C(70)	37(3)	36(3)	69(3)	16(2)	-14(2)	5(2)
C(71)	40(3)	26(2)	53(3)	9(2)	-16(2)	-3(2)
C(72)	39(2)	22(2)	39(2)	2(2)	-11(2)	-1(2)
N(1)	18(2)	18(2)	26(2)	2(1)	0(1)	1(1)
C(73)	30(2)	24(2)	30(2)	4(2)	-1(2)	-1(2)
C(74)	32(2)	43(2)	29(2)	8(2)	6(2)	-4(2)
C(75)	27(2)	24(2)	33(2)	10(2)	8(2)	3(2)
C(76)	36(2)	21(2)	51(3)	3(2)	9(2)	5(2)
C(77)	18(2)	17(2)	37(2)	1(2)	4(2)	-2(2)
C(78)	26(2)	23(2)	53(3)	2(2)	3(2)	3(2)
C(79)	23(2)	23(2)	28(2)	-2(2)	3(2)	-1(2)
C(80)	39(2)	39(2)	31(2)	2(2)	4(2)	-8(2)
N(2)	23(2)	26(2)	74(3)	5(2)	-2(2)	0(1)
C(81)	83(4)	137(6)	130(6)	-35(5)	-62(4)	21(4)
C(82)	163(6)	193(7)	82(4)	-7(5)	-14(4)	152(6)
C(87)	102(5)	101(6)	325(12)	-135(7)	-21(6)	51(4)
C(88)	203(7)	95(5)	81(4)	-20(4)	-84(5)	71(5)
C(84)	37(3)	83(4)	188(6)	70(4)	-4(4)	-11(3)
C(86)	41(3)	45(4)	432(13)	37(6)	26(5)	-25(3)
C(83)	51(4)	860(30)	85(5)	14/(9)	-13(4)	-172(9)
C(85)	830(30)	15(4)	134(7)	14(4)	217(11)	45(8)

	X	у	Z	U(eq)
H(2)	1371	6524	1378	49
H(3)	1372	4276	1277	58
H(4)	1155	3527	713	58
H(5)	865	4880	257	58
H(6)	896	7067	358	43
H(8)	2178	8091	439	33
H(9)	2682	9230	-22	42
H(10)	2245	11260	-154	51
H(11)	1258	12094	160	51
H(12)	754	10942	621	44
H(14)	-166	9106	520	40
H(15)	-1430	9188	649	46
H(16)	-1818	9015	1222	52
H(17)	-958	8723	1671	63
H(18)	290	8655	1543	44
H(20)	2474	7812	1217	28
H(21)	3278	8688	1631	$\frac{1}{32}$
H(22)	2957	10541	1924	32
H(24)	1051	10679	1368	28
H(26)	2563	14294	1717	40
H(27)	3640	15189	1951	46
H(28)	4131	14431	2478	43
H(29)	3562	12760	2769	41
H(30)	2510	11814	2531	36
H(32)	1411	9715	2224	40
H(33)	748	8974	2699	48
H(34)	81	10389	3051	51
H(35)	54	12552	2899	52
H(36)	698	13282	2416	43
H(38)	4929	6193	1417	29
H(39)	3645	6065	1326	33
H(40)	3174	5734	762	34
H(41)	3976	5496	290	35
H(42)	5246	5613	382	27
H(44)	6168	8282	1445	27
H(45)	6242	10487	1384	32
H(46)	6289	11407	826	35
H(47)	6247	10100	332	37
H(48)	6165	7920	395	33
H(50)	7346	6942	528	36
H(51)	7978	5880	91	47
H(52)	7666	3791	-60	41
H(53)	6755	2751	262	38
H(54)	6107	3822	688	31
H(56)	5815	4324	1457	30
H(58)	7564	4543	2127	33
H(59)	8011	6277	1808	22
	0011	0277	1000	32

Table 5. Hydrogen coordinates (x 10⁴) and isotropic displacement parameters (Å²x 10³) for $\{[NEt_4][Ph_3BP^{m-Ph_2}]\}_2$.

H(62)	5538	1871	2651	40
H(63)	4970	2669	3146	48
H(64)	4908	4858	3242	45
H(65)	5442	6243	2840	40
H(66)	5993	5462	2336	35
H(68)	7159	728	1894	43
H(69)	8217	-228	2127	56
H(70)	8766	580	2641	57
H(71)	8241	2333	2916	48
H(72)	7213	3311	2677	40
H(73A)	3775	2770	386	33
H(73B)	3711	1316	266	33
H(74A)	5072	2605	400	52
H(74B)	4762	2219	19	52
H(74C)	5016	1135	290	52
H(75A)	4847	317	834	34
H(75B)	4211	-21	1108	34
H(76A)	3511	-959	649	54
H(76B)	4299	-1641	695	54
H(76C)	4165	-650	382	54
H(77A)	3089	1018	1119	29
H(77B)	2886	831	714	29
H(78A)	2931	3245	1057	51
H(78B)	2188	2501	951	51
H(78C)	2719	3048	652	51
H(79A)	4872	2477	958	29
H(79B)	4150	3353	948	29
H(80A)	3736	2386	1467	54
H(80B)	4530	3033	1526	54
H(80C)	4466	1522	1477	54
H(81A)	9537	3950	1436	140
H(81B)	8754	3477	1564	140
H(82A)	9132	1868	1737	219
H(82B)	9891	2657	1746	219
H(82C)	9720	1702	1428	219
H(87A)	9402	1654	914	211
H(87B)	9900	2897	860	211
H(88A)	8967	1734	373	190
H(88B)	9634	2700	299	190
H(88C)	8830	3239	391	190
H(84A)	7814	1947	1423	154
H(84B)	7320	1971	1071	154
H(84C)	7377	3215	1313	154
H(86A)	9198	5950	1155	259
H(86B)	8827	6093	773	259
H(86C)	9653	5554	812	259
H(83A)	7931	3498	919	400
H(83B)	8215	2097	897	400
H(85A)	8881	4357	685	391
H(85B)	8414	4756	1008	391
- *				

Empirical formula	C ₃₈ H ₅₃ BNP
Formula weight	565.59
Crystal Habit	acicular
Crystal Color	colorless
Crystal size	0.474 x 0.18 x 0.081 mm ³

Table 6. Crystal data and structure refinement for $\{[NEt_4][Ph_3BP^{m-iPr2}]\}_2$.

Data Collection

Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Data collection temperature	98(2) K	
Unit cell dimensions	a = 9.8900(8) Å b = 20.1253(16) Å c = 16.7970(14) Å	$\alpha = 90^{\circ}$ $\beta = 92.835(2)^{\circ}$ $\gamma = 90^{\circ}$
Volume	3339.2(5) Å ³	
Z	4	
Crystal system	Monoclinic	
Space group	P2(1)	
Density (calculated)	1.125 Mg/m ³	
F(000)	1232	
θ range for data collection	1.58 to 28.60°	
Completeness to $\theta = 28.60^{\circ}$	94.5 %	
Index ranges	$-13 \le h \le 13, -27 \le k \le 26, -21$	$\leq l \leq 22$
Reflections collected	50901	
Independent reflections	15665 [R(int) = 0.0696]	
Absorption coefficient	0.109 mm ⁻¹	
Absorption correction	None	
Structure solut	ion and refinement	
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	direct methods	
Secondary solution method	Difference Fourier Map	
Hydrogen placement	calculated positions	

Structure refinement program

SHELXL-97 (Sheldrick, 1997)

Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	15665 / 1 / 755
Goodness-of-fit on F ²	1.614
Final R indices [I>2sigma(I)]	R1 = 0.0659, wR2 = 0.0917
R indices (all data)	R1 = 0.1066, wR2 = 0.0973
Absolute structure parameter	0.48(8)
Largest diff. peak and hole	0.725 and -0.468 e.Å ⁻³

Table 7. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters $(Å^2x \ 10^3)$ for $\{[NEt_4][Ph_3BP^{m-iPr^2}]\}_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	X	У	Z	U(eq)
B(1)	174(3)	7420(2)	2274(2)	23(1)
P(1)	524(1)	10077(1)	2851(1)	29(1)
C(1)	278(3)	7186(2)	3221(2)	21(1)
C(2)	453(3)	7627(2)	3852(2)	24(1)
C(3)	635(3)	7437(2)	4646(2)	$\frac{28(1)}{28(1)}$
C(4)	640(3)	6774(2)	4844(2)	36(1)
C(5)	457(3)	6315(2)	4247(2)	37(1)
C(6)	289(3)	6520(2)	3457(2)	31(1)
C(0)	1708(3)	7415(2)	1963(2)	24(1)
C(8)	2529(3)	6854(2)	2079(2)	$\frac{2}{32(1)}$
C(0)	2329(3) 3843(3)	6827(2)	1853(2)	32(1) 37(1)
C(3)	4420(3)	7360(2)	1033(2) 1482(2)	$\frac{37(1)}{37(1)}$
C(10)	4420(3)	7020(2)	1402(2) 1350(2)	$\frac{37(1)}{37(1)}$
C(11)	3039(3) 2217(2)	7929(2) 7040(2)	1550(2)	$\frac{3}{(1)}$
C(12)	2517(5)	7940(2) 6999(2)	1302(2) 1720(2)	$\frac{51(1)}{10(1)}$
C(15)	-739(3)	0000(2) 6702(2)	1/39(2)	19(1) 20(1)
C(14)	-505(3)	6/93(2)	930(2)	29(1)
C(15)	-1442(3)	6393(2)	441(2)	33(1)
C(16)	-2503(3)	6080(2)	768(2)	33(1)
C(17)	-2/41(3)	6153(2)	1563(2)	2/(1)
C(18)	-1882(3)	6565(2)	2029(2)	26(1)
C(19)	-537(3)	8163(1)	2194(2)	18(1)
C(20)	95(3)	8748(2)	2460(2)	21(1)
C(21)	-493(3)	9383(2)	2445(2)	20(1)
C(22)	-1797(3)	9427(2)	2102(2)	28(1)
C(23)	-2458(3)	8872(2)	1819(2)	35(1)
C(24)	-1838(3)	8249(2)	1870(2)	31(1)
C(25)	-55(3)	10134(2)	3885(2)	31(1)
C(26)	487(3)	9537(2)	4361(2)	38(1)
C(27)	-1556(3)	10212(2)	3972(2)	33(1)
C(28)	-283(3)	10825(2)	2385(2)	29(1)
C(29)	292(3)	11447(2)	2777(2)	37(1)
C(30)	17(3)	10835(2)	1497(2)	38(1)
B(2)	4396(3)	3909(2)	2780(2)	22(1)
P(2)	4289(1)	1304(1)	1983(1)	26(1)
C(31)	4283(3)	4174(2)	1837(2)	21(1)
C(32)	4483(3)	3779(2)	1176(2)	31(1)
C(33)	4305(3)	4000(2)	400(2)	38(1)
C(34)	3966(3)	4652(2)	245(2)	40(1)
C(35)	3792(3)	5068(2)	888(2)	37(1)
C(36)	3953(3)	4833(2)	1652(2)	32(1)
C(37)	5303(3)	4442(2)	3305(2)	21(1)
C(38)	6405(3)	4780(2)	2993(2)	25(1)
C(39)	7786(3)	5173(2)	3444(2)	$\frac{23(1)}{32(1)}$
C(40)	7200(3) 711A(3)	57/9(2)	4242(2)	32(1)
C(41)	6051(2)	32 + 9(2)	7272(2)	30(1)
C(41)	5172(2)	4732(2)	4374(2) 1115(2)	$\frac{37(1)}{28(1)}$
C(42)	31/2(3)	+3+0(2)	$\frac{113(2)}{2001(2)}$	20(1) 21(1)
U(43)	2838(3)	300/(2)	3091(2)	21(1)

C(44)	2121(3)	4477(2)	3211(2)	34(1)
C(45)	790(3)	4480(2)	3424(2)	39(1)
C(46)	101(3)	3897(2)	3539(2)	32(1)
C(47)	762(3)	3310(2)	3445(2)	24(1)
C(48)	2106(3)	3305(2)	3228(2)	22(1)
C(49)	5133(3)	3180(2)	2853(2)	19(1)
C(50)	4614(3)	2608(1)	2479(2)	18(1)
C(51)	5197(3)	1983(2)	2523(2)	22(1)
C(52)	6401(3)	1912(2)	2974(2)	21(1)
C(53)	6955(3)	2458(2)	3372(2)	24(1)
C(54)	6331(3)	3066(2)	3314(2)	20(1)
C(55)	5129(3)	1298(2)	1013(2)	28(1)
C(56)	4776(3)	1941(2)	549(2)	38(1)
C(57)	6644(3)	1190(2)	1046(2)	34(1)
C(58)	4984(3)	545(2)	2461(2)	28(1)
C(59)	4453(3)	-70(2)	1993(2)	39(1)
C(60)	4603(3)	492(2)	3332(2)	34(1)
N(1)	4428(2)	2497(1)	5642(2)	29(1)
C(61)	9200(4)	4527(2)	1290(2)	50(1)
C(62)	10218(3)	5068(2)	1328(2)	60(1)
C(63)	9668(4)	4109(2)	-68(2)	49(1)
C(64)	8533(4)	4497(2)	-434(2)	54(1)
C(65)	10804(4)	3619(2)	1137(2)	54(1)
C(66)	11180(3)	2946(2)	783(2)	50(1)
C(67)	8351(4)	3441(2)	838(2)	48(1)
C(68)	8177(4)	3133(2)	1623(2)	66(1)
N(2)	9502(2)	3903(1)	809(2)	25(1)
C(69)	5598(3)	2986(2)	5667(2)	38(1)
C(70)	6036(4)	3231(2)	6479(2)	57(1)
C(71)	3234(3)	2796(2)	6028(2)	43(1)
C(72)	2731(3)	3470(2)	5711(2)	58(1)
C(73)	4759(3)	1868(2)	6085(2)	40(1)
C(74)	5921(3)	1480(2)	5795(2)	67(1)
C(75)	4095(3)	2369(2)	4761(2)	38(1)
C(76)	3003(3)	1888(2)	4554(2)	42(1)

B(1)-C(7)	1.628(4)	C(25)-H(25)	1.0000
B(1)-C(13)	1.650(5)	C(26)-H(26A)	0.9800
B(1)-C(19)	1.654(4)	C(26)-H(26B)	0.9800
B(1)-C(1)	1.657(4)	C(26)-H(26C)	0.9800
P(1)-C(21)	1.833(3)	C(27)-H(27A)	0.9800
P(1)-C(25)	1.859(3)	C(27)-H(27B)	0.9800
P(1)-C(28)	1.859(3)	C(27)-H(27C)	0.9800
C(1)-C(2)	1.387(4)	C(28)-C(29)	1.512(4)
C(1)-C(6)	1.397(4)	C(28)-C(30)	1.534(4)
C(2)-C(3)	1.390(4)	C(28)-H(28)	1.0000
C(2)-H(2)	0.9500	C(29)-H(29A)	0.9800
C(3)-C(4)	1.376(4)	C(29)-H(29B)	0.9800
C(3)-H(3)	0.9500	C(29)-H(29C)	0.9800
C(4)-C(5)	1.368(4)	C(30)-H(30A)	0.9800
C(4)-H(4)	0.9500	C(30)-H(30B)	0.9800
C(5)-C(6)	1.392(4)	C(30)-H(30C)	0.9800
C(5)-H(5)	0.9500	B(2)-C(37)	1.629(4)
C(6)-H(6)	0.9500	B(2)-C(49)	1.640(5)
C(7)-C(12)	1.388(4)	B(2)-C(43)	1.653(4)
C(7)-C(8)	1.400(4)	B(2)-C(31)	1.669(5)
C(8)-C(9)	1.373(4)	P(2)-C(58)	1.842(3)
C(8)-H(8)	0.9500	P(2)-C(51)	1.849(3)
C(9)-C(10)	1.392(5)	P(2)-C(55)	1.865(3)
С(9)-Н(9)	0.9500	C(31)-C(32)	1.388(4)
C(10)-C(11)	1.379(4)	C(31)-C(36)	1.397(4)
C(10)-H(10)	0.9500	C(32)-C(33)	1.380(4)
C(11)-C(12)	1.383(4)	C(32)-H(32)	0.9500
C(11)-H(11)	0.9500	C(33)-C(34)	1.376(5)
C(12)-H(12)	0.9500	C(33)-H(33)	0.9500
C(13)-C(14)	1.385(4)	C(34)-C(35)	1.384(4)
C(13)-C(18)	1.395(4)	C(34)-H(34)	0.9500
C(14)-C(15)	1.421(4)	C(35)-C(36)	1.370(4)
C(14)-H(14)	0.9500	C(35)-H(35)	0.9500
C(15)-C(16)	1.363(4)	C(36)-H(36)	0.9500
C(15)-H(15)	0.9500	C(37)-C(42)	1.388(4)
C(16)-C(17)	1.374(4)	C(37)-C(38)	1.408(4)
C(16)-H(16)	0.9500	C(38)-C(39)	1.375(4)
C(17)-C(18)	1.400(4)	C(38)-H(38)	0.9500
C(17)-H(17)	0.9500	C(39)-C(40)	1.367(4)
C(18)-H(18)	0.9500	C(39)-H(39)	0.9500
C(19)-C(24)	1.384(4)	C(40)-C(41)	1.372(4)
C(19)-C(20)	1.396(4)	C(40)-H(40)	0.9500
C(20)-C(21)	1.403(4)	C(41)-C(42)	1.380(4)
C(20)-H(20)	0.9500	C(41)-H(41)	0.9500
C(21)-C(22)	1.389(4)	C(42)-H(42)	0.9500
C(22)-C(23)	1.368(4)	C(43)-C(48)	1.401(4)
C(22)-H(22)	0.9500	C(43)-C(44)	1.403(4)
C(23)-C(24)	1.396(4)	C(44)-C(45)	1.380(4)
C(23)-H(23)	0.9500	C(44)-H(44)	0.9500
C(24)-H(24)	0.9500	C(45)-C(46)	1.375(4)
C(25)-C(27)	1.507(4)	C(45)-H(45)	0.9500
C(25)-C(26)	1.525(4)	C(46)-C(47)	1.364(4)

Table 8. Bond lengths [Å] and angles [°] for $\{[NEt_4][Ph_3BP^{m-iPr2}]\}_2$.

C(46)-H(46)	0.9500	C(66)-H(66C)	0.9800
C(47)-C(48)	1.396(4)	C(67)-N(2)	1.473(4)
C(47)-H(47)	0.9500	C(67)-C(68)	1.474(5)
C(48)-H(48)	0.9500	C(67)-H(67A)	0.9900
C(49)-C(50)	1.397(4)	C(67)-H(67B)	0.9900
C(49)-C(54)	1.401(4)	C(68)-H(68A)	0.9800
C(50)-C(51)	1.383(4)	C(68)-H(68B)	0.9800
C(50)-H(50)	0.9500	C(68)-H(68C)	0.9800
C(51)-C(52)	1.387(4)	C(69)-C(70)	1.493(4)
C(52)-C(53)	1.385(4)	C(69)-H(69A)	0.9900
C(52)-H(52)	0.9500	C(69)-H(69B)	0.9900
C(53)-C(54)	1.372(4)	C(70)-H(70A)	0.9800
C(53)-H(53)	0.9500	C(70)-H(70B)	0.9800
C(54)-H(54)	0.9500	C(70)-H(70C)	0.9800
C(55)-C(57)	1.512(4)	C(71)-C(72)	1.530(4)
C(55)-C(56)	1.542(4)	C(71)-H(71A)	0.9900
C(55)-H(55)	1.0000	C(71)-H(71B)	0.9900
C(56)-H(56A)	0.9800	C(72)-H(72A)	0.9800
C(56)-H(56B)	0.9800	C(72)-H(72B)	0.9800
C(56)-H(56C)	0.9800	C(72)-H(72C)	0 9800
C(57)-H(57A)	0.9800	C(73)-C(74)	1 491(4)
C(57)-H(57B)	0.9800	C(73)-H(73A)	0 9900
C(57)-H(57C)	0.9800	C(73)-H(73B)	0.9900
C(58)- $C(60)$	1 533(4)	C(74)-H(74A)	0.9800
C(58)- $C(59)$	1 546(4)	C(74)-H(74B)	0.9800
C(58)-H(58)	1 0000	C(74)-H(74C)	0.9800
C(59)-H(59A)	0.9800	C(75)-C(76)	1480(4)
C(59)-H(59B)	0.9800	C(75) - H(75A)	0.9900
C(59)-H(59C)	0.9800	C(75)-H(75B)	0.9900
C(60)-H(60A)	0.9800	C(76)-H(76A)	0.9900
C(60)-H(60B)	0.9800	C(76)-H(76B)	0.9800
C(60)-H(60C)	0.9800	C(76)-H(76C)	0.9800
N(1)-C(73)	1 496(4)	C(10) II(10C)	0.9000
N(1) - C(71)	1.490(4)	C(7)-B(1)-C(13)	109.0(3)
N(1) - C(69)	1.501(4) 1 517(4)	C(7)-B(1)-C(19)	109.0(3) 112 3(3)
N(1)-C(75)	1.517(4)	C(13)-B(1)-C(19)	108.5(2)
C(61)-C(62)	1.321(+) 1.483(5)	C(7)-B(1)-C(1)	106.9(2)
C(61)-C(02)	1.532(4)	C(13)-B(1)-C(1)	110.9(2)
C(61) - N(2) C(61) + U(61A)	0.0000	C(13)- $D(1)$ - $C(1)$	100.1(3) 100.0(3)
C(01)-H(01R)	0.9900	C(19)-D(1)-C(1) C(21)-P(1)-C(25)	109.9(3) 101.83(15)
$C(01)$ - $\Pi(01D)$ $C(62) \Pi(62A)$	0.9900	$C(21) - \Gamma(1) - C(23)$ $C(21) - \Gamma(1) - C(28)$	101.03(13) 104.15(14)
$C(02)$ - $\Pi(02R)$ $C(62)$ $\Pi(62R)$	0.9800	$C(21)$ - $\Gamma(1)$ - $C(28)$	104.13(14) 101.42(15)
$C(02)-\Pi(02D)$ $C(62) \Pi(62C)$	0.9800	C(23) - F(1) - C(28)	101.42(13) 112 $4(2)$
$C(02)-\Pi(02C)$ C(62) C(64)	1.476(4)	C(2) - C(1) - C(0) C(2) - C(1) - C(0)	113.4(3) 122.4(2)
C(03)-C(04) C(62) N(2)	1.4/0(4) 1.547(4)	C(2)-C(1)-B(1)	123.4(3) 122.0(2)
C(03)-IN(2) C(62) II(62 A)	1.347(4)	C(0)-C(1)-B(1)	125.0(5) 124.2(2)
$C(03)-\Pi(03A)$	0.9900	C(1) - C(2) - C(3)	124.3(3)
C(03)-H(03B)	0.9900	C(1)-C(2)-H(2)	117.9
C(04)-H(04A)	0.9800	C(3)-C(2)-H(2)	11/.9
C(04)-H(04B)	0.9800	C(4) - C(3) - C(2)	119.8(3)
C(04)-H(04C)	0.9800	C(4)-C(5)-H(5)	120.1
C(03)-N(2)	1.489(4)	C(2)-C(3)-H(3)	120.1
C(05) - C(00)	1.354(4)	C(5) - C(4) - C(3)	118.7(3)
C(05)-H(05A)	0.9900	C(5)-C(4)-H(4)	120.7
C(65)-H(65B)	0.9900	C(3)-C(4)-H(4)	120.7
C(00)-H(00A)	0.9800	C(4)-C(5)-C(6)	120.2(3)
C(66)-H(66B)	0.9800	C(4)-C(5)-H(5)	119.9

C(6)-C(5)-H(5)	119.9	C(19)-C(24)-H(24)	118.9
C(5)-C(6)-C(1)	123.7(3)	C(23)-C(24)-H(24)	118.9
C(5)-C(6)-H(6)	118.2	C(27)-C(25)-C(26)	110.7(3)
C(1)-C(6)-H(6)	118.2	C(27)-C(25)-P(1)	116.6(2)
C(12)-C(7)-C(8)	114.6(3)	C(26)-C(25)-P(1)	109.0(2)
C(12)-C(7)-B(1)	125.1(3)	C(27)-C(25)-H(25)	106.7
C(8)-C(7)-B(1)	120.3(3)	C(26)-C(25)-H(25)	106.7
C(9)-C(8)-C(7)	123.0(3)	P(1)-C(25)-H(25)	106.7
C(9)-C(8)-H(8)	118.5	C(25)-C(26)-H(26A)	109.5
C(7)-C(8)-H(8)	118.5	C(25)-C(26)-H(26B)	109.5
C(8)-C(9)-C(10)	120 5(3)	H(26A)-C(26)-H(26B)	109.5
C(8)-C(9)-H(9)	119.8	C(25)-C(26)-H(26C)	109.5
C(10)-C(9)-H(9)	119.8	H(26A)-C(26)-H(26C)	109.5
C(11)-C(10)-C(9)	118 3(3)	H(26B)-C(26)-H(26C)	109.5
C(11)- $C(10)$ - $H(10)$	120.8	C(25)-C(27)-H(27A)	109.5
C(9)-C(10)-H(10)	120.8	C(25)-C(27)-H(27B)	109.5
C(10)-C(11)-C(12)	119 8(3)	H(27A)-C(27)-H(27B)	109.5
C(10)- $C(11)$ - $H(11)$	120.1	C(25)-C(27)-H(27C)	109.5
C(12)-C(11)-H(11)	120.1	H(27A)-C(27)-H(27C)	109.5
C(12) - C(12) - C(7)	123.8(3)	H(27R) - C(27) - H(27C)	109.5
C(11) - C(12) - H(12)	118.1	C(29)-C(28)-C(30)	109.0
C(7)-C(12)-H(12)	118.1	C(29)-C(28)-P(1)	109.0(3) 110.0(2)
C(14)-C(13)-C(18)	115 3(3)	C(20) - C(20) - P(1)	108.7(2)
C(14)-C(13)-B(1)	121 3(3)	C(20)-C(28)-H(28)	100.7(2)
C(14)-C(13)-B(1)	121.3(3) 123 0(3)	C(20)-C(20)-H(20)	109.7
C(13)-C(14)-C(15)	123.0(3) 122 5(3)	P(1)-C(28)-H(28)	109.7
C(13)-C(14)-H(14)	118 7	$C(28)-C(29)-H(29\Delta)$	109.7
C(15)-C(14)-H(14)	118.7	C(28)-C(29)-H(29R)	109.5
C(16)-C(15)-C(14)	110.7	H(29A)-C(29)-H(29B)	109.5
C(16)-C(15)-H(15)	120.5	C(28)-C(29)-H(29C)	109.5
C(14)-C(15)-H(15)	120.5	H(29A)-C(29)-H(29C)	109.5
C(15)-C(16)-C(17)	120.9	H(29R) - C(29) - H(29C)	109.5
C(15)-C(16)-H(16)	119.5	C(28)-C(30)-H(30A)	109.5
C(17)- $C(16)$ -H(16)	119.5	C(28)-C(30)-H(30B)	109.5
C(16)-C(17)-C(18)	118.6(3)	H(30A)-C(30)-H(30B)	109.5
C(16)-C(17)-H(17)	120.7	C(28)-C(30)-H(30C)	109.5
C(18)-C(17)-H(17)	120.7	H(30A)-C(30)-H(30C)	109.5
C(13)-C(18)-C(17)	123.5(3)	H(30R) - C(30) - H(30C)	109.5
C(13)-C(18)-H(18)	118.3	C(37)-B(2)-C(49)	109.5 108.5(2)
C(17)-C(18)-H(18)	118.3	C(37)-B(2)-C(43)	100.3(2) 110.1(3)
C(24)-C(19)-C(20)	114 4(3)	C(49)-B(2)-C(43)	110.1(3) 111.7(3)
C(24) - C(19) - B(1)	121 9(3)	C(37)-B(2)-C(31)	108.2(3)
C(20)-C(19)-B(1)	121.9(3) 123 7(3)	C(49)-B(2)-C(31)	100.2(3) 111 5(3)
C(19)-C(20)-C(21)	125.7(3)	C(43)-B(2)-C(31)	106.8(2)
C(19)-C(20)-C(21)	117.2	C(58) - P(2) - C(51)	100.0(2) 103 74(14)
C(21)-C(20)-H(20)	117.2	C(58)-P(2)-C(55)	103.74(14) 101.74(15)
$C(21)-C(20)-\Pi(20)$	116.2(3)	C(51) - P(2) - C(55)	101.74(13) 101.03(14)
C(22)-C(21)-C(20)	125 0(2)	C(31) - C(31) - C(36)	101.93(14) 114.0(3)
$C(22)-C(21)-\Gamma(1)$ C(20)-C(21)-P(1)	125.9(2) 117 9(2)	C(32)-C(31)-B(2)	124.8(3)
C(23)-C(21)-C(21)	120.6(3)	C(32)-C(31)-B(2)	124.0(3) 121 2(3)
C(23)-C(22)-C(21)	110.7	C(33)-C(31)-D(2)	121.2(3) 123.7(3)
C(23)-C(22)-H(22)	110.7	C(33)-C(32)-C(31)	123.7(3)
$C(21) - C(22) - \Pi(22)$ C(22) - C(23) - C(24)	120.8(3)	C(31) - C(32) - H(32)	118.2
C(22) - C(23) - C(24) C(22) - C(23) - H(23)	119.6	C(34)- $C(33)$ - $C(32)$	120 3(3)
C(24)-C(23)-H(23)	119.6	C(34)-C(33)-H(33)	1199
C(19)-C(24)-C(23)	122 2(3)	C(32) - C(33) - H(33)	119.9
(1) (2) (2)	(-)	(32) (33) (1(33))	11/./
C(33)-C(34)-C(35)	117.9(3)	C(51)-C(52)-H(52)	120.3
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C(33)-C(34)-H(34)	121.0	C(54)-C(53)-C(52)	120.5(3)
C(35)-C(34)-H(34)	121.0	C(54)-C(53)-H(53)	119.7
C(36)-C(35)-C(34)	120.6(3)	C(52)-C(53)-H(53)	119.7
С(36)-С(35)-Н(35)	119.7	C(53)-C(54)-C(49)	123.4(3)
C(34)-C(35)-H(35)	119.7	C(53)-C(54)-H(54)	118.3
C(35)-C(36)-C(31)	123.5(3)	C(49)-C(54)-H(54)	118.3
С(35)-С(36)-Н(36)	118.3	C(57)-C(55)-C(56)	109.8(3)
С(31)-С(36)-Н(36)	118.3	C(57)-C(55)-P(2)	116.9(2)
C(42)-C(37)-C(38)	114.0(3)	C(56)-C(55)-P(2)	109.7(2)
C(42)-C(37)-B(2)	123.3(3)	C(57)-C(55)-H(55)	106.6
C(38)-C(37)-B(2)	122.2(3)	C(56)-C(55)-H(55)	106.6
C(39)-C(38)-C(37)	123.6(3)	P(2)-C(55)-H(55)	106.6
C(39)-C(38)-H(38)	118.2	C(55)-C(56)-H(56A)	109.5
C(37)-C(38)-H(38)	118.2	C(55)-C(56)-H(56B)	109.5
C(40)-C(39)-C(38)	119.9(3)	H(56A)-C(56)-H(56B)	109.5
C(40)-C(39)-H(39)	120.1	C(55)-C(56)-H(56C)	109.5
C(38)-C(39)-H(39)	120.1	H(56A)-C(56)-H(56C)	109.5
C(39)-C(40)-C(41)	118.8(3)	H(56B)-C(56)-H(56C)	109.5
C(39)-C(40)-H(40)	120.6	C(55)-C(57)-H(57A)	109.5
C(41)-C(40)-H(40)	120.6	C(55)-C(57)-H(57B)	109.5
C(40)-C(41)-C(42)	120.9(3)	H(57A)-C(57)-H(57B)	109.5
C(40)-C(41)-H(41)	119.6	C(55)-C(57)-H(57C)	109.5
C(42)-C(41)-H(41)	119.6	H(57A)-C(57)-H(57C)	109.5
C(41)-C(42)-C(37)	122.8(3)	H(57B)-C(57)-H(57C)	109.5
C(41)-C(42)-H(42)	118.6	C(60)-C(58)-C(59)	109.6(3)
C(37)-C(42)-H(42)	118.6	C(60)-C(58)-P(2)	111.8(2)
C(48)-C(43)-C(44)	114.5(3)	C(59)-C(58)-P(2)	109.4(2)
C(48)-C(43)-B(2)	124.9(3)	C(60)-C(58)-H(58)	108.7
C(44)-C(43)-B(2)	120.6(3)	C(59)-C(58)-H(58)	108.7
C(45)-C(44)-C(43)	122.5(3)	P(2)-C(58)-H(58)	108.7
C(45)-C(44)-H(44)	118.8	C(58)-C(59)-H(59A)	109.5
C(43)-C(44)-H(44)	118.8	C(58)-C(59)-H(59B)	109.5
C(46)-C(45)-C(44)	121.2(3)	H(59A)-C(59)-H(59B)	109.5
C(46)-C(45)-H(45)	119.4	C(58)-C(59)-H(59C)	109.5
C(44)-C(45)-H(45)	119.4	H(59A)-C(59)-H(59C)	109.5
C(47)-C(46)-C(45)	118.7(3)	H(59B)-C(59)-H(59C)	109.5
C(47)-C(46)-H(46)	120.7	C(58)-C(60)-H(60A)	109.5
C(45)-C(46)-H(46)	120.7	C(58)-C(60)-H(60B)	109.5
C(46)-C(47)-C(48)	120.3(3)	H(60A)-C(60)-H(60B)	109.5
C(46)-C(47)-H(47)	119.9	C(58)-C(60)-H(60C)	109.5
C(48)-C(47)-H(47)	119.9	H(60A)-C(60)-H(60C)	109.5
C(47)-C(48)-C(43)	122.9(3)	H(60B)-C(60)-H(60C)	109.5
C(47)-C(48)-H(48)	118.6	C(73)-N(1)-C(71)	106.3(3)
C(43)-C(48)-H(48)	118.6	C(73)-N(1)-C(69)	112.7(2)
C(50)-C(49)-C(54)	113.3(3)	C(71)-N(1)-C(69)	110.1(3)
C(50)-C(49)-B(2)	123.5(3)	C(73)-N(1)-C(75)	111.8(3)
C(54)-C(49)-B(2)	123.2(3)	C(71)-N(1)-C(75)	110.5(3)
C(51)-C(50)-C(49)	125.6(3)	C(69)-N(1)-C(75)	105.4(2)
C(51)-C(50)-H(50)	117.2	C(62)-C(61)-N(2)	118.4(3)
C(49)-C(50)-H(50)	117.2	C(62)-C(61)-H(61A)	107.7
C(50)-C(51)-C(52)	117.9(3)	N(2)-C(61)-H(61A)	107.7
C(50)-C(51)-P(2)	117.1(2)	C(62)-C(61)-H(61B)	107.7
C(52)-C(51)-P(2)	125.1(2)	N(2)-C(61)-H(61B)	107.7
C(53)-C(52)-C(51)	119.3(3)	H(61A)-C(61)-H(61B)	107.1
C(53)-C(52)-H(52)	120.3	C(61)-C(62)-H(62A)	109.5

C(61)-C(62)-H(62B)	109.5	C(70)-C(69)-H(69A)	108.5
H(62A)-C(62)-H(62B)	109.5	N(1)-C(69)-H(69A)	108.5
C(61)-C(62)-H(62C)	109.5	C(70)-C(69)-H(69B)	108.5
H(62A)-C(62)-H(62C)	109.5	N(1)-C(69)-H(69B)	108.5
H(62B)-C(62)-H(62C)	109.5	H(69A)-C(69)-H(69B)	107.5
C(64)-C(63)-N(2)	115.1(3)	C(69)-C(70)-H(70A)	109.5
C(64)-C(63)-H(63A)	108.5	C(69)-C(70)-H(70B)	109.5
N(2)-C(63)-H(63A)	108.5	H(70A)-C(70)-H(70B)	109.5
C(64)-C(63)-H(63B)	108.5	C(69)-C(70)-H(70C)	109.5
N(2)-C(63)-H(63B)	108.5	H(70A)-C(70)-H(70C)	109.5
H(63A)-C(63)-H(63B)	107.5	H(70B)-C(70)-H(70C)	109.5
C(63)-C(64)-H(64A)	109.5	N(1)-C(71)-C(72)	117.0(3)
C(63)-C(64)-H(64B)	109.5	N(1)-C(71)-H(71A)	108.1
H(64A)-C(64)-H(64B)	109.5	C(72)-C(71)-H(71A)	108.1
C(63)-C(64)-H(64C)	109.5	N(1)-C(71)-H(71B)	108.1
H(64A)-C(64)-H(64C)	109.5	C(72)-C(71)-H(71B)	108.1
H(64B)-C(64)-H(64C)	109.5	H(71A)-C(71)-H(71B)	107.3
N(2)-C(65)-C(66)	114.6(3)	C(71)-C(72)-H(72A)	109.5
N(2)-C(65)-H(65A)	108.6	C(71)-C(72)-H(72B)	109.5
C(66)-C(65)-H(65A)	108.6	H(72A)-C(72)-H(72B)	109.5
N(2)-C(65)-H(65B)	108.6	C(71)-C(72)-H(72C)	109.5
C(66)-C(65)-H(65B)	108.6	H(72A)-C(72)-H(72C)	109.5
H(65A)-C(65)-H(65B)	107.6	H(72B)-C(72)-H(72C)	109.5
C(65)-C(66)-H(66A)	109.5	C(74)-C(73)-N(1)	115.7(3)
C(65)-C(66)-H(66B)	109.5	C(74)-C(73)-H(73A)	108.4
H(66A)-C(66)-H(66B)	109.5	N(1)-C(73)-H(73A)	108.4
C(65)-C(66)-H(66C)	109.5	C(74)-C(73)-H(73B)	108.4
H(66A)-C(66)-H(66C)	109.5	N(1)-C(73)-H(73B)	108.4
H(66B)-C(66)-H(66C)	109.5	H(73A)-C(73)-H(73B)	107.4
N(2)-C(67)-C(68)	114.9(3)	C(73)-C(74)-H(74A)	109.5
N(2)-C(67)-H(67A)	108.6	С(73)-С(74)-Н(74В)	109.5
C(68)-C(67)-H(67A)	108.6	H(74A)-C(74)-H(74B)	109.5
N(2)-C(67)-H(67B)	108.6	C(73)-C(74)-H(74C)	109.5
C(68)-C(67)-H(67B)	108.6	H(74A)-C(74)-H(74C)	109.5
H(67A)-C(67)-H(67B)	107.5	H(74B)-C(74)-H(74C)	109.5
C(67)-C(68)-H(68A)	109.5	C(76)-C(75)-N(1)	117.4(3)
C(67)-C(68)-H(68B)	109.5	С(76)-С(75)-Н(75А)	108.0
H(68A)-C(68)-H(68B)	109.5	N(1)-C(75)-H(75A)	108.0
C(67)-C(68)-H(68C)	109.5	C(76)-C(75)-H(75B)	108.0
H(68A)-C(68)-H(68C)	109.5	N(1)-C(75)-H(75B)	108.0
H(68B)-C(68)-H(68C)	109.5	H(75A)-C(75)-H(75B)	107.2
C(67)-N(2)-C(65)	113.6(3)	C(75)-C(76)-H(76A)	109.5
C(67)-N(2)-C(61)	109.2(3)	C(75)-C(76)-H(76B)	109.5
C(65)-N(2)-C(61)	107.9(3)	H(76A)-C(76)-H(76B)	109.5
C(67)-N(2)-C(63)	108.7(2)	C(75)-C(76)-H(76C)	109.5
C(65)-N(2)-C(63)	109.0(3)	H(76A)-C(76)-H(76C)	109.5
C(61)-N(2)-C(63)	108.4(3)	H(76B)-C(76)-H(76C)	109.5
C(70)-C(69)-N(1)	115.2(3)		

Table 9. Anisotropic displacement parameters (Å²x 10³) for {[NEt₄][Ph₃BP^{*m*-iPr²}]}₂. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h² a*²U¹¹ + ... + 2 h k a* b* U¹²].

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
$\overline{\mathbf{P}(1)}$	24(2)	24(2)	21(2)	1(2)	3(2)	6(2)
$\mathbf{D}(1)$ $\mathbf{D}(1)$	24(2) 26(1)	24(2) 22(1)	$\frac{21(2)}{38(1)}$	1(2) 1(1)	$\frac{3(2)}{1(1)}$	0(2)
C(1)	20(1) 19(2)	$\frac{22(1)}{10(2)}$	33(1) 23(2)	$\frac{1(1)}{3(2)}$	1(1) 0(1)	3(1)
C(1)	19(2)	19(2) 10(2)	23(2)	$\frac{3(2)}{2(2)}$	0(1)	3(1) 2(1)
C(2)	20(2)	19(2)	$\frac{27(2)}{20(2)}$	-2(2)	0(2)	3(1)
C(3)	39(2)	20(2) 24(2)	20(2)	1(2) 5(2)	3(2)	-4(2)
C(4)	40(2)	34(2)	20(2) 21(2)	3(2)	1(2) 12(2)	-4(2)
C(5)	58(2)	20(2)	31(2)	8(2)	-12(2)	-6(2)
C(6)	44(2)	22(2)	$\frac{2}{2}$	-3(2)	-10(2)	-1(2)
C(7)	29(2)	19(2)	22(2)	-5(2)	-6(2)	2(2)
C(8)	24(2)	33(2)	39(2)	-8(2)	5(2)	3(2)
C(9)	30(2)	34(2)	48(2)	-9(2)	1(2)	7(2)
C(10)	23(2)	52(3)	36(2)	-15(2)	12(2)	6(2)
C(11)	32(2)	44(2)	34(2)	6(2)	14(2)	3(2)
C(12)	30(2)	34(2)	29(2)	3(2)	9(2)	5(2)
C(13)	22(2)	13(2)	23(2)	-3(1)	0(1)	7(1)
C(14)	36(2)	21(2)	29(2)	6(2)	2(2)	1(2)
C(15)	48(2)	33(2)	17(2)	1(2)	-5(2)	1(2)
C(16)	34(2)	24(2)	37(2)	-1(2)	-18(2)	3(2)
C(17)	21(2)	18(2)	43(2)	-2(2)	-5(2)	5(1)
C(18)	29(2)	21(2)	27(2)	-2(2)	-1(2)	5(2)
C(19)	20(2)	15(2)	19(2)	-1(1)	1(1)	3(1)
C(20)	15(2)	24(2)	22(2)	3(2)	2(1)	3(1)
C(21)	22(2)	17(2)	20(2)	2(1)	0(1)	3(1)
C(22)	31(2)	19(2)	33(2)	-2(2)	0(2)	5(2)
C(23)	28(2)	30(2)	44(2)	-6(2)	-13(2)	12(2)
C(24)	33(2)	23(2)	37(2)	-1(2)	-6(2)	-1(2)
C(25)	39(2)	21(2)	33(2)	-5(2)	-7(2)	1(2)
C(26)	48(2)	32(2)	32(2)	-4(2)	-6(2)	3(2)
C(27)	46(2)	23(2)	30(2)	-1(2)	2(2)	0(2)
C(28)	30(2)	18(2)	39(2)	1(2)	6(2)	2(2)
C(29)	39(2)	29(2)	43(2)	-3(2)	9(2)	2(2)
C(30)	43(2)	31(2)	42(2)	5(2)	17(2)	-1(2)
B(2)	23(2)	21(2)	22(2)	-4(2)	-3(2)	2(2)
P(2)	24(1)	21(1)	34(1)	-5(1)	-1(1)	3(1)
C(31)	18(2)	20(2)	25(2)	0(2)	2(1)	-3(1)
C(32)	37(2)	25(2)	30(2)	9(2)	9(2)	6(2)
C(33)	54(2)	39(3)	21(2)	1(2)	9(2)	9(2)
C(34)	47(2)	43(3)	29(2)	13(2)	5(2)	1(2)
C(35)	55(2)	21(2)	34(2)	6(2)	-9(2)	0(2)
C(36)	49(2)	22(2)	26(2)	2(2)	-5(2)	-5(2)
C(37)	24(2)	16(2)	21(2)	6(1)	0(1)	5(1)
C(38)	30(2)	22(2)	24(2)	-2(2)	0(2)	1(2)
C(39)	26(2)	25(2)	44(2)	2(2)	-2(2)	0(2)
C(40)	37(2)	19(2)	40(2)	-11(2)	-17(2)	1(2)
C(41)	49(2)	39(3)	26(2)	-4(2)	-8(2)	11(2)
C(42)	30(2)	27(2)	26(2)	-3(2)	-1(2)	1(2)
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C(43)	23(2)	25(2)	16(2)	-3(2)	-1(1)	1(2)
C(44)	29(2)	17(2)	55(2)	-2(2)	7(2)	-4(2)
C(45)	29(2)	27(2)	59(3)	-2(2)	8(2)	9(2)
C(46)	24(2)	37(2)	36(2)	-11(2)	8(2)	-2(2)
C(47)	24(2)	27(2)	22(2)	2(2)	2(1)	-5(2)
C(48)	28(2)	20(2)	18(2)	-2(1)	3(1)	2(1)
C(49)	21(2)	26(2)	12(2)	6(1)	3(1)	-3(1)
C(50)	21(2)	19(2)	14(2)	3(1)	1(1)	4(1)
C(51)	21(2)	28(2)	17(2)	4(2)	5(1)	2(2)
C(52)	23(2)	20(2)	22(2)	2(2)	3(1)	4(1)
C(53)	19(2)	34(2)	18(2)	4(2)	0(1)	-1(2)
C(54)	28(2)	17(2)	17(2)	-1(1)	0(1)	-1(1)
C(55)	35(2)	22(2)	25(2)	-4(2)	-10(1)	5(2)
C(56)	51(2)	31(2)	29(2)	-2(2)	-11(2)	10(2)
C(57)	45(2)	39(2)	19(2)	-2(2)	2(2)	5(2)
C(58)	27(2)	22(2)	36(2)	-2(2)	11(2)	1(2)
C(59)	42(2)	22(2)	55(3)	-6(2)	11(2)	0(2)
C(60)	32(2)	30(2)	40(2)	2(2)	8(2)	5(2)
N(1)	28(2)	31(2)	30(2)	5(1)	8(1)	0(1)
C(61)	64(3)	40(3)	47(3)	1(2)	11(2)	3(2)
C(62)	46(2)	36(2)	94(3)	-25(2)	-17(2)	4(2)
C(63)	49(2)	53(3)	45(3)	-10(2)	5(2)	-8(2)
C(64)	86(3)	39(3)	36(2)	17(2)	7(2)	1(2)
C(65)	37(2)	60(3)	63(3)	1(2)	-2(2)	7(2)
C(66)	39(2)	35(2)	75(3)	-31(2)	-6(2)	8(2)
C(67)	50(2)	44(3)	51(3)	0(2)	2(2)	3(2)
C(68)	71(3)	85(3)	45(3)	22(2)	22(2)	37(3)
N(2)	26(2)	25(2)	25(2)	-6(1)	5(1)	-3(1)
C(69)	30(2)	31(2)	53(2)	-5(2)	11(2)	-9(2)
C(70)	55(3)	52(3)	61(3)	-12(2)	-23(2)	2(2)
C(71)	36(2)	36(2)	59(3)	-9(2)	20(2)	4(2)
C(72)	43(2)	32(2)	100(4)	-4(2)	15(2)	4(2)
C(73)	42(2)	35(2)	41(2)	5(2)	-14(2)	9(2)
C(74)	47(2)	42(3)	107(4)	-9(2)	-31(2)	15(2)
C(75)	47(2)	38(2)	31(2)	1(2)	0(2)	4(2)
C(76)	56(2)	34(2)	35(2)	6(2)	-12(2)	2(2)

Table 10. Hydrogen coordinates (x 10⁴) and isotropic displacement parameters (Å²x 10³) for $\{[NEt_4][Ph_3BP^{m-iPr^2}]\}_2$.

	х	У	Z	U(eq)
	440	0000	2724	20
H(2)	449	8088	3/34	29
H(3)	/55	//65	5051	34
H(4)	/68	6637	5383	43
H(5)	446	5855	43/3	44
H(6)	1/4	6189	3056	38
H(8)	2161	64/4	2325	38
H(9)	4363	6435	1950	45
H(10)	5329	/353	1324	44
H(11)	4008	8307	1100	44
H(12)	1/96	8329	14/4	3/
H(14)	184	/003	/0/	34
H(15)	-1291	6346	-110	39
H(16)	-3086	5806	442	39
H(1/)	-34/3	5928	1/90	33
H(18)	-20/4	6629	2573	31
H(20)	1003	8/14	2668	25
H(22)	-2234	9847	2064	33
H(23)	-3349	8911	1586	41
H(24)	-2327	/8/2	16/4	3/
H(25)	387	10536	4130	38
H(26A)	299	9595	4924	56
H(26B)	1467	9501	4307	56
H(26C)	44	9131	4157	56
H(2/A)	-2041	9863	3668	50
H(2/B)	-1846	10649	3769	50
H(2/C)	-1756	10176	4536	50
H(28)	-1284	10808	2444	34
H(29A)	1279	11448	2745	55
H(29B)	60	11457	3337	55
H(29C)	-89	11839	2502	55
H(30A)	-424	11221	1241	57
H(30B)	-331	10427	1242	5/
H(30C)	997	10863	1441	5/
H(32)	4/5/	3331	1262	3/
H(33)	4417	3700	-29	45
H(34)	3855	4812	-286	4/
H(35)	3008	5521	/98	44
H(36)	3835	5134	2079	39
H(38)	6548	4/35	2441	31
H(39)	8012	5391	3202	38
H(40)	//20	5516	4560	39
H(41)	5919	4982	5127	46
H(42)	4446	4329	4365	34
H(44)	2567	4889	3144	40
H(45)	343	4892	3492	46
H(40)	-81/	3903	3080	39
П(4/) Ц(49)	3UD 2545	2902	5527 2170	29
П(48) Ц(50)	2545	2889	31/U 21/0	20
п(30)	5/90	2001	2108	22
H(52)	6842	1493	3010	20
H(53)	(722	2411	3687	28
H(34)	6/32	3429	3600	24
н(55)	4/19	923	694	55

H(56A)	5219	2320	820	56
H(56B)	3793	2007	524	56
H(56C)	5093	1905	6	56
H(57A)	6982	1240	511	51
H(57B)	6849	741	1245	51
H(57C)	7084	1517	1404	51
H(58)	5993	557	2445	34
H(59A)	4852	-473	2233	59
H(59B)	4705	-37	1437	59
H(59C)	3465	-91	2011	59
H(60A)	3615	488	3357	50
H(60B)	4975	873	3633	50
H(60C)	4976	80	3564	50
H(61A)	8337	4716	1068	60
H(61R)	9046	4387	1843	60
H(62A)	11096	4889	1522	89
H(62R)	9931	5415	1693	89
H(62C)	10300	5258	795	89
$H(63\Delta)$	10507	4374	-96	59
H(63R)	9784	3702	-389	59
H(61A)	7688	1218	-302	81
H(64R)	8693	4577	_997	81
H(64C)	8465	4023	-156	81
H(65A)	10750	3560	1721	64
H(05R)	10730	3040	1/21	04 64
H(65D)	10562	2603	065	04 75
H(00A)	10302	2003	905	75
H(66C)	12111	2832	200	75
$H(67\Lambda)$	11107 9470	2972	200	73 59
H(0/A) H(67D)	7512	3083	443 677	50
$H(68\Lambda)$	0037	2030	1821	100
11(00A) 11(69D)	9037 7496	2939	1621	100
$\Pi(00D)$	7400	2703	1372	100
$\Pi(0\delta C)$ $\Pi(60\Lambda)$	6282	3472 2770	1998	100
$\Pi(09A)$	0362 5227	2770	5221	43
$\Pi(09D)$	5070	3373	3331	43
$\Pi(70A)$	5272	2540	6/22	83 85
$\Pi(70D)$	6245	2055	6911	83 85
$\Pi(70C)$	0343	2833	0811	83 52
H(/IA) H(71D)	3409	2844	0005 5072	52
H(/1B)	24/3	2477	5972	52 97
H(72A)	3404	3/90	5//1	87
H(72B)	1962	3010	6013 5140	87
H(72C)	2446	3427	5146	8/
H(/3A)	4956	1980	6653	48
H(73B)	3946	1580	6057	48
H(/4A)	5/54	13/6	5229	100
H(/4B)	6020	1066	6100	100
H(74C)	6752	1743	5866	100
H(/5A)	3847	2799	4507	46
H(75B)	4930	2212	4520	46
H(76A)	3260	1448	4764	63
H(76B)	2862	1863	3974	63
H(76C)	2164	2032	4789	63

Table 11. Crystal data and structure refinement for $\{NBu_4\}\{[Ph_3BP^{p-iPr2}]RhX(NBD)\}$.Empirical formula $C_{53}H_{77}BBr_{0.6}Cl_{0.4}NPRh$ Formula weight988.21

Crystal Habit	rounded blade	
Crystal Color	orange	
Crystal size	0.37 x 0.11 x 0.22 mm ³	
Da	ta Collection	
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Data collection temperature	98(2) K	
Unit cell dimensions	a = 15.8487(10) Å b = 15.6527(10) Å c = 20.3787(13) Å	$\alpha = 90^{\circ}$ $\beta = 102.6390(10)^{\circ}$ $\gamma = 90^{\circ}$
Volume	4932.9(5) Å ³	
Ζ	4	
Crystal system	Monoclinic	
Space group	P2 ₁	
Density (calculated)	1.331 Mg/m ³	
F(000)	2076	
θ range for data collection	1.66 to 28.59°	
Completeness to $\theta = 28.59^{\circ}$	94.5%	
Index ranges	$-21 \le h \le 21, -20 \le k \le 20, -27$	$\leq l \leq 27$
Reflections collected	91118	
Independent reflections	11928 [R(int) = 0.0884]	
Absorption coefficient	1.278 mm ⁻¹	
Absorption correction	None	
Structure so	olution and refinement	
Structure solution program	SHELXS-97 (Sheldrick, 1990))
Primary solution method	direct methods	
Secondary solution method	difference Fourier map	
Hydrogen placement	calculated positions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997))
Refinement method	Full-matrix least-squares on F ²	2
Data / restraints / parameters	11928 / 0 / 532	
Goodness-of-fit on F ²	1.551	
Final R indices [I>2 σ (I)]	R1 = 0.0432, wR2 = 0.0646	
R indices (all data)	R1 = 0.0945, wR2 = 0.0705	
Type of weighting scheme used	calc	
Weighting scheme used	calc w=1/[^2^(Fo^2^)+(0.0000	$(P)^{2^+0.000P}$ where

$P = (Fo^2 + 2Fc^2)/3$	
Max shift/error	0.035
Average shift/error	0.001
Largest diff. peak and hole	0.980 and -0.670 e·Å ⁻³

Special Refinement Details:

Halide occupancy was modeled reasonably as 60% bromide and 40% chloride. The structure was otherwise unremarkable.

Table 12. Atomic coordinates ($x \ 10^4$) and equivalent isotropic displacement parameters (Å²x 10³) for {NBu₄} {[Ph₃BP^{*p*-iPr²}]RhX(NBD)}. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	X	У	Z	U(eq)
Rh	55(1)	6868(1)	3120(1)	16(1)
Br	-1523(1)	6703(1)	2738(1)	23(1)
Cl	-1523(1)	6703(1)	2738(1)	23(1)
Р	211(1)	7589(1)	2152(1)	15(1)
В	3530(2)	6758(2)	1001(2)	15(1)
C(1)	3827(2)	7591(2)	613(1)	15(1)
C(2)	3675(2)	7666(2)	-83(2)	22(1)
C(3)	3906(2)	8393(2)	-398(2)	26(1)
C(4)	4288(2)	9076(2)	-24(2)	26(1)
C(5)	4450(2)	9024(2)	666(2)	26(1)
C(6)	4228(2)	8294(2)	975(2)	22(1)
C(7)	4362(2)	6453(2)	1600(2)	17(1)
C(8)	5203(2)	6479(2)	1491(2)	23(1)
C(9)	5914(2)	6164(2)	1959(2)	28(1)
C(10)	5806(2)	5822(2)	2556(2)	33(1)
C(11)	4996(2)	5818(2)	2694(2)	31(1)
C(12)	4283(2)	6127(2)	2225(2)	24(1)
C(13)	3271(2)	5986(2)	439(1)	12(1)
C(14)	3866(2)	5416(2)	272(1)	14(1)
C(15)	3657(2)	4839(2)	-257(1)	18(1)
C(16)	2831(2)	4813(2)	-647(1)	18(1)
C(17)	2214(2)	5362(2)	-495(1)	18(1)
C(18)	2431(2)	5926(2)	34(1)	16(1)
C(20)	2219(2)	6386(2)	1576(1)	17(1)
C(21)	1511(2)	6564(2)	1847(1)	17(1)
C(22)	1192(2)	7396(2)	1848(1)	16(1)
C(23)	1624(2)	8028(2)	1561(1)	16(1)
C(24)	2344(2)	7832(2)	1302(1)	16(1)
C(25)	-649(2)	7341(2)	1392(1)	20(1)
C(26)	-606(2)	7898(2)	784(1)	27(1)
C(27)	-644(2)	6404(2)	1215(2)	28(1)
C(29)	-741(2)	9036(2)	2352(2)	22(1)
C(30)	868(2)	9137(2)	2763(1)	20(1)
C(32)	1226(2)	7202(2)	3794(1)	18(1)
C(33)	1123(2)	5726(2)	3972(1)	21(1)
C(34)	1461(2)	6153(2)	4658(2)	23(1)
C(35)	953(2)	6992(2)	4456(1)	19(1)
C(36)	39(2)	6638(2)	4182(1)	19(1)
C(37)	137(2)	5864(2)	3887(1)	22(1)
N	6588(1)	8278(1)	3565(1)	15(1)
C(38)	5737(2)	8697(2)	3610(2)	17(1)
C(39)	4917(2)	8245(2)	3271(2)	27(1)
C(40)	4149(2)	8685(2)	3464(2)	27(1)
C(41)	3291(2)	8288(3)	3130(2)	47(1)
C(42)	6663(2)	8204(2)	2839(1)	18(1)
C(43)	6776(2)	9044(2)	2501(1)	21(1)
C(44)	6774(2)	8920(2)	1763(1)	25(1)
C(45)	6927(2)	9773(2)	1450(2)	35(1)
C(46)	7297(2)	8831(2)	3974(1)	16(1)
C(47)	8221(2)	8518(2)	4022(1)	16(1)
C(48)	8858(2)	9242(2)	4241(2)	20(1)

C(49)	9788(2)	8945(2)	4410(2)	23(1)	
C(50)	6644(2)	7375(2)	3836(1)	19(1)	
C(51)	6545(2)	7257(2)	4555(2)	27(1)	
C(52)	6498(2)	6306(2)	4710(2)	31(1)	
C(53)	7317(2)	5806(2)	4677(2)	43(1)	
C(19)	2678(2)	7013(2)	1304(1)	13(1)	
C(31)	1319(2)	6420(2)	3489(2)	22(1)	
C(28)	138(2)	8768(2)	2219(1)	17(1)	

Table 13. Bond lengths [Å] and angles [°] for $\{NBu_4\}\{[Ph_3BP^{p-iPr2}]RhX(NBD)\}$.

Rh-C(31)	2.101(3)	Rh-C(37)	2.200(3)
Rh-C(32)	2.119(3)	Rh-P	2.3321(8)
Rh-C(36)	2.199(3)	Rh-Br	2.4653(5)

P-C(22)	1.819(3)	C(27)-H(27A)	0.9800
P-C(28)	1.857(3)	C(27)-H(27B)	0.9800
P-C(25)	1.866(3)	C(27)-H(27C)	0.9800
B-C(1)	1.647(4)	C(29)-C(28)	1.535(4)
B-C(19)	1.652(4)	C(29)-H(29A)	0.9800
B-C(13)	1.652(4)	C(29)-H(29B)	0.9800
B-C(7)	1.659(4)	C(29)-H(29C)	0.9800
C(1)-C(2)	1.390(4)	C(30)-C(28)	1.529(4)
C(1)-C(6)	1.397(4)	C(30)-H(30A)	0.9800
C(2)-C(3)	1.394(4)	C(30)-H(30B)	0.9800
C(2)-H(2)	0.9500	C(30)-H(30C)	0.9800
C(3)-C(4)	1.376(4)	C(32)-C(31)	1.394(4)
C(3)-H(3)	0.9500	C(32)-C(35)	1.540(4)
C(4)-C(5)	1.374(4)	C(32)-H(32)	1.0000
C(4)-H(4)	0.9500	C(33)-C(34)	1.536(4)
C(5)-C(6)	1 387(4)	C(33)-C(31)	1.543(4)
C(5)-H(5)	0.9500	C(33)-C(37)	1.548(4)
C(6)-H(6)	0.9500	C(33)-H(33)	1 0000
C(7)- $C(8)$	1 399(4)	C(34)-C(35)	1 547(4)
C(7)- $C(12)$	1.000(1)	C(34)-H(34A)	0 9900
C(8)-C(9)	1 397(4)	C(34)-H(34B)	0.9900
C(8)-H(8)	0.9500	C(35)-C(36)	1 538(4)
C(9)- $C(10)$	1 372(4)	C(35) - H(35)	1 0000
C(9)-H(9)	0.9500	C(36)- $C(37)$	1 376(4)
C(10)- $C(11)$	1 373(4)	C(36)-H(36)	1.0000
C(10)-H(10)	0.9500	C(37)-H(37)	1 0000
C(11)- $C(12)$	1 399(4)	N-C(50)	1.513(3)
C(11)-C(12) C(11)-H(11)	0.9500	N-C(42)	1.515(3) 1.514(3)
C(12)-H(12)	0.9500	N-C(46)	1.514(3) 1.515(3)
$C(12)-\Pi(12)$ C(13)-C(14)	1.394(4)	N-C(38)	1.515(5) 1.521(3)
C(13) - C(18)	1.094(4)	C(38)- $C(39)$	1.521(5) 1 508(4)
C(14)-C(15)	1 390(4)	C(38) - H(38A)	0.9900
C(14)-C(15)	0.9500	C(38)-H(38R)	0.9900
C(14)-11(14) C(15)-C(16)	1 376(4)	C(39)-C(40)	1.522(4)
C(15)-U(15)	0.9500	C(39) - H(39A)	0 0000
$C(15)$ - $\Pi(15)$ C(16) $C(17)$	1.387(4)	C(39) - H(39R) C(30) + H(30R)	0.9900
C(10)-C(17) C(16) H(16)	0.9500	$C(39) - \Pi(39B)$ C(40) C(41)	0.9900 1 514(4)
C(10)-11(10) C(17) $C(18)$	1,277(4)	C(40) - C(41)	0.0000
C(17) - C(10) C(17) - U(17)	0.0500	C(40) - H(40R) C(40) - H(40R)	0.9900
$C(17) - \Pi(17)$ C(18) H(18)	0.9300	C(40) - H(40B) C(41) + H(41A)	0.9900
C(10)-11(10) C(20) $C(21)$	1.384(4)	C(41) - H(41R) C(41) - H(41R)	0.9800
C(20) - C(21)	1.364(4)	C(41) - H(41B)	0.9800
C(20) - C(19)	1.400(4)	$C(41) - \Pi(41C)$	0.9800 1.512(4)
C(20)- $H(20)$	0.9500	C(42) - C(43)	1.515(4)
C(21)-C(22)	1.398(4)	$C(42) - \Pi(42A)$	0.9900
C(21)-H(21)	0.9500	C(42)- $H(42B)C(42)$ - $C(44)$	0.9900
C(22)-C(23)	1.402(4)	C(43) - C(44)	1.510(4)
C(23)-C(24)	1.391(4)	C(43)-H(43A)	0.9900
C(23)-H(23)	0.9500	C(43)-H(43B)	0.9900
C(24) - C(19)	1.38/(4)	C(44) - C(45)	1.523(4)
C(24)-H(24)	0.9500	C(44)-H(44A)	0.9900
C(25) - C(27)	1.512(4)	C(44)-H(44B)	0.9900
U(25)-U(26)	1.529(4)	C(45)-H(45A)	0.9800
C(25)-H(25)	1.0000	C(45)-H(45B)	0.9800
C(26)-H(26A)	0.9800	C(45)-H(45C)	0.9800
C(26)-H(26B)	0.9800	C(46)-C(47)	1.527(4)
C(26)-H(26C)	0.9800	C(46)-H(46A)	0.9900

C(46)-H(46B)	0.9900	C(1)-C(2)-H(2)	118.8
C(47)-C(48)	1.519(4)	C(3)-C(2)-H(2)	118.8
C(47)-H(47A)	0.9900	C(4)-C(3)-C(2)	120.4(3)
C(47)-H(47B)	0.9900	C(4)-C(3)-H(3)	119.8
C(48)-C(49)	1.512(4)	C(2)-C(3)-H(3)	119.8
C(48)-H(48A)	0.9900	C(5)-C(4)-C(3)	118.8(3)
C(48)-H(48B)	0.9900	C(5)-C(4)-H(4)	120.6
C(49)-H(49A)	0.9800	C(3)-C(4)-H(4)	120.6
C(49)-H(49B)	0.9800	C(4)-C(5)-C(6)	120.3(3)
C(49)-H(49C)	0.9800	C(4)- $C(5)$ - $H(5)$	119.8
C(50)- $C(51)$	1 519(4)	C(6)-C(5)-H(5)	119.8
C(50) - H(50A)	0.9900	C(5)-C(6)-C(1)	122.6(3)
C(50)-H(50B)	0.9900	C(5)- $C(6)$ - $H(6)$	118 7
C(51)-C(52)	1 526(4)	C(1)-C(6)-H(6)	118.7
C(51) - H(51A)	0.9900	C(8)-C(7)-C(12)	115.6(3)
C(51)-H(51B)	0.9900	C(8)-C(7)-B	120.4(3)
C(52)-C(53)	1 529(4)	C(12)-C(7)-B	123.9(3)
C(52) - H(52A)	0.9900	C(9)-C(8)-C(7)	123.9(3) 122.4(3)
C(52) - H(52R)	0.9900	C(9)-C(8)-H(8)	118.8
C(52) H(52B) C(53)-H(53A)	0.9800	C(7)- $C(8)$ -H(8)	118.8
C(53)-H(53R)	0.9800	C(10)- $C(9)$ - $C(8)$	120.3(3)
C(53) - H(53C)	0.9800	C(10) - C(9) - H(9)	119.9
C(31)-H(31)	1 0000	C(8)-C(9)-H(9)	119.9
C(28)-H(28)	1 0000	C(9)-C(10)-C(11)	119.9 119.1(3)
C(20) II(20)	1.0000	C(9)- $C(10)$ - $H(10)$	120.4
C(31)-Rh- $C(32)$	38 59(10)	C(11)-C(10)-H(10)	120.1
C(31)-Rh- $C(36)$	78.97(11)	C(10)- $C(11)$ - $C(12)$	120.4 120.7(3)
C(32)-Rh- $C(36)$	66 40(11)	C(10) - C(11) - H(11)	119.6
C(31)-Rh- $C(37)$	66 66(12)	C(12)-C(11)-H(11)	119.6
C(32)-Rh- $C(37)$	78.94(11)	C(12) - C(12) - C(7)	121 8(3)
C(36)-Rh- $C(37)$	3645(10)	C(11) - C(12) - H(12)	119.1
C(31)-Rh-P	$101\ 24(8)$	C(7)- $C(12)$ -H(12)	119.1
C(32)-Rh-P	100.90(8)	C(14)-C(13)-C(18)	114 6(3)
C(36)-Rh-P	159 66(8)	C(14)-C(13)-B	1240(3)
C(37)-Rh-P	161.04(8)	C(18)-C(13)-B	121.0(2)
C(31)-Rh-Br	154 23(9)	C(15) - C(14) - C(13)	123.0(2) 123.1(3)
C(32)-Rh-Br	156 22(8)	C(15) - C(14) - H(14)	118.4
C(36)-Rh-Br	93 69(8)	C(13)-C(14)-H(14)	118.4
C(37)-Rh-Br	92.75(8)	C(16)-C(15)-C(14)	1202(3)
P-Rh-Br	94 10(2)	C(16)-C(15)-H(15)	119.9
C(22)-P- $C(28)$	105 14(14)	C(14)-C(15)-H(15)	119.9
C(22)-P- $C(25)$	101.92(13)	C(15)-C(16)-C(17)	118 7(3)
C(28)-P- $C(25)$	102.78(13)	C(15)-C(16)-H(16)	120.6
C(22)-P-Rh	117 69(10)	C(17)- $C(16)$ - $H(16)$	120.6
C(28)-P-Rh	113 52(10)	C(18)-C(17)-C(16)	120 3(3)
C(25)-P-Rh	114.07(10)	C(18)-C(17)-H(17)	119.8
C(1)-B-C(19)	109.3(2)	C(16)-C(17)-H(17)	119.8
C(1)-B- $C(13)$	107.5(2)	C(17)-C(18)-C(13)	123.0(3)
C(19)-B- $C(13)$	109.7(2)	C(17)-C(18)-H(18)	118.5
C(1)-B-C(7)	108.5(2)	C(13)-C(18)-H(18)	118.5
C(19)-B-C(7)	112.2(2)	C(21)-C(20)-C(19)	123.5(3)
C(13)-B-C(7)	109.7(2)	C(21)-C(20)-H(20)	118.3
C(2)-C(1)-C(6)	115.5(3)	C(19)-C(20)-H(20)	118.3
C(2)-C(1)-B	123.5(3)	C(20)-C(21)-C(22)	120.9(3)
C(6)-C(1)-B	121.0(3)	C(20)-C(21)-H(21)	119.5
C(1)-C(2)-C(3)	122.3(3)	C(22)-C(21)-H(21)	119.5

C(21)-C(22)-C(23)	116.5(3)	H(34A)-C(34)-H(34B)	110.3
C(21)-C(22)-P	119.4(2)	C(36)-C(35)-C(32)	100.4(2)
C(23)-C(22)-P	123.9(2)	C(36)-C(35)-C(34)	100.7(2)
C(24)-C(23)-C(22)	121.3(3)	C(32)-C(35)-C(34)	100.6(2)
C(24)-C(23)-H(23)	119.4	C(36)-C(35)-H(35)	117.3
C(22)-C(23)-H(23)	119.4	C(32)-C(35)-H(35)	117.3
C(19)-C(24)-C(23)	123.1(3)	C(34)-C(35)-H(35)	117.3
C(19)-C(24)-H(24)	118.4	C(37)-C(36)-C(35)	106.7(3)
C(23)-C(24)-H(24)	118.4	C(37)-C(36)-Rh	71.82(16)
C(27)-C(25)-C(26)	110.8(2)	C(35)-C(36)-Rh	94.93(17)
C(27)-C(25)-P	1110(2)	C(37)-C(36)-H(36)	123 3
C(26)-C(25)-P	113 6(2)	C(35)-C(36)-H(36)	123.3
C(27)-C(25)-H(25)	107.0	Rh-C(36)-H(36)	123.3
C(26)-C(25)-H(25)	107.0	C(36)-C(37)-C(33)	106.4(3)
P-C(25)-H(25)	107.0	C(36)-C(37)-Rh	71 72(17)
C(25)-C(26)-H(26A)	109.5	C(33)-C(37)-Rh	94.60(17)
C(25)-C(26)-H(26B)	109.5	C(36)-C(37)-H(37)	123.5
H(26A)-C(26)-H(26B)	109.5	C(33)-C(37)-H(37)	123.5
C(25)-C(26)-H(26C)	109.5	Rh-C(37)-H(37)	123.5
H(26A)-C(26)-H(26C)	109.5	C(50)-N- $C(42)$	105.9(2)
H(26B)-C(26)-H(26C)	109.5	C(50)-N- $C(46)$	110.7(2)
C(25)-C(27)-H(27A)	109.5	C(42)-N-C(46)	112.0(2)
C(25)-C(27)-H(27B)	109.5	C(50)-N-C(38)	111.2(2)
H(27A)-C(27)-H(27B)	109.5	C(42)-N- $C(38)$	110.7(2)
C(25)-C(27)-H(27C)	109.5	C(46)-N-C(38)	106.3(2)
H(27A)-C(27)-H(27C)	109.5	C(39)-C(38)-N	117.2(2)
H(27B)-C(27)-H(27C)	109.5	C(39)-C(38)-H(38A)	108.0
C(28)-C(29)-H(29A)	109.5	N-C(38)-H(38A)	108.0
C(28)-C(29)-H(29B)	109.5	C(39)-C(38)-H(38B)	108.0
H(29A)-C(29)-H(29B)	109.5	N-C(38)-H(38B)	108.0
C(28)-C(29)-H(29C)	109.5	H(38A)-C(38)-H(38B)	107.2
H(29A)-C(29)-H(29C)	109.5	C(38)-C(39)-C(40)	109.1(3)
H(29B)-C(29)-H(29C)	109.5	C(38)-C(39)-H(39A)	109.9
C(28)-C(30)-H(30A)	109.5	C(40)-C(39)-H(39A)	109.9
C(28)-C(30)-H(30B)	109.5	C(38)-C(39)-H(39B)	109.9
H(30A)-C(30)-H(30B)	109.5	C(40)-C(39)-H(39B)	109.9
C(28)-C(30)-H(30C)	109.5	H(39A)-C(39)-H(39B)	108.3
H(30A)-C(30)-H(30C)	109.5	C(41)-C(40)-C(39)	112.9(3)
H(30B)-C(30)-H(30C)	109.5	C(41)-C(40)-H(40A)	109.0
C(31)-C(32)-C(35)	106.3(2)	C(39)-C(40)-H(40A)	109.0
C(31)-C(32)-Rh	70.00(17)	C(41)-C(40)-H(40B)	109.0
C(35)-C(32)-Rh	98.11(18)	C(39)-C(40)-H(40B)	109.0
С(31)-С(32)-Н(32)	123.0	H(40A)-C(40)-H(40B)	107.8
С(35)-С(32)-Н(32)	123.0	C(40)-C(41)-H(41A)	109.5
Rh-C(32)-H(32)	123.0	C(40)-C(41)-H(41B)	109.5
C(34)-C(33)-C(31)	101.2(2)	H(41A)-C(41)-H(41B)	109.5
C(34)-C(33)-C(37)	100.6(2)	C(40)-C(41)-H(41C)	109.5
C(31)-C(33)-C(37)	99.8(2)	H(41A)-C(41)-H(41C)	109.5
C(34)-C(33)-H(33)	117.4	H(41B)-C(41)-H(41C)	109.5
C(31)-C(33)-H(33)	117.4	C(43)-C(42)-N	114.8(2)
C(37)-C(33)-H(33)	117.4	C(43)-C(42)-H(42A)	108.6
C(33)-C(34)-C(35)	94.0(2)	N-C(42)-H(42A)	108.6
C(33)-C(34)-H(34A)	112.9	C(43)-C(42)-H(42B)	108.6
C(35)-C(34)-H(34A)	112.9	N-C(42)-H(42B)	108.6
C(33)-C(34)-H(34B)	112.9	H(42A)-C(42)-H(42B)	107.5
C(35)-C(34)-H(34B)	112.9	C(42)-C(43)-C(44)	111.4(2)

C(42)-C(43)-H(43A)	109.4	H(49B)-C(49)-H(49C)	109.5
C(44)-C(43)-H(43A)	109.4	N-C(50)-C(51)	117.2(2)
C(42)-C(43)-H(43B)	109.4	N-C(50)-H(50A)	108.0
C(44)-C(43)-H(43B)	109.4	С(51)-С(50)-Н(50А)	108.0
H(43A)-C(43)-H(43B)	108.0	N-C(50)-H(50B)	108.0
C(43)-C(44)-C(45)	109.7(3)	С(51)-С(50)-Н(50В)	108.0
C(43)-C(44)-H(44A)	109.7	H(50A)-C(50)-H(50B)	107.3
C(45)-C(44)-H(44A)	109.7	C(50)-C(51)-C(52)	109.8(3)
C(43)-C(44)-H(44B)	109.7	C(50)-C(51)-H(51A)	109.7
C(45)-C(44)-H(44B)	109.7	C(52)-C(51)-H(51A)	109.7
H(44A)-C(44)-H(44B)	108.2	C(50)-C(51)-H(51B)	109.7
C(44)-C(45)-H(45A)	109.5	C(52)-C(51)-H(51B)	109.7
C(44)-C(45)-H(45B)	109.5	H(51A)-C(51)-H(51B)	108.2
H(45A)-C(45)-H(45B)	109.5	C(51)-C(52)-C(53)	114.2(3)
C(44)-C(45)-H(45C)	109.5	C(51)-C(52)-H(52A)	108.7
H(45A)-C(45)-H(45C)	109.5	C(53)-C(52)-H(52A)	108.7
H(45B)-C(45)-H(45C)	109.5	C(51)-C(52)-H(52B)	108.7
N-C(46)-C(47)	115.9(2)	C(53)-C(52)-H(52B)	108.7
N-C(46)-H(46A)	108.3	H(52A)-C(52)-H(52B)	107.6
C(47)-C(46)-H(46A)	108.3	C(52)-C(53)-H(53A)	109.5
N-C(46)-H(46B)	108.3	C(52)-C(53)-H(53B)	109.5
C(47)-C(46)-H(46B)	108.3	H(53A)-C(53)-H(53B)	109.5
H(46A)-C(46)-H(46B)	107.4	C(52)-C(53)-H(53C)	109.5
C(48)-C(47)-C(46)	110.2(2)	H(53A)-C(53)-H(53C)	109.5
C(48)-C(47)-H(47A)	109.6	H(53B)-C(53)-H(53C)	109.5
C(46)-C(47)-H(47A)	109.6	C(24)-C(19)-C(20)	114.6(3)
C(48)-C(47)-H(47B)	109.6	С(24)-С(19)-В	124.5(3)
C(46)-C(47)-H(47B)	109.6	С(20)-С(19)-В	120.9(3)
H(47A)-C(47)-H(47B)	108.1	C(32)-C(31)-C(33)	106.1(3)
C(49)-C(48)-C(47)	112.9(2)	C(32)-C(31)-Rh	71.41(17)
C(49)-C(48)-H(48A)	109.0	C(33)-C(31)-Rh	98.82(19)
C(47)-C(48)-H(48A)	109.0	C(32)-C(31)-H(31)	122.7
C(49)-C(48)-H(48B)	109.0	C(33)-C(31)-H(31)	122.7
C(47)-C(48)-H(48B)	109.0	Rh-C(31)-H(31)	122.7
H(48A)-C(48)-H(48B)	107.8	C(30)-C(28)-C(29)	109.9(2)
C(48)-C(49)-H(49A)	109.5	C(30)-C(28)-P	112.3(2)
C(48)-C(49)-H(49B)	109.5	C(29)-C(28)-P	111.0(2)
H(49A)-C(49)-H(49B)	109.5	C(30)-C(28)-H(28)	107.8
C(48)-C(49)-H(49C)	109.5	C(29)-C(28)-H(28)	107.8
H(49A)-C(49)-H(49C)	109.5	P-C(28)-H(28)	107.8

Table 14. Anisotropic displacement parameters $(Å^2 x \ 10^3)$ for $\{NBu_4\} \{[Ph_3BP^{p-1}]RhX(NBD)\}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2h k a^{*} b^{*} U^{12}]$.

	U^{11}	U ²²	U ³³	U ²³	U ¹³	U^{12}
Rh	16(1)	18(1)	15(1)	0(1)	5(1)	1(1)
Br	16(1)	32(1)	22(1)	-3(1)	6(1)	2(1)
Cl	16(1)	32(1)	22(1)	-3(1)	6(1)	2(1)
Р	16(1)	16(1)	14(1)	-1(1)	3(1)	1(1)
В	19(2)	12(2)	14(2)	-3(2)	3(1)	1(2)
C(1)	10(2)	14(2)	23(2)	-1(1)	6(1)	3(1)
C(2)	23(2)	17(2)	28(2)	1(1)	11(2)	-1(1)
C(3)	30(2)	24(2)	27(2)	5(2)	13(2)	0(2)
C(4)	21(2)	18(2)	40(2)	9(2)	10(2)	-5(2)
C(5)	21(2)	18(2)	37(2)	-3(2)	0(2)	-5(1)
C(6)	20(2)	21(2)	23(2)	1(1)	2(1)	-1(1)
C(7)	21(2)	10(2)	19(2)	-8(1)	1(1)	2(1)
C(8)	24(2)	18(2)	26(2)	-11(1)	4(2)	3(1)
C(9)	19(2)	30(2)	32(2)	-18(2)	-1(2)	3(2)
C(10)	32(2)	23(2)	33(2)	-9(2)	-13(2)	9(2)
C(11) C(12)	42(2)	21(2) 15(2)	23(2)	1(2) 1(1)	-3(2)	-4(2)
C(12) C(13)	20(2) 16(2)	13(2)	$\frac{2}{(2)}$	-1(1)	0(2) 6(1)	-2(1)
C(13) C(14)	10(2) 12(2)	$\frac{9(2)}{17(2)}$	11(2) 15(2)	4(1)	6(1)	-3(1)
C(14) C(15)	12(2) 19(2)	17(2) 16(2)	22(2)	-(1)	13(2)	2(1)
C(15)	27(2)	18(2)	11(2)	-3(1)	6(1)	-6(1)
C(17)	18(2)	19(2)	15(2)	3(1)	-1(1)	-2(1)
C(18)	19(2)	11(2)	17(2)	4(1)	4(1)	4(1)
C(20)	22(2)	12(2)	16(2)	-1(1)	3(1)	2(1)
C(21)	22(2)	14(2)	16(2)	2(1)	8(1)	-1(1)
C(22)	20(2)	18(2)	11(2)	-1(1)	5(1)	0(1)
C(23)	19(2)	12(2)	15(2)	-2(1)	2(1)	3(1)
C(24)	19(2)	16(2)	14(2)	2(1)	3(1)	-3(1)
C(25)	18(2)	24(2)	16(2)	-5(1)	0(1)	-2(1)
C(26)	31(2)	30(2)	16(2)	-1(1)	-1(2)	-1(2)
C(27)	35(2)	27(2)	20(2)	-7(2)	5(2)	-11(2)
C(29)	21(2)	24(2)	21(2)	5(1)	7(2)	8(2)
C(30)	22(2)	19(2)	19(2)	-5(1)	3(1)	2(1)
C(32)	12(2)	20(2)	22(2)	4(1)	1(1)	3(1)
C(33)	28(2)	$\frac{1}{(2)}$	20(2)	4(1)	7(2)	0(1) 5(2)
C(34) C(35)	23(2) 23(2)	23(2) 19(2)	20(2) 16(2)	-1(1)	4(2) 3(1)	3(2) 3(1)
C(36)	25(2)	$\frac{19(2)}{23(2)}$	10(2) 11(2)	-1(1)	9(1)	$\frac{3(1)}{1(1)}$
C(37)	30(2)	18(2)	17(2)	7(1)	7(2)	-3(2)
N	14(1)	14(1)	16(1)	-2(1)	2(1)	1(1)
C(38)	18(2)	16(2)	17(2)	-2(1)	$\frac{2}{5(1)}$	5(1)
C(39)	18(2)	41(2)	21(2)	-9(2)	0(1)	1(2)
C(40)	22(2)	31(2)	29(2)	7(2)	6(2)	5(2)
C(41)	19(2)	90(3)	30(2)	-10(2)	-1(2)	7(2)
C(42)	20(2)	20(2)	14(2)	-3(1)	4(1)	2(2)
C(43)	25(2)	20(2)	17(2)	3(1)	3(1)	3(1)
C(44)	23(2)	31(2)	19(2)	2(2)	1(2)	-6(2)
C(45)	44(2)	41(2)	21(2)	5(2)	7(2)	-8(2)
C(46)	19(2)	14(2)	15(2)	-1(1)	4(1)	-3(1)
C(47)	18(2)	18(2)	13(2)	1(1)	3(1)	0(1)
C(48)	15(2)	21(2)	24(2)	-4(1)	6(1) 7(2)	-2(1)
C(49)	23(2)	25(2)	24(2)	-6(2)	/(2)	-1(2)
U(30)	21(2)	11(2)	23(2)	2(1)	3(1)	1(1)

C(51)	31(2)	26(2)	27(2)	5(2)	10(2)	0(2)	
C(52)	27(2)	30(2)	35(2)	15(2)	5(2)	1(2)	
C(53)	40(2)	36(2)	53(3)	18(2)	7(2)	6(2)	
C(19)	14(2)	15(2)	10(1)	-2(1)	1(1)	-2(1)	
C(31)	15(2)	31(2)	21(2)	6(2)	5(1)	8(1)	
C(28)	16(2)	18(2)	15(2)	1(1)	3(1)	2(1)	

Table 15. Hydrogen coordinates (x 10⁴) and isotropic displacement parameters (Å 2 x 10 ³) for{NBu₄} {[Ph₃BP^{p-iPr2}]RhX(NBD)}.

Х	У	Z	U(eq)

H(2)	3405	7206	-353	26
H(3)	3799	8416	-875	31
H(4)	4437	9576	-237	31
H(5)	4715	9489	932	32
H(6)	4353	8270	1453	26
H(8)	5294	6720	1084	28
H(0)	6474	6186	1864	34
H(10)	6286	5502	2860	30
H(10) H(11)	4020	5602	2112	37
H(12)	4920	5002 6117	2222	28
$\Pi(12)$ $\Pi(14)$	3729	5422	522	20
$\Pi(14)$ $\Pi(15)$	4442	3422	240	21
$\Pi(13)$	4080	4401	-349	21
$\Pi(10)$	2080	4420	-1014	22
H(1/)	1039	5548	-/30	22
H(18)	1994	6292	128	19
H(20)	2405	5809	15/3	20
H(21)	1237	6114	2035	20
H(23)	1421	8600	1542	19
H(24)	2620	8282	1116	19
H(25)	-1217	7461	1512	24
H(26A)	-30	7851	685	40
H(26B)	-719	8494	883	40
H(26C)	-1042	7705	394	40
H(27A)	-1151	6274	857	42
H(27B)	-664	6059	1613	42
H(27C)	-116	6270	1060	42
H(29A)	-836	8746	2756	33
H(29B)	-1201	8877	1966	33
H(29C)	-748	9656	2418	33
H(30A)	848	9762	2742	31
H(30B)	1426	8937	2690	31
H(30C)	797	8948	3206	31
H(32)	1570	7720	3735	22
H(33)	1325	5132	3911	25
H(34A)	2095	6237	4763	27
H(34B)	1280	5851	5031	27
H(35)	1018	7454	4803	23
H(36)	-467	6779	4382	23
H(37)	-288	5386	3853	26
H(38A)	5730	8764	4092	20
H(38B)	5726	9277	3416	20
$H(30\Delta)$	4942	7639	3410	33
H(30R)	4852	8262	2777	33
H(40A)	4052	8655	3058	33
H(40R)	4217	0205	3336	22
$\Pi(40D)$ $\Pi(41A)$	2199	9293	3330	33 71
$\Pi(41A)$ $\Pi(41D)$	2026	8574	2042	71
$\Pi(41D)$ $\Pi(41C)$	2020	0JJY 7675	2000	/1
$\Pi(41C)$ $\Pi(42A)$	5505	/0/3	3228	/1
$\Pi(42A)$	/101	/031	2019	21
$\Pi(42\mathbf{B})$	0130	/919	2380	21
H(43A)	/329	9310	2/30	25
H(43B)	6301	9437	2544	25
H(44A)	6211	8680	1527	30
H(44B)	7234	8512	1716	30

H(45A)	6474	10178	1502	53
H(45B)	6912	9692	970	53
H(45C)	7493	9999	1675	53
H(46A)	7197	8879	4436	19
H(46B)	7245	9411	3776	19
H(47A)	8349	8044	4351	20
H(47B)	8281	8298	3579	20
H(48A)	8786	9670	3876	24
H(48B)	8723	9524	4641	24
H(49A)	9878	8562	4800	35
H(49B)	10171	9440	4515	35
H(49C)	9918	8639	4024	35
H(50A)	7212	7136	3802	22
H(50B)	6193	7030	3539	22
H(51A)	6011	7545	4616	33
H(51B)	7043	7518	4869	33
H(52A)	6004	6052	4386	37
H(52B)	6382	6241	5165	37
H(53A)	7424	5846	4223	65
H(53B)	7241	5205	4788	65
H(53C)	7809	6046	5001	65
H(31)	1739	6331	3194	27
H(28)	189	9019	1778	20

Empirical formula C ₁₀₂ H ₁₂₂ B ₂ BrN ₃ OP ₂ Pt			
Formula weight	1764.59		
Crystal Habit	plate		
Crystal Color	colorless		
Crystal size	0.27 x 0.26 x 0.13 mm ³		
D	ata Collection		
Type of diffractometer	CCD area detector		
Wavelength	0.71073 Å		
Data collection temperature	98(2) K		
Unit cell dimensions	a = 10.1511(18) Å b = 17.534(3) Å c = 24.912(4) Å	$\alpha = 76.949(3)^{\circ}$ $\beta = 85.774(3)^{\circ}$ $\gamma = 83.253(3)^{\circ}$	
Volume	4284.4(13) Å ³		
Z	2		
Crystal system	Triclinic		
Space group	P-1		
Density (calculated)	ted) 1.368 Mg/m^3		
F(000)	1832		
θ range for data collection	1.30 to 28.59°		
Completeness to $\theta = 28.59^{\circ}$	91.7%		
Index ranges	$-13 \le h \le 13, -23 \le k \le 23, -33$	$\leq l \leq 32$	
Reflections collected	89517		
Independent reflections	20077 [R(int) = 0.0702]		
Absorption coefficient	2.193 mm ⁻¹		
Absorption correction	None		
Structure s	olution and refinement		
Structure solution program	SHELXS-97 (Sheldrick, 1990))	
Primary solution method	direct methods		
Secondary solution method	differential Fourier Map		
Hydrogen placement	calculated positions		
Structure refinement program	SHELXL-97 (Sheldrick, 1997))	
Refinement method	d Full-matrix least-squares on F ²		
Data / restraints / parameters 20077 / 0 / 1013			
Goodness-of-fit on F ²	1.103		
Final R indices [I> $2\sigma(I)$]	R1 = 0.0413, wR2 = 0.0947		

Table 16.	Crystal data and structure refinement	nt for {ASN} ₂ {[Ph ₃ BP	$^{m-Ph2}]_2$ PtMe ₂ $\}.$

$P = (Fo^2 + 2Fc^2)/3$	
Max shift/error	2.395
Average shift/error	0.045
Largest diff. peak and hole	2.339 and -1.763 e·Å ⁻³

The complex co-crystallized with [ASN]Br and one highly disordered molecule of Et_2O .

	Х	У	Z	U(eq)
D ₁ (1)	10120/1)	0.407(1)	2225(1)	12(1)
Pt(1)	10128(1)	949/(1)	3235(1)	13(1)
B(1)	6405(4)	11/48(3)	795(2)	22(1)
C(1)	11053(4)	10408(2)	3431(2)	24(1)
C(2)	11622(4)	8741(2)	3719(2)	19(1)
P(1)	8598(1)	10426(1)	2768(1)	14(1)
C(3)	6407(4)	11635(3)	157(2)	26(1)
C(4)	7209(5)	12067(3)	-263(2)	36(1)
C(5)	7317(5)	11946(3)	-798(2)	44(1)
C(6)	6609(5)	11397(3)	-939(2)	36(1)
C(7)	5789(5)	10980(3)	-546(2)	33(1)
C(8)	5706(4)	11095(2)	-4(2)	28(1)
C(9)	4985(4)	11535(2)	1137(2)	21(1)
C(10)	4719(4)	10747(2)	1322(2)	25(1)
C(11)	3560(4)	10522(2)	1614(2)	25(1)
C(12)	2597(4)	11090(3)	1748(2)	25(1)
C(13)	2812(4)	11869(3)	1579(2)	24(1)
C(14)	3979(4)	12091(2)	1282(2)	19(1)
C(15)	6696(4)	12659(2)	790(2)	28(1)
C(16)	5932(5)	13306(3)	481(3)	47(2)
C(17)	6189(6)	14093(3)	465(3)	58(2)
C(18)	7220(7)	14251(3)	730(3)	54(2)
C(19)	7990(7)	13636(3)	1031(2)	47(2)
C(20)	7713(5)	12860(3)	1060(2)	32(1)
C(21)	7570(4)	11123(2)	1130(2)	17(1)
C(22)	7605(3)	11024(2)	1706(2)	15(1)
C(23)	8530(4)	10501(2)	2030(2)	14(1)
C(24)	9513(3)	10060(2)	1769(2)	15(1)
C(25)	9527(4)	10148(2)	1201(2)	18(1)
C(26)	8571(4)	10667(2)	890(2)	18(1)
C(20)	8757(4)	11460(2)	2784(2)	18(1)
C(28)	9405(4)	11941(2)	2345(2)	21(1)
C(29)	9584(4)	12711(2)	2361(2)	25(1)
C(30)	9125(4)	12711(2) 13012(2)	2301(2) 2821(2)	26(1)
C(31)	8495(4)	12537(2)	3260(2)	25(1)
C(31)	8316(4)	12337(2) 11768(2)	3200(2) 3243(2)	23(1) 21(1)
C(32)	6946(3)	10204(2)	32+3(2) 3008(2)	15(1)
C(33)	5764(4)	10294(2) 10343(2)	3098(2)	13(1) 18(1)
C(34)	4577(A)	10343(2) 10220(2)	2032(2) 3142(2)	21(1)
C(33)	4377(4)	10220(2) 10062(2)	3142(2) 3712(2)	21(1) 22(1)
C(30) C(37)	4331(4) 5710(4)	10003(2) 10017(2)	$\frac{3712(2)}{3082(2)}$	23(1) 22(1)
C(37)	5/19(4)	10017(2) 10120(2)	3962(2)	23(1) 10(1)
U(30)	0908(4)	10120(2)	$\frac{3077(2)}{2101(2)}$	19(1)
D(2)	9/09(4)	3033(2)	2191(2) 2151(1)	10(1) 12(1)
$\Gamma(2)$	924/(1)	$\frac{83}{6(1)}$	5151(1) 1027(2)	12(1)
C(39)	82/4(4)	6046(2)	1957(2)	18(1)
C(40)	/556(4)	6/96(2)	1815(2)	18(1)
C(41)	6268(4)	6924(2)	1621(2)	23(1)

Table 17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å²x 10³) for $\{ASN\}_2\{[Ph_3BP^{m-Ph_2}]_2PtMe_2\}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

C(12)	5(50(4)	(205(2))	1521(2)	$\mathbf{O}(1)$
C(42)	5652(4)	6305(3)	1531(2)	26(1)
C(43)	6344(4)	5558(3)	1636(2)	26(1)
C(44)	7618(4)	5431(2)	1833(2)	21(1)
C(45)	10736(4)	5424(2)	1751(2)	17(1)
C(46)	11176(4)	5884(2)	1246(2)	23(1)
C(47)	11994(5)	5574(3)	860(2)	28(1)
C(48)	12412(5)	4767(3)	962(2)	31(1)
C(40)	12 + 12(5) 11072(5)	4707(3)	1446(2)	20(1)
C(49)	11975(3)	4293(3)	1440(2)	30(1)
C(50)	11157(4)	4616(2)	1833(2)	23(1)
C(51)	9692(4)	5228(2)	2803(2)	16(1)
C(52)	10870(4)	4897(2)	3067(2)	20(1)
C(53)	10876(4)	4377(2)	3578(2)	23(1)
C(54)	9677(4)	4176(2)	3855(2)	23(1)
C(55)	8500(4)	4496(2)	3613(2)	24(1)
C(56)	8514(4)	5016(2)	3098(2)	20(1)
C(57)	10424(4)	6602(2)	2302(2)	15(1)
C(58)	9690(3)	7124(2)	2502(2) 2596(2)	14(1)
C(50)	10222(4)	7124(2)	2570(2)	17(1)
C(39)	10223(4)	7743(2)	2/44(1)	15(1)
C(60)	11549(4)	7870(2)	2589(2)	15(1)
C(61)	12313(4)	7360(2)	2307(2)	17(1)
C(62)	11759(4)	6746(2)	2170(2)	17(1)
C(63)	9005(4)	7722(2)	3837(2)	18(1)
C(64)	8989(4)	6909(3)	3917(2)	26(1)
C(65)	8661(5)	6466(3)	4437(2)	35(1)
C(66)	8357(5)	6825(3)	4880(2)	40(1)
C(67)	8417(5)	7620(3)	4807(2)	39(1)
C(68)	8740(4)	8068(3)	4287(2)	28(1)
C(60)	7587(4)	8008(3)	$\frac{4207(2)}{2882(2)}$	$\frac{20(1)}{14(1)}$
C(09)	(458(4)	8443(2)	2003(2)	14(1)
C(70)	6458(4)	8311(2)	3232(2)	1/(1)
C(71)	5214(4)	8386(2)	3017(2)	21(1)
C(72)	5077(4)	8594(2)	2454(2)	21(1)
C(73)	6195(4)	8737(2)	2096(2)	18(1)
C(74)	7439(4)	8660(2)	2312(2)	15(1)
N(1)	1621(4)	2218(2)	9990(1)	24(1)
C(75)	764(5)	2718(3)	10318(2)	42(1)
C(76)	956(6)	3565(3)	10040(2)	45(1)
C(77)	2344(6)	3514(3)	9748(2)	38(1)
C(78)	2862(4)	2644(2)	9871(2)	26(1)
C(79)	1025(5)	2011(2) 2181(3)	9459(2)	28(1)
C(79)	1768(5)	1451(3)	9+39(2) 0212(2)	20(1)
C(80)	1/08(3)	1431(3)	9312(2)	32(1)
C(81)	1858(5)	869(3)	9868(2)	38(1)
C(82)	1896(5)	1360(3)	10297(2)	31(1)
N(2)	3507(3)	5920(2)	4021(2)	24(1)
C(83)	4001(4)	3560(2)	2959(2)	24(1)
C(84)	5217(5)	3915(3)	2664(2)	37(1)
C(85)	5494(6)	3482(3)	2193(2)	49(1)
C(86)	5261(5)	2645(3)	2457(2)	30(1)
C(87)	4785(4)	2212(2)	3487(2)	24(1)
C(88)	3547(5)	2102(3)	3876(2)	$\frac{2}{30(1)}$
C(89)	2361(5)	2258(3)	3400(2)	36(1)
C(0)	2301(3)	2230(3)	3477(2)	22(1)
U(90)	298/(3)	2341(3)	2919(2)	33(1)
IN(3)	4264(3)	2688(2)	2948(1)	22(1)
C(91)	4887(4)	5831(2)	4246(2)	25(1)
C(92)	5755(4)	6202(2)	3751(2)	25(1)
C(93)	4985(4)	6216(3)	3236(2)	26(1)
C(94)	3794(4)	5770(3)	3454(2)	26(1)

2797(4)	6728(2)	4023(2)	28(1)
2201(4)	6664(3)	4613(2)	27(1)
2134(5)	5770(3)	4845(2)	30(1)
2570(4)	5385(3)	4372(2)	27(1)
5129(1)	3704(1)	4293(1)	24(1)
4678(9)	8179(5)	4712(4)	87(3)
3609(13)	8487(5)	5058(4)	93(4)
1190(40)	10366(8)	4943(7)	560(50)
2969(14)	8974(14)	5167(9)	406(16)
1710(30)	9540(30)	5086(9)	910(60)
	$2797(4) \\2201(4) \\2134(5) \\2570(4) \\5129(1) \\4678(9) \\3609(13) \\1190(40) \\2969(14) \\1710(30)$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	$\begin{array}{ccccccc} 2797(4) & 6728(2) & 4023(2) \\ 2201(4) & 6664(3) & 4613(2) \\ 2134(5) & 5770(3) & 4845(2) \\ 2570(4) & 5385(3) & 4372(2) \\ 5129(1) & 3704(1) & 4293(1) \\ 4678(9) & 8179(5) & 4712(4) \\ 3609(13) & 8487(5) & 5058(4) \\ 1190(40) & 10366(8) & 4943(7) \\ 2969(14) & 8974(14) & 5167(9) \\ 1710(30) & 9540(30) & 5086(9) \\ \end{array}$

Pt(1)-C(1)	2.107(4)	C(22)-H(22)	0.9500
Pt(1)-C(2)	2.141(4)	C(23)-C(24)	1.402(5)
Pt(1)-P(1)	2.2885(10)	C(24) - C(25)	1.387(5)
Pt(1)-P(2)	2.3096(10)	C(24)-H(24)	0.9500
B(1)-C(21)	1.651(6)	C(25)-C(26)	1.399(5)
B(1)-C(9)	1.656(6)	C(25)-H(25)	0.9500
B(1)-C(3)	1 645(7)	C(26) - H(26)	0.9500
B(1)-C(15)	1 655(6)	C(27)-C(28)	1 394(6)
C(1)-H(1A)	0.9800	C(27)-C(32)	1 395(6)
C(1)-H(1B)	0.9800	C(28)-C(29)	1 393(5)
C(1)-H(1C)	0.9800	C(28) - H(28)	0.9500
C(2)-H(2A)	0.9800	C(29)-C(30)	1 396(6)
C(2) - H(2B)	0.9800	C(29)-H(29)	0.9500
C(2)-H(2C)	0.9800	C(30)-C(31)	1 381(6)
P(1)-C(23)	1 819(4)	C(30)-H(30)	0.9500
P(1)-C(33)	1.828(4)	C(31)-C(32)	1 393(5)
P(1)-C(27)	1 848(4)	C(31)-H(31)	0.9500
C(3)-C(8)	1 392(6)	C(32)-H(32)	0.9500
C(3) - C(4)	1 411(6)	C(32) - C(34)	1 397(5)
C(4)-C(5)	1 391(7)	C(33)-C(38)	1.097(5) 1.403(5)
C(4)-H(4)	0.9500	C(34)-C(35)	1 395(5)
C(5)-C(6)	1 385(7)	C(34)-H(34)	0.9500
C(5) - H(5)	0.9500	C(35)-C(36)	1 382(6)
C(6)-C(7)	1 375(7)	C(35) - H(35)	0.9500
C(6)-H(6)	0.9500	C(36)-C(37)	1 391(6)
C(7)-C(8)	1404(7)	C(36)-H(36)	0.9500
C(7)-H(7)	0.9500	C(37)-C(38)	1 387(5)
C(8)-H(8)	0.9500	C(37)-H(37)	0.9500
C(9)-C(14)	1 413(6)	C(38)-H(38)	0.9500
C(9)-C(10)	1 407(6)	B(2)-C(45)	1 650(6)
C(10)-C(11)	1 386(6)	B(2)-C(39)	1 656(6)
C(10)-H(10)	0.9500	B(2)-C(51)	1 653(6)
C(11)-C(12)	1 391(6)	B(2)-C(57)	1 653(5)
C(11)-H(11)	0.9500	P(2)-C(59)	1.825(4)
C(12)-C(13)	1 373(6)	P(2)-C(69)	1 840(4)
C(12)-H(12)	0.9500	P(2)-C(63)	1 848(4)
C(13)-C(14)	1.396(6)	C(39)-C(40)	1.407(5)
C(13)-H(13)	0.9500	C(39)-C(44)	1 413(5)
C(14)-H(14)	0.9500	C(40)-C(41)	1.403(5)
C(15)-C(20)	1.393(7)	C(40)-H(40)	0.9500
C(15)-C(16)	1.403(6)	C(41)-C(42)	1.383(6)
C(16)-C(17)	1.425(8)	C(41)-H(41)	0.9500
C(16)-H(16)	0.9500	C(42)-C(43)	1.390(6)
C(17)-C(18)	1.363(10)	C(42)-H(42)	0.9500
C(17)-H(17)	0.9500	C(43)-C(44)	1.392(6)
C(18)-C(19)	1.364(9)	C(43)-H(43)	0.9500
C(18)-H(18)	0.9500	C(44)-H(44)	0.9500
C(19)-C(20)	1.406(6)	C(45)-C(50)	1.404(5)
C(19)-H(19)	0.9500	C(45)-C(46)	1.404(6)
С(20)-Н(20)	0.9500	C(46)-C(47)	1.387(6)
C(21)-C(26)	1.402(5)	C(46)-H(46)	0.9500
C(21)-C(22)	1.407(5)	C(47)-C(48)	1.399(6)
C(22)-C(23)	1.397(5)	C(47)-H(47)	0.9500

Table 18. Bond lengths [Å] and angles [°] for $\{ASN\}_2\{[Ph_3BP^{m-Ph_2}]_2PtMe_2\}$.

C(48)-C(49)	1.378(6)	C(76)-H(76A)	0.9900
C(48)-H(48)	0.9500	C(76)-H(76B)	0.9900
C(49)-C(50)	1.397(6)	C(77)-C(78)	1.524(6)
C(49)-H(49)	0.9500	C(77)-H(77A)	0.9900
C(50)-H(50)	0.9500	C(77)-H(77B)	0.9900
C(51)-C(56)	1.400(5)	C(78)-H(78A)	0.9900
C(51)-C(52)	1.408(5)	C(78)-H(78B)	0.9900
C(52)-C(53)	1.388(6)	C(79)-C(80)	1.511(6)
C(52)-H(52)	0.9500	C(79)-H(79A)	0.9900
C(53)-C(54)	1.396(6)	C(79)-H(79B)	0.9900
C(53)-H(53)	0.9500	C(80)-C(81)	1.526(7)
C(54)-C(55)	1.379(6)	C(80)-H(80A)	0.9900
C(54)-H(54)	0.9500	C(80)-H(80B)	0.9900
C(55)-C(56)	1.397(6)	C(81)-C(82)	1.522(7)
C(55)-H(55)	0.9500	C(81)-H(81A)	0.9900
C(56)-H(56)	0.9500	C(81)-H(81B)	0.9900
C(57)-C(58)	1.411(5)	C(82)-H(82A)	0.9900
C(57)-C(62)	1.409(5)	C(82)-H(82B)	0.9900
C(58)-C(59)	1.402(5)	N(2)-C(94)	1.496(6)
C(58)-H(58)	0.9500	N(2)-C(98)	1.505(5)
C(59)- $C(60)$	1 402(5)	N(2)-C(95)	1 513(5)
C(60)- $C(61)$	1.390(5)	N(2)-C(91)	1.525(5)
C(60)-H(60)	0.9500	C(83)-C(84)	1.513(6)
C(61)- $C(62)$	1 389(5)	C(83)-N(3)	1 526(5)
C(61)-H(61)	0.9500	C(83)-H(83A)	0 9900
C(62)-H(62)	0.9500	C(83)-H(83B)	0.9900
C(63)- $C(68)$	1 387(6)	C(84)-C(85)	1 529(7)
C(63)- $C(64)$	1 395(6)	C(84)-H(84A)	0.9900
C(64)- $C(65)$	1 391(6)	C(84)-H(84B)	0.9900
C(64)-H(64)	0.9500	C(85)-C(86)	1 505(7)
C(65)-C(66)	1 388(8)	C(85) - H(85A)	0.9900
C(65)- $H(65)$	0.9500	C(85)-H(85B)	0.9900
C(66)- $C(67)$	1 372(8)	C(86)-N(3)	1 537(5)
C(66)- $H(66)$	0.9500	C(86)-H(86A)	0.9900
C(67)- $C(68)$	1 393(6)	C(86)-H(86B)	0.9900
C(67)-C(00)	0.9500	C(87)-N(3)	1 508(5)
C(68)-H(68)	0.9500	C(87)-C(88)	1.500(5)
C(60)-C(70)	1 396(5)	C(87)-H(87A)	0.0000
C(69)-C(74)	1.390(3)	C(87)-H(87R)	0.9900
C(09)-C(74) C(70)-C(71)	1 300(5)	C(87)-G(89)	0.9900 1 5/3(7)
C(70) + C(71) C(70) + H(70)	0.9500	C(88) + C(89)	1.343(7)
C(70)-11(70) C(71) $C(72)$	1 280(6)	C(88) - H(88A)	0.9900
C(71)- $C(72)C(71)$ $H(71)$	0.9500	C(80) - H(80B) C(80) C(90)	0.9900
$C(71)-\Pi(71)$ C(72) $C(72)$	1.401(6)	C(89) - C(90)	1.316(7)
C(72)- $C(73)$	0.0500	$C(89) - \Pi(89A)$	0.9900
$C(72) - \Pi(72)$ $C(72) - \Omega(74)$	0.9300	$C(09) - \Pi(09B)$	0.9900
C(73)-C(74) C(72) $U(72)$	1.368(3)	C(90) - N(3)	1.309(3)
$C(73)-\Pi(73)$	0.9500	C(90) - H(90A)	0.9900
U(74)-H(74) V(1) C(75)	0.9500	C(90)-H(90B) C(01) $C(02)$	0.9900
N(1)-C(73) N(1)-C(79)	1.493(6)	C(91)-C(92)	1.527(6)
N(1) - C(70)	1.313(0)	$C(91) - \Pi(91A)$	0.9900
N(1)-C(79) N(1)-C(82)	1.514(5)	C(91)-H(91B)	0.9900
$N(1)-C(\delta 2)$	1.529(5)	C(92) - C(93)	1.544(6)
U(75)-U(76)	1.519(8)	C(92)-H(92A)	0.9900
U(75)-H(75A)	0.9900	C(92) - H(92B)	0.9900
U(7)-H(7)B)	0.9900	C(93)-C(94)	1.516(6)
C(76)-C(77)	1.540(8)	C(93)-H(93A)	0.9900

C(93)-H(93B)	0.9900	C(23)-P(1)-Pt(1)	117.59(12)
C(94)-H(94A)	0.9900	C(33)-P(1)-Pt(1)	109.60(13)
C(94)-H(94B)	0.9900	C(27)-P(1)-Pt(1)	116.34(12)
C(95)-C(96)	1.534(6)	C(8)-C(3)-C(4)	115.4(4)
C(95)-H(95A)	0.9900	C(8)-C(3)-B(1)	124.0(4)
C(95)-H(95B)	0.9900	C(4)-C(3)-B(1)	120.4(4)
C(96)-C(97)	1.550(6)	C(5)-C(4)-C(3)	122.2(5)
C(96)-H(96A)	0 9900	C(5)-C(4)-H(4)	118.9
C(96)-H(96B)	0.9900	C(3)-C(4)-H(4)	118.9
C(97)- $C(98)$	1 501(6)	C(6)-C(5)-C(4)	120.4(4)
C(97)-H(97A)	0.9900	C(6)-C(5)-H(5)	119.8
C(97)-H(97B)	0.9900	C(4)-C(5)-H(5)	119.8
C(98)-H(98A)	0.9900	C(5)-C(6)-C(7)	119.2(5)
C(98)-H(98B)	0.9900	C(5) - C(6) - H(6)	120.4
C(102) - C(101)	1.466(13)	C(7)-C(6)-H(6)	120.4
C(102)-C(101) C(102)-H(10A)	0.9800	C(7)-C(0)-H(0)	120.4 120.0(5)
$C(102)$ - $\Pi(10R)$ $C(102)$ $\Pi(10R)$	0.9800	C(6) - C(7) - C(8)	120.0(3)
$C(102)$ - $\Pi(10D)$ $C(102)$ $\Pi(10C)$	0.9800	C(0)-C(7)-H(7)	120.0
$C(102)$ - $\Pi(10C)$ C(101) O(1)	1.082(15)	C(8)-C(7)-H(7) C(3)-C(8)-C(7)	120.0 122.7(4)
C(101) - O(1) C(101) - U(10D)	0.0000	C(3)-C(8)-C(7)	122.7(4)
$C(101) - \Pi(10D)$ $C(101) - \Pi(10D)$	0.9900	$C(3)-C(8)-\Pi(8)$	110.0
$C(101) - \Pi(10E)$ C(100) C(00)	1.45(4)	C(14) C(0) C(10)	110.0 114.4(4)
C(100) - C(99)	1.43(4)	C(14) - C(9) - C(10)	114.4(4) 125.2(2)
C(100)-H(10F) C(100)-H(10C)	0.9911	C(14)-C(9)-B(1)	125.3(3) 120.2(4)
C(100)-H(10G)	0.9929	C(10)-C(9)-B(1)	120.2(4)
C(100)-H(10H)	0.9930	C(11) - C(10) - C(9)	123.6(4)
O(1) - C(99)	1.52(3)	C(11)-C(10)-H(10)	118.2
C(99)-H(99A)	0.9900	C(9)-C(10)-H(10)	118.2
С(99)-Н(99В)	0.9900	C(10) - C(11) - C(12)	119.9(4)
$C(1)$ $D_1(1)$ $C(2)$	04.10(15)	C(10)-C(11)-H(11)	120.0
C(1)-Pt(1)-C(2)	84.19(15)	C(12)-C(11)-H(11)	120.0
C(1)-Pt(1)-P(1)	88.94(11)	C(13)-C(12)-C(11)	118.7(4)
C(2)-Pt(1)-P(1)	172.86(10)	C(13)-C(12)-H(12)	120.6
C(1)-Pt(1)-P(2)	170.80(12)	C(11)-C(12)-H(12)	120.6
C(2)-Pt(1)-P(2)	87.54(10)	C(12)-C(13)-C(14)	121.0(4)
P(1)-Pt(1)-P(2)	99.17(3)	C(12)-C(13)-H(13)	119.5
C(21)-B(1)-C(9)	105.8(3)	C(14)-C(13)-H(13)	119.5
C(21)-B(1)-C(3)	109.8(3)	C(13)-C(14)-C(9)	122.3(4)
C(9)-B(1)-C(3)	111.2(3)	C(13)-C(14)-H(14)	118.9
C(21)-B(1)-C(15)	109.4(3)	C(9)-C(14)-H(14)	118.9
C(9)-B(1)-C(15)	111.1(3)	C(20)-C(15)-C(16)	114.1(4)
C(3)-B(1)-C(15)	109.5(3)	C(20)-C(15)-B(1)	125.0(4)
Pt(1)-C(1)-H(1A)	109.5	C(16)-C(15)-B(1)	120.9(5)
Pt(1)-C(1)-H(1B)	109.5	C(15)-C(16)-C(17)	121.4(6)
H(1A)-C(1)-H(1B)	109.5	C(15)-C(16)-H(16)	119.3
Pt(1)-C(1)-H(1C)	109.5	C(17)-C(16)-H(16)	119.3
H(1A)-C(1)-H(1C)	109.5	C(18)-C(17)-C(16)	121.7(5)
H(1B)-C(1)-H(1C)	109.5	C(18)-C(17)-H(17)	119.2
Pt(1)-C(2)-H(2A)	109.5	C(16)-C(17)-H(17)	119.2
Pt(1)-C(2)-H(2B)	109.5	C(17)-C(18)-C(19)	118.6(5)
H(2A)-C(2)-H(2B)	109.5	C(17)-C(18)-H(18)	120.7
Pt(1)-C(2)-H(2C)	109.5	C(19)-C(18)-H(18)	120.7
H(2A)-C(2)-H(2C)	109.5	C(18)-C(19)-C(20)	119.8(6)
H(2B)-C(2)-H(2C)	109.5	C(18)-C(19)-H(19)	120.1
C(23)-P(1)-C(33)	109.43(17)	C(20)-C(19)-H(19)	120.1
C(23)-P(1)-C(27)	100.84(17)	C(15)-C(20)-C(19)	124.5(5)
C(33)-P(1)-C(27)	101.64(16)	C(15)-C(20)-H(20)	117.8

C(19)-C(20)-H(20)	117.8	C(45)-B(2)-C(51)	110.8(3)
C(26)-C(21)-C(22)	115.1(3)	C(39)-B(2)-C(51)	110.1(3)
C(26)-C(21)-B(1)	125.5(4)	C(45)-B(2)-C(57)	110.0(3)
C(22)-C(21)-B(1)	119.4(3)	C(39)-B(2)-C(57)	114.4(3)
C(23)-C(22)-C(21)	124.0(3)	C(51)-B(2)-C(57)	104.6(3)
C(23)-C(22)-H(22)	118.0	C(59)-P(2)-C(69)	101 54(17)
C(21)-C(22)-H(22)	118.0	C(59)-P(2)-C(63)	$104\ 23(17)$
C(24)-C(23)-C(22)	118 5(3)	C(69)-P(2)-C(63)	100.53(17)
C(24)-C(23)-P(1)	118 5(3)	C(59)-P(2)-Pt(1)	11742(12)
C(22)-C(23)-P(1)	122 7(3)	C(69)-P(2)-Pt(1)	120.45(11)
C(22) = C(23) + C(23)	119 3(3)	C(63)-P(2)-Pt(1)	11031(13)
C(25) - C(24) - C(25)	120.3	C(40)-C(39)-C(44)	115.0(4)
C(23) - C(24) - H(24)	120.3	C(40) - C(39) - B(2)	1261(3)
C(24)-C(25)-C(26)	120.5	C(40) = C(39) = B(2)	120.1(3) 118 9(3)
C(24)-C(25)-C(20)	110.7	C(41)-C(40)-C(39)	122.8(4)
C(24)-C(25)-H(25)	119.7	C(41)-C(40)-U(57)	118.6
C(25)-C(26)-C(21)	122 A(A)	C(39) - C(40) - H(40)	118.6
C(25)-C(26)-H(26)	1122.4(4)	C(42)-C(41)-C(40)	120.5(4)
C(21) - C(26) - H(26)	118.8	C(42) - C(41) - C(40) C(42) - C(41) - H(41)	110.8
$C(21)$ - $C(20)$ - $\Pi(20)$ C(28) $C(27)$ $C(22)$	118 1(2)	$C(42)$ - $C(41)$ - $\Pi(41)$	119.8
C(28) - C(27) - C(32) C(28) - C(27) - D(1)	1202(3)	$C(40)-C(41)-\Pi(41)$ C(41)-C(42)-C(43)	119.0 118.2(4)
C(20)-C(27)-I(1) C(22)-C(27)-I(1)	120.2(3) 121 6(3)	C(41) - C(42) - C(43) C(41) - C(42) - H(42)	110.2(4)
$C(32)-C(27)-\Gamma(1)$	121.0(3)	$C(41) - C(42) - \Pi(42)$ $C(42) - C(42) - \Pi(42)$	120.9
C(27) - C(28) - C(29)	121.0(4)	$C(43)-C(42)-\Pi(42)$	120.9 121.2(4)
C(27)- $C(28)$ - $H(28)$	119.5	C(44) - C(43) - C(42) C(44) - C(43) - U(42)	121.2(4)
$C(29)$ - $C(20)$ - $\Pi(20)$ C(20) $C(20)$	119.3 120.2(4)	C(44) - C(43) - H(43)	119.4
C(30)-C(29)-C(28) C(20)-C(20)-H(20)	110.0	$C(42) - C(43) - \Pi(43)$ C(42) - C(44) - C(20)	117.4 122.2(4)
C(28)-C(29)-H(29)	119.9	C(43)-C(44)-C(59) C(43)-C(44)-H(44)	122.3(4)
C(20)-C(20)-C(20)	119.9 119.2(A)	C(43)-C(44)-H(44)	118.9
C(31) - C(30) - C(29) C(31) - C(30) - H(30)	120 4	C(59)-C(44)-H(44)	116.9 115.1(A)
C(29) - C(30) - H(30)	120.4	C(50)-C(45)-B(2)	113.1(4) 124.6(3)
C(30) - C(31) - C(32)	120.4	C(46)-C(45)-B(2)	124.0(3) 120 3(3)
C(30)-C(31)-H(31)	110.8	C(40) - C(45) - D(2)	120.3(3) 123 0(4)
C(32)-C(31)-H(31)	119.8	C(47)-C(46)-C(45)	118 5
C(31)-C(32)-C(27)	121 1(4)	C(45)-C(46)-H(46)	118.5
C(31) - C(32) - U(32)	110 5	C(45) - C(47) - C(48)	120.1(4)
C(27) - C(32) - H(32)	119.5	C(46)-C(47)-U(48) C(46)-C(47)-U(47)	120.1(4)
C(34)-C(33)-C(38)	118.8(3)	C(48)-C(47)-H(47)	120.0
C(34)-C(33)-P(1)	126 6(3)	C(49)-C(48)-C(47)	120.0 118 6(4)
C(38)-C(33)-P(1)	114 6(3)	C(49)-C(48)-U(48)	120.7
C(33)-C(34)-C(35)	119.8(4)	C(47) - C(48) - H(48)	120.7
C(33)-C(34)-H(34)	120.1	C(48)-C(49)-C(50)	120.7 120.5(4)
C(35)-C(34)-H(34)	120.1	C(48)-C(49)-C(50)	110 7
C(36)-C(35)-C(34)	120.1 120.7(4)	C(50)-C(49)-H(49)	119.7
C(36) - C(35) - H(35)	110 7	C(40)-C(50)-C(45)	117.7 122.6(A)
C(34)-C(35)-H(35)	119.7	C(49)-C(50)-C(45)	118 7
C(35)-C(36)-C(37)	120 1(4)	C(45) - C(50) - H(50)	118.7
C(35)-C(36)-H(36)	110.0	C(56)-C(51)-C(52)	115.7 115 $A(A)$
C(37)-C(36)-H(36)	119.9	C(56)-C(51)-B(2)	124.8(3)
C(38)-C(37)-C(36)	119 5(4)	C(52)- $C(51)$ - $B(2)$	119 8(3)
C(38)-C(37)-H(37)	120.2	C(52)-C(51)-D(2)	1227(4)
C(36)-C(37)-H(37)	120.2	C(53)-C(52)-H(52)	118.6
C(37)-C(38)-C(33)	121 0(4)	C(51)-C(52)-H(52)	118.6
C(37)-C(38)-H(38)	119.5	C(52)-C(53)-C(54)	119 9(4)
C(33)-C(38)-H(38)	119.5	C(52)-C(53)-H(53)	120.1
C(45)-B(2)-C(39)	107 1(3)	C(54)-C(53)-H(53)	120.1

C(55)-C(54)-C(53)	119.2(4)	C(73)-C(72)-H(72)	120.0
C(55)-C(54)-H(54)	120.4	C(74)-C(73)-C(72)	119.5(4)
C(53)-C(54)-H(54)	120.4	C(74)-C(73)-H(73)	120.2
C(54)-C(55)-C(56)	120.1(4)	C(72)-C(73)-H(73)	120.2
C(54)-C(55)-H(55)	119.9	C(73)-C(74)-C(69)	120.8(3)
C(56)-C(55)-H(55)	119.9	C(73)-C(74)-H(74)	119.6
C(55)-C(56)-C(51)	122.7(4)	C(69)-C(74)-H(74)	119.6
C(55)-C(56)-H(56)	118.7	C(75)-N(1)-C(78)	101.7(3)
C(51)-C(56)-H(56)	118.7	C(75)-N(1)-C(79)	113.2(3)
C(58)-C(57)-C(62)	114.7(3)	C(78)-N(1)-C(79)	110.6(3)
C(58)-C(57)-B(2)	120.7(3)	C(75)-N(1)-C(82)	113.5(4)
C(62)-C(57)-B(2)	124.3(3)	C(78)-N(1)-C(82)	112.9(3)
C(59)-C(58)-C(57)	123.5(3)	C(79)-N(1)-C(82)	105.0(3)
C(59)-C(58)-H(58)	118.2	N(1)-C(75)-C(76)	106.1(4)
C(57)-C(58)-H(58)	118.2	N(1)-C(75)-H(75A)	110.5
C(60)-C(59)-C(58)	119.0(3)	C(76)-C(75)-H(75A)	110.5
C(60)-C(59)-P(2)	119.3(3)	N(1)-C(75)-H(75B)	110.5
C(58)-C(59)-P(2)	121.6(3)	C(76)-C(75)-H(75B)	110.5
C(61)-C(60)-C(59)	119.2(3)	H(75A)-C(75)-H(75B)	108.7
C(61)-C(60)-H(60)	120.4	C(75)-C(76)-C(77)	104.3(4)
C(59)-C(60)-H(60)	120.4	C(75)-C(76)-H(76A)	110.9
C(62)-C(61)-C(60)	120.4(3)	C(77)-C(76)-H(76A)	110.9
C(62)-C(61)-H(61)	119.8	C(75)-C(76)-H(76B)	110.9
C(60)-C(61)-H(61)	119.8	C(77)-C(76)-H(76B)	110.9
C(61)-C(62)-C(57)	123.1(3)	H(76A)-C(76)-H(76B)	108.9
C(61)-C(62)-H(62)	118.4	C(78)-C(77)-C(76)	105.9(4)
C(57)-C(62)-H(62)	118.4	C(78)-C(77)-H(77A)	110.5
C(68)-C(63)-C(64)	118.8(4)	C(76)-C(77)-H(77A)	110.5
C(68)-C(63)-P(2)	117.7(3)	C(78)-C(77)-H(77B)	110.6
C(64)-C(63)-P(2)	123.3(3)	C(76)-C(77)-H(77B)	110.5
C(63)-C(64)-C(65)	120.0(4)	H(77A)-C(77)-H(77B)	108.7
C(63)-C(64)-H(64)	120.0	N(1)-C(78)-C(77)	104.4(4)
C(65)-C(64)-H(64)	120.0	N(1)-C(78)-H(78A)	110.9
C(66)-C(65)-C(64)	120.6(5)	C(77)-C(78)-H(78A)	110.9
C(66)-C(65)-H(65)	119.7	N(1)-C(78)-H(78B)	110.9
C(64)-C(65)-H(65)	119.7	C(77)-C(78)-H(78B)	110.9
C(67)-C(66)-C(65)	119.6(4)	H(78A)-C(78)-H(78B)	108.9
C(67)-C(66)-H(66)	120.2	N(1)-C(79)-C(80)	103.3(3)
C(65)-C(66)-H(66)	120.2	N(1)-C(79)-H(79A)	111.1
C(66)-C(67)-C(68)	120.2(5)	C(80)-C(79)-H(79A)	111.1
C(66)-C(67)-H(67)	119.9	N(1)-C(79)-H(79B)	111.1
C(68)-C(67)-H(67)	119.9	C(80)-C(79)-H(79B)	111.1
C(63)-C(68)-C(67)	120.8(4)	H(79A)-C(79)-H(79B)	109.1
C(63)-C(68)-H(68)	119.6	C(79)-C(80)-C(81)	103.1(4)
C(67)-C(68)-H(68)	119.6	C(79)-C(80)-H(80A)	111.1
C(70)-C(69)-C(74)	118.8(3)	C(81)-C(80)-H(80A)	111.1
C(70)-C(69)-P(2)	121.9(3)	C(79)-C(80)-H(80B)	111.1
C(74)-C(69)-P(2)	119.3(3)	C(81)-C(80)-H(80B)	111.1
C(69)-C(70)-C(71)	120.5(4)	H(80A)-C(80)-H(80B)	109.1
C(69)-C(70)-H(70)	119.8	C(82)-C(81)-C(80)	106.1(4)
C(71)-C(70)-H(70)	119.8	C(82)-C(81)-H(81A)	110.5
C(72)-C(71)-C(70)	120.4(4)	C(80)-C(81)-H(81A)	110.5
C(72)-C(71)-H(71)	119.8	C(82)-C(81)-H(81B)	110.5
C(70)-C(71)-H(71)	119.8	C(80)-C(81)-H(81B)	110.5
C(71)-C(72)-C(73)	120.0(4)	H(81A)-C(81)-H(81B)	108.7
C(71)-C(72)-H(72)	120.0	C(81)-C(82)-N(1)	105.9(4)

C(81)-C(82)-H(82A)	110.5	N(3)-C(90)-H(90B)	111.0
N(1)-C(82)-H(82A)	110.5	C(89)-C(90)-H(90B)	111.0
C(81)-C(82)-H(82B)	110.6	H(90A)-C(90)-H(90B)	109.0
N(1)-C(82)-H(82B)	110.6	C(90)-N(3)-C(87)	102.3(3)
H(82A)-C(82)-H(82B)	108.7	C(90)-N(3)-C(83)	111.2(3)
C(94)-N(2)-C(98)	113.7(3)	C(87)-N(3)-C(83)	111.0(3)
C(94)-N(2)-C(95)	113.3(3)	C(90)-N(3)-C(86)	114.4(3)
C(98)-N(2)-C(95)	102.3(3)	C(87)-N(3)-C(86)	112.5(3)
C(94)-N(2)-C(91)	102.9(3)	C(83)-N(3)-C(86)	105.7(3)
C(98)-N(2)-C(91)	113.9(3)	N(2)-C(91)-C(92)	104.1(3)
C(95)-N(2)-C(91)	111.1(3)	N(2)-C(91)-H(91A)	110.9
C(84)-C(83)-N(3)	104.3(3)	C(92)-C(91)-H(91A)	111.0
C(84)-C(83)-H(83A)	110.9	N(2)-C(91)-H(91B)	110.9
N(3)-C(83)-H(83A)	110.9	C(92)-C(91)-H(91B)	110.9
C(84)-C(83)-H(83B)	110.9	H(91A)-C(91)-H(91B)	109.0
N(3)-C(83)-H(83B)	110.9	C(91)-C(92)-C(93)	105.8(3)
H(83A)-C(83)-H(83B)	108.9	C(91)-C(92)-H(92A)	110.6
C(83)-C(84)-C(85)	102.2(4)	C(93)-C(92)-H(92A)	110.6
C(83)-C(84)-H(84A)	111.3	C(91)-C(92)-H(92B)	110.6
C(85)-C(84)-H(84A)	111.3	C(93)-C(92)-H(92B)	110.6
C(83)-C(84)-H(84B)	111.3	H(92A)-C(92)-H(92B)	108.7
C(85)-C(84)-H(84B)	111.3	C(94)-C(93)-C(92)	105.2(3)
H(84A)-C(84)-H(84B)	109.2	C(94)-C(93)-H(93A)	110.7
C(86)-C(85)-C(84)	104.0(4)	C(92)-C(93)-H(93A)	110.7
C(86)-C(85)-H(85A)	110.9	C(94)-C(93)-H(93B)	110.7
C(84)-C(85)-H(85A)	110.9	C(92)-C(93)-H(93B)	110.7
C(86)-C(85)-H(85B)	111.0	H(93A)-C(93)-H(93B)	108.8
C(84)-C(85)-H(85B)	111.0	N(2)-C(94)-C(93)	103.9(3)
H(85A)-C(85)-H(85B)	109.0	N(2)-C(94)-H(94A)	111.0
C(85)-C(86)-N(3)	106.1(4)	C(93)-C(94)-H(94A)	111.0
C(85)-C(86)-H(86A)	110.5	N(2)-C(94)-H(94B)	111.0
N(3)-C(86)-H(86A)	110.5	C(93)-C(94)-H(94B)	111.0
C(85)-C(86)-H(86B)	110.5	H(94A)-C(94)-H(94B)	109.0
N(3)-C(86)-H(86B)	110.5	N(2)-C(95)-C(96)	104.6(3)
H(86A)-C(86)-H(86B)	108.7	N(2)-C(95)-H(95A)	110.8
N(3)-C(87)-C(88)	104.6(3)	C(96)-C(95)-H(95A)	110.8
N(3)-C(87)-H(87A)	110.8	N(2)-C(95)-H(95B)	110.8
C(88)-C(87)-H(87A)	110.8	C(96)-C(95)-H(95B)	110.8
N(3)-C(87)-H(87B)	110.8	H(95A)-C(95)-H(95B)	108.9
C(88)-C(87)-H(87B)	110.8	C(95)-C(96)-C(97)	104 9(3)
H(87A)-C(87)-H(87B)	108.9	C(95)- $C(96)$ - $H(96A)$	110.8
C(87)-C(88)-C(89)	105 7(4)	C(97)- $C(96)$ - $H(96A)$	110.8
C(87)-C(88)-H(88A)	110.6	C(95)-C(96)-H(96B)	110.8
C(89)-C(88)-H(88A)	110.6	C(97)- $C(96)$ - $H(96B)$	110.8
C(87)-C(88)-H(88B)	110.6	H(96A)-C(96)-H(96B)	108.8
C(89)-C(88)-H(88B)	110.6	C(98)-C(97)-C(96)	105.6(4)
H(88A)-C(88)-H(88B)	108.7	C(98)- $C(97)$ - $H(97A)$	110.6
C(90)- $C(89)$ - $C(88)$	104.7(4)	C(96)- $C(97)$ - $H(97A)$	110.6
C(90)-C(89)-H(89A)	110 8	C(98)-C(97)-H(97R)	110.0
C(88)-C(89)-H(89A)	110.8	C(96)-C(97)-H(97B)	110.6
C(90) - C(80) - H(80R)	110.8	$H(97A)_{-}C(07)_{-}H(07B)$	108.8
$C(88)_{C(89)_{-H(80R)}}$	110.8	C(97) - C(97) - H(97D)	104.5(3)
$H(80\Delta)_C(80)_H(80P)$	108.0	C(97) - C(98) - H(08A)	110 8
$N(3)_C(0)_C(0)$	103.7(3)	N(2) - C(20) - H(20A)	110.0
N(3) - C(90) - C(09) N(3) - C(00) - H(00A)	105.7(5)	$\Gamma(2)$ -C(20)- $\Pi(20A)$ C(07)-C(08)- $\Pi(08D)$	110.9
C(80) = C(00) = H(00A)	111.0	N(2) C(00) U(00D)	110.7
C(09)-C(90)-П(90A)	111.0	IN(2)-C(30)-A(30D)	110.9

H(98A)-C(98)-H(98B)	108.9
C(101)-C(102)-H(10A)	109.5
C(101)-C(102)-H(10B)	109.9
H(10A)-C(102)-H(10B)	109.5
C(101)-C(102)-H(10C)	109.0
H(10A)-C(102)-H(10C)	109.5
H(10B)-C(102)-H(10C)	109.5
O(1)-C(101)-C(102)	150.8(18)
O(1)-C(101)-H(10D)	97.5
C(102)-C(101)-H(10D)	99.7
O(1)-C(101)-H(10E)	98.2
C(102)-C(101)-H(10E)	100.1
H(10D)-C(101)-H(10E)	104.2
C(99)-C(100)-H(10F)	111.1
C(99)-C(100)-H(10G)	110.7
H(10F)-C(100)-H(10G)	108.0
C(99)-C(100)-H(10H)	110.5
H(10F)-C(100)-H(10H)	108.4
H(10G)-C(100)-H(10H)	108.1
C(101)-O(1)-C(99)	150.2(16)
C(100)-C(99)-O(1)	145(5)
C(100)-C(99)-H(99A)	101.8
O(1)-C(99)-H(99A)	100.5
C(100)-C(99)-H(99B)	101.1
O(1)-C(99)-H(99B)	99.3
H(99A)-C(99)-H(99B)	104.7

Table 19. Anisotropic displacement parameters $(Å^2x \ 10^3)$ for $\{ASN\}_2\{[Ph_3BP^{m-Ph_2}]_2PtMe_2\}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2h k a^{*} b^{*} U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
$\overline{Pt(1)}$	10(1)	13(1)	19(1)	-7(1)	-1(1)	0(1)
B(1)	16(2)	19(2)	25(2)	4(2)	1(2)	1(2)
C(1)	10(2) 14(2)	19(2) 18(2)	43(3)	-13(2)	-7(2)	2(2)
C(1)	14(2) 11(2)	10(2) 19(2)	30(2)	-16(2)	1(2)	0(1)
P(1)	11(2) 11(1)	11(1)	20(1)	-6(1)	1(2) 1(1)	-1(1)
C(3)	16(2)	29(2)	25(1)	7(2)	-2(2)	1(1)
C(3)	33(3)	50(3)	23(2) 22(2)	5(2)	-2(2) -5(2)	-18(2)
$C(\tau)$	45(3)	63(4)	22(2) 23(2)	5(2)	-3(2)	-10(2)
C(5)	45(3)	40(3)	$\frac{23(2)}{17(2)}$	3(2)	-5(2)	-27(3)
C(0)	$\frac{40(3)}{34(3)}$	10(2)	$\frac{1}{(2)}$	-1(2)	-0(2)	-3(2)
C(7)	34(3)	19(2) 18(2)	$\frac{42(3)}{32(2)}$	-1(2) 1(2)	5(2)	$\frac{0(2)}{1(2)}$
C(0)	20(2) 17(2)	10(2) 22(2)	$\frac{32(2)}{10(2)}$	1(2)	3(2)	-1(2)
C(9)	$\frac{1}{(2)}$	23(2)	19(2)	1(2)	-3(2)	-1(2)
C(10) C(11)	10(2)	22(2)	20(2)	4(2)	0(2)	1(2)
C(11)	20(2)	22(2)	29(2) 10(2)	4(2)	-2(2)	-3(2)
C(12)	$\frac{1}{(2)}$	30(2)	19(2)	-2(2)	1(2)	-7(2)
C(15)	19(2)	32(2)	21(2) 16(2)	-9(2)	-1(2)	-2(2)
C(14)	20(2)	22(2)	10(2)	-2(2)	-4(2)	-3(2)
C(15)	23(2)	19(2)	36(2)	2(2)	13(2)	3(2)
C(10)	28(3)	31(3)	66(4) (0(4)	$\frac{1}{(2)}$	12(2)	3(2)
C(17)	58(4) 72(4)	21(2)	69(4)	21(3)	36(3)	19(2)
C(18)	73(4)	24(3)	60(4)	-9(3)	36(3)	-10(3)
C(19)	/5(4)	27(3)	39(3)	-13(2)	26(3)	-1/(3)
C(20)	44(3)	17(2)	36(3)	-8(2)	14(2)	-9(2)
C(21)	15(2)	11(2)	24(2)	0(1)	2(2)	-3(1)
C(22)	11(2)	11(2)	24(2)	-6(1)	2(1)	-2(1)
C(23)	15(2)	12(2)	16(2)	-4(1)	1(1)	-5(1)
C(24)	11(2)	10(2)	25(2)	-5(1)	1(1)	-1(1)
C(25)	15(2)	17(2)	23(2)	-7(2)	4(2)	-1(1)
C(26)	19(2)	16(2)	20(2)	-3(1)	1(2)	-1(1)
C(27)	12(2)	14(2)	29(2)	-8(2)	-4(2)	2(1)
C(28)	17(2)	18(2)	30(2)	-10(2)	2(2)	-3(2)
C(29)	19(2)	19(2)	39(2)	-8(2)	3(2)	-7(2)
C(30)	21(2)	15(2)	45(3)	-14(2)	-2(2)	-4(2)
C(31)	20(2)	23(2)	38(2)	-18(2)	3(2)	-3(2)
C(32)	17(2)	19(2)	29(2)	-10(2)	1(2)	-1(2)
C(33)	12(2)	11(2)	25(2)	-9(1)	4(1)	-2(1)
C(34)	17(2)	13(2)	25(2)	-7(2)	1(2)	-1(1)
C(35)	13(2)	18(2)	33(2)	-11(2)	-1(2)	-1(1)
C(36)	13(2)	24(2)	34(2)	-7(2)	6(2)	-6(2)
C(37)	23(2)	24(2)	21(2)	-6(2)	6(2)	-5(2)
C(38)	14(2)	17(2)	26(2)	-5(2)	1(2)	-2(1)
B(2)	14(2)	13(2)	22(2)	-6(2)	-2(2)	1(2)
P(2)	11(1)	12(1)	14(1)	-4(1)	0(1)	-1(1)
C(39)	20(2)	16(2)	19(2)	-4(2)	-1(2)	-3(1)
C(40)	18(2)	16(2)	22(2)	-6(2)	-1(2)	-2(1)
C(41)	21(2)	22(2)	28(2)	-7(2)	-2(2)	2(2)

C(42)	17(2)	32(2)	30(2)	-8(2)	-3(2)	-3(2)
C(43)	28(2)	25(2)	28(2)	-6(2)	-4(2)	-12(2)
C(44)	24(2)	16(2)	26(2)	-7(2)	-2(2)	-5(2)
C(45)	18(2)	17(2)	20(2)	-9(2)	-2(2)	-2(1)
C(46)	27(2)	20(2)	22(2)	-6(2)	-3(2)	-1(2)
C(47)	36(2)	32(2)	18(2)	-7(2)	4(2)	-7(2)
C(48)	34(2)	33(2)	30(2)	-18(2)	9(2)	-3(2)
C(49)	38(3)	19(2)	34(2)	-14(2)	7(2)	-1(2)
C(50)	28(2)	17(2)	27(2)	-9(2)	2(2)	-4(2)
C(51)	20(2)	12(2)	19(2)	-8(1)	3(2)	-3(1)
C(52)	20(2)	17(2)	23(2)	-7(2)	1(2)	-4(2)
C(53)	23(2)	23(2)	24(2)	-6(2)	-4(2)	-1(2)
C(54)	34(2)	19(2)	16(2)	-4(2)	3(2)	-1(2)
C(55)	24(2)	24(2)	24(2)	-10(2)	9(2)	-5(2)
C(56)	19(2)	21(2)	23(2)	-11(2)	0(2)	0(2)
C(57)	17(2)	14(2)	14(2)	-4(1)	-2(1)	0(1)
C(58)	10(2)	14(2)	18(2)	-2(1)	-1(1)	-1(1)
C(59)	15(2)	11(2)	13(2)	-4(1)	1(1)	0(1)
C(60)	14(2)	13(2)	17(2)	-3(1)	0(1)	-4(1)
C(61)	13(2)	17(2)	19(2)	-2(1)	2(1)	-2(1)
C(62)	15(2)	17(2)	17(2)	-3(1)	2(1)	2(1)
C(63)	12(2)	22(2)	17(2)	3(2)	0(1)	-3(1)
C(64)	28(2)	28(2)	23(2)	2(2)	-8(2)	-12(2)
C(65)	35(3)	37(3)	29(2)	11(2)	-11(2)	-19(2)
C(66)	27(2)	60(3)	21(2)	18(2)	-1(2)	-11(2)
C(67)	32(3)	59(3)	19(2)	-1(2)	7(2)	4(2)
C(68)	26(2)	34(2)	20(2)	-1(2)	3(2)	3(2)
C(69)	14(2)	9(2)	19(2)	-5(1)	-1(1)	-2(1)
C(70)	16(2)	12(2)	22(2)	-2(1)	2(2)	-1(1)
C(71)	13(2)	16(2)	34(2)	-5(2)	5(2)	-3(1)
C(72)	15(2)	13(2)	38(2)	-9(2)	-8(2)	1(1)
C(73)	22(2)	13(2)	21(2)	-8(1)	-3(2)	0(1)
C(74)	15(2)	9(2)	21(2)	-5(1)	3(1)	-4(1)
N(1)	25(2)	26(2)	20(2)	-6(1)	1(1)	0(1)
C(75)	32(3)	63(4)	33(3)	-20(2)	1(2)	4(2)
C(76)	56(3)	41(3)	41(3)	-24(2)	-19(3)	21(3)
C(77)	59(3)	22(2)	34(3)	-5(2)	-13(2)	0(2)
C(78)	28(2)	25(2)	26(2)	-6(2)	-2(2)	-3(2)
C(79)	30(2)	33(2)	22(2)	-6(2)	-5(2)	-2(2)
C(80)	41(3)	30(2)	29(2)	-13(2)	3(2)	-9(2)
C(81)	46(3)	28(2)	38(3)	-7(2)	4(2)	-3(2)
C(82)	34(2)	29(2)	27(2)	2(2)	0(2)	-8(2)
N(2)	23(2)	18(2)	29(2)	-5(1)	1(1)	0(1)
C(83)	28(2)	20(2)	25(2)	-9(2)	0(2)	2(2)
C(84)	43(3)	30(2)	37(3)	-13(2)	13(2)	-7(2)
C(85)	61(4)	44(3)	42(3)	-18(2)	22(3)	-6(3)
C(86)	33(2)	35(2)	24(2)	-13(2)	0(2)	6(2)
C(87)	25(2)	21(2)	28(2)	-8(2)	-2(2)	1(2)
C(88)	36(2)	23(2)	32(2)	-11(2)	9(2)	-7(2)
C(89)	25(2)	28(2)	59(3)	-19(2)	4(2)	-9(2)
C(90)	27(2)	32(2)	46(3)	-21(2)	-9(2)	-3(2)
N(3)	22(2)	23(2)	25(2)	-13(1)	-2(1)	2(1)
C(91)	31(2)	20(2)	26(2)	-8(2)	-7(2)	0(2)
C(92)	20(2)	23(2)	35(2)	-9(2)	-2(2)	-2(2)
C(93)	25(2)	28(2)	24(2)	-5(2)	0(2)	0(2)
C(94)	24(2)	26(2)	27(2)	-6(2)	-5(2)	0(2)

C(95)	27(2)	22(2)	33(2)	-7(2)	-3(2)	4(2)
C(96)	25(2)	28(2)	29(2)	-9(2)	-2(2)	1(2)
C(97)	31(2)	31(2)	28(2)	-6(2)	3(2)	-3(2)
C(98)	28(2)	24(2)	29(2)	-4(2)	1(2)	-6(2)
Br(1)	28(1)	21(1)	25(1)	-8(1)	-5(1)	-3(1)
C(102)	82(6)	73(5)	94(6)	21(5)	-18(5)	-28(4)
C(101)	161(12)	57(4)	66(5)	-27(4)	-47(7)	17(6)
C(100)	1400(130)	139(14)	77(10)	-60(12)	-170(30)	330(40)
O(1)	173(13)	620(30)	600(30)	-540(30)	-78(16)	87(16)
C(99)	490(40)	2000(130)	360(30)	-860(60)	-280(30)	760(60)

	х	У	Z	U(eq)
H(1A)	11814	10181	3656	36
H(1B)	10416	10712	3637	36
H(1C)	11359	10755	3089	36
H(2A)	12503	8875	3565	28
H(2B)	11534	8192	3713	28
H(2C)	11512	8809	4100	28
H(4)	7691	12453	-177	43
H(5)	7879	12242	-1068	53
H(6)	6690	11311	-1304	43
H(7)	5277	10614	-641	40
H(8)	5149	10791	263	33
H(10)	5369	10346	1242	30
H(11)	3424	9981	1722	30
H(12)	1805	10942	1953	29
H(13)	2158	12263	1666	28
H(14)	4099	12634	1174	23
H(16)	5229	13219	278	57
H(17)	5628	14518	266	70
H(18)	7399	14778	705	65
H(19)	8712	13731	1221	56
H(20)	8255	12445	1280	39
H(22)	6960	11333	1885	18
H(24)	10162	9705	1005	18
H(25)	10102	9852	1022	22
H(25)	8601	10713	502	22
П(20) Ц(28)	0730	11740	2032	22
П(20) Ц(20)	9730	12022	2032	23
$\Pi(29)$	0242	13032	2037	21
П(30) П(21)	9245	15556	2033	51 20
$\Pi(31)$	8182	12/30	3370 2540	30 25
H(32)	/88/	11447	3549	25
H(34)	5/69	10461	2440	21
H(35)	3778	10244	2960	25
H(36)	3735	9987	3919	28
H(37)	5702	9915	43/4	27
H(38)	7709	10072	3862	23
H(40)	7960	7235	1866	22
H(41)	5816	7440	1551	28
H(42)	4779	6387	1400	31
H(43)	5940	5126	1572	31
H(44)	8062	4913	1899	25
H(46)	10900	6433	1166	27
H(47)	12271	5910	526	34
H(48)	12986	4551	703	37
H(49)	12227	3742	1517	36
H(50)	10877	4275	2164	28
H(52)	11695	5035	2888	24
u(52)	11605	4159	3739	28

Table 20. Hydrogen coordinates (x 10⁴) and isotropic displacement parameters (Å²x 10³) for $\{ASN\}_2\{[Ph_3BP^{m-Ph_2}]_2PtMe_2\}$.

$\mathbf{U}(5A)$	0672	2022	1206	20
11(34) 11(55)	7072	3823	4200	20
H(55)	/6/8	4363	3/9/	28
H(56)	7691	5235	2942	24
H(58)	8785	7052	2698	17
H(60)	11922	8297	2675	17
H(61)	13219	7432	2208	20
H(62)	12306	6407	1978	20
H(64)	9203	6658	3617	31
H(65)	8645	5914	4490	42
H(66)	8108	6522	5232	47
H(67)	8239	7865	5112	47
H(68)	8778	8618	4240	34
H(70)	6542	8170	3620	20
U(71)	4452	8202	2258	20
$\Pi(/1)$	4433	0292	3238	20
H(72)	4224	8042	2309	20
H(73)	6104	8885	1/09	22
H(74)	8198	8755	2070	17
H(75A)	1034	2597	10704	50
H(75B)	-179	2624	10317	50
H(76A)	921	3895	10316	54
H(76B)	266	3789	9771	54
H(77A)	2286	3721	9345	46
H(77B)	2940	3822	9891	46
H(78A)	3388	2504	9549	32
H(78B)	3424	2510	10194	32
H(79A)	1169	2655	9167	34
H(79B)	61	2131	9515	34
H(80A)	2663	1556	9145	38
H(80R)	1274	1253	9052	38
$H(81\Lambda)$	1077	565	9032	45
H(81R)	2672	107	0873	45
$\Pi(01D)$ $\Pi(02A)$	2072	1269	10450	45
H(02A) H(02D)	1210	1208	10433	27
$H(\delta 2B)$	1210	1224	10596	37
$H(\delta 3A)$	3188	3803	2705	29
H(83B)	3900	3632	3344	29
H(84A)	5972	3812	2910	44
H(84B)	5029	4489	2523	44
H(85A)	4883	3704	1892	59
H(85B)	6421	3514	2042	59
H(86A)	6102	2335	2586	36
H(86B)	4893	2394	2191	36
H(87A)	5419	2496	3630	29
H(87B)	5236	1697	3441	29
H(88A)	3463	2479	4122	36
H(88B)	3595	1560	4106	36
H(89A)	1805	1814	3590	43
H(89B)	1802	2747	3538	43
H(90A)	3165	1822	2818	39
H(90R)	2405	2695	2646	39
H(91A)	5203	5269	4383	30
$H(01\mathbf{R})$	J20J 1005	6111	4505	20
H(02A)	400J 6676	5005	4343	20
$\frac{11(32A)}{11(02D)}$	0020	3003 (712	3/40 2771	30
H(92B)	5903	0/43	3//1	30
H(93A)	4696	6764	3047	31
H(93B)	5544	5955	2973	31
H(94A)	3027	5972	3220	31
H(94B)	4007	5200	3467	31
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H(95A)	2091	6864	3753	34
H(95B)	3428	7134	3931	34
H(96A)	1304	6954	4613	33
H(96B)	2773	6878	4836	33
H(97A)	2733	5573	5154	36
H(97B)	1218	5662	4979	36
H(98A)	1801	5343	4162	33
H(98B)	3027	4852	4505	33
H(10A)	4417	8304	4328	130
H(10B)	4842	7607	4841	130
H(10C)	5489	8421	4735	130
H(10D)	2921	8149	5022	111
H(10E)	3963	8246	5425	111
H(10F)	226	10414	5012	837
H(10G)	1408	10581	4553	837
H(10H)	1593	10659	5170	837
H(99A)	1264	9329	4821	1095
H(99B)	1220	9369	5443	1095