SUPPLEMENTARY INFORMATION

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PROCEDURES

**General comments:** All reactions and manipulations were carried out under an atmosphere of dry argon using standard Schlenk techniques or in the glovebox. All solvents were sparged with argon and dried using an MBRAUN Solvent Purification System (SPS) and degassed with 3 freeze-pump-thaw cycles. Deuterated solvents were dried over alumina or molecular sieves and degassed with 3 freeze-pump-thaw cycles. NMR spectra were recorded on Bruker Avance 300, 400 or 500 systems. The chemical shifts are given as $\delta$ values and were referenced against residual solvent signals for $^1$H (5.32, and 7.16 ppm for CD$_2$Cl$_2$ and C$_6$D$_6$ respectively) and $^{13}$C (53.84 and 128.06 ppm for CD$_2$Cl$_2$ and C$_6$D$_6$ respectively). The $^{11}$B NMR spectra were referenced to an external BF$_3$.Et$_2$O sample. The $^{31}$P NMR spectra were referenced to an external 85% H$_3$PO$_4$ sample. Solid-state NMR experiments were recorded on a Bruker Avance 400 spectrometer equipped with a 3.2-mm probe. Samples were spun between 12 kHz at the magic angle using ZrO$_2$ rotors. Melting points were determined with a Stuart SMP40 melting point apparatus and are not corrected. Mass spectra were recorded on a Waters LCT mass spectrometer. X-Band EPR data were recorded using an Elexsys ESP 500, operating at a microwave frequency of approximately 9.5 GHz. All spectra were recorded using a microwave power of 2 mW, across a sweep width of 140 G (centered at 3400 G) with a modulation amplitude of 1 G. At the end of the measurement, the first spectrum was remeasured to verify that no decomposition occurred and to verify the reliability of the integral values.
Based on a poorly described literature procedure.\textsuperscript{i}

To a stirred suspension of solvent free (2,4,6-triisopropylphenyl)lithium (1.42 g, 6.8 mmol) in 10 mL pentane, was added at -80°C neat BBr\textsubscript{3} (0.64 mL, 1.69 g, 6.8 mmol). The suspension was warmed to RT and stirred overnight. The beige suspension was filtered and the solid extracted twice with 10 mL of pentane. The combined organic phases were evaporated to dryness to yield 2 grams of crude product. This crude product was recrystallized from pentane to yield 1.4 g (56\%) of the product as colorless needles, suitable for a single crystal x-ray diffraction study.

\textsuperscript{1}H NMR (300 MHz, 298 K, C\textsubscript{6}D\textsubscript{6}): δ 6.99 (s, 2H, H\textsubscript{Ar}), 2.87 (sept, 2H, \textsuperscript{3}J\textsubscript{HH} = 6.8 Hz, CH(CH\textsubscript{3})), 2.71 (sept, 21H, \textsuperscript{3}J\textsubscript{HH} = 6.7 Hz, CH(CH\textsubscript{3})), 1.20 (d, 12H, \textsuperscript{3}J\textsubscript{HH} = 6.8 Hz, CH\textsubscript{3}), 1.16 (d, 6H, \textsuperscript{3}J\textsubscript{HH} = 6.7 Hz, CH\textsubscript{3}).

\textsuperscript{11}B \{\textsuperscript{1}H\} NMR (96.3 MHz, 298 K, C\textsubscript{6}D\textsubscript{6}): δ 62.6.

\textbf{Compound 1a}

Under argon, (8-iodonaphthalen-1-yl)diphenylphosphane (1.8 g, 4.1 mmol) was suspended in 16 mL of Et\textsubscript{2}O. At -80°C and under stirring, \textit{n}-butyllithium (2.6 mL, 1.6 M solution in hexane, 4.2 mmol) was added. After two hours at -60°C, the yellow suspension was cooled to -80°C and the solvent filtered out with a cannula. The yellow solid was dissolved in 10 mL of toluene at -60°C. A solution of dibromide (2,4,6 triisopropylphenyl)borane (1.38 g, 3.7 mmol) in 10 mL of toluene was added slowly. The solution was allowed to warm up to RT and the red solution stirred overnight. The red solution was filtered off from the white solid. The white solid was washed with 5 mL of toluene and extracted the solid 3 times with 10 mL of DCM. The combined solutions were evaporated to dryness to yield 643 mg (29\%) of product as a white powder. Mp. 207 °C.

**Compound 2a and [2a]₂**

To a solution of (8-(bromo(2,4,6 triisopropylphenyl)boryl)naphthalen-1-yl)diphenylphosphane (200 mg, 0.33 mmol) in 4 mL of toluene was added 1% sodium amalgam (1.0 g, 0.43 mmol) and the reaction stirred vigorously. The next day, the stirring was stopped and an hour later the dark red solution was carefully decanted onto a glass filter. After the filtration and washing with 1 mL of toluene, the solution was let to stand for 24 hours and checked for the presence of grey mercury particles, if these formed the solution was filtered once more. The solvent was evaporated to dryness and washed 3 times with 1 mL of pentanes to yield 150 mg (86%) of [2a]₂. The product could be further purified by recrystallization from diethyl ether. Mp. 95 °C (decomposition).

**Compound 3**

To a stirred red solution of 2a (18 mg, 0.038 mmol) in 1 mL of toluene was added a solution of TEMPO free radical in 1 mL of Et₂O (6 mg, 0.038 mmol). The solution discolored in a few minutes. The solvent was evaporated and the oil dissolved in 1 mL of pentane. The product crystalized out at -20°C to yield in total 11 mg (42%) of colorless cubes. Mp. 148 °C.
Compound 4

To a red solution of 2a (18 mg, 0.038 mmol) in 1 mL of toluene was added a solution of triphenylmethylchloride (6 mg, 0.038 mmol) in 1 mL of Et₂O. The next day, the light orange solution was filtered and evaporated to dryness. The resulting solid was washed 2 times with 0.5 mL of pentanes to yield 14 mg (66%) of colorless solid. Mp. 161 °C.

At room temperature the 2,4,6 triisopropylphenyl group is rotating slowly and gives in the NMR spectra broad signals. Hence the ¹H and ¹³C were recorded at 253 K.

Compound 1b

Under argon, (8-iodonaphthalen-1-yl)diphenylphosphane (0.475 g, 1.1 mmol) was suspended in 4 mL of Et₂O. At -60°C and under stirring, n-butyllithium (0.7 mL, 1.6 M solution in hexane, 1.1 mmol) was added. After an hour at -60°C, the yellow suspension was cooled to -80°C and the solvent filtered out with a cannula. The yellow solid was dissolved in 5 mL of toluene at -60°C. A solution of dibromide(2,6 dimesitylphenyl)borane® (0.500 g, 1.0 mmol) in 10 mL of toluene was added slowly. The solution was allowed to warm up to RT and stirred overnight. The red solution was filtered off from the white solid and the solid extracted with 10 more mL of toluene. The solution was allowed to warm up to RT and stirred overnight. The red solution was filtered off from the white solid and the solid extracted with 10 more mL of toluene. The white solid washed 3 times with 5 mL of pentanes and 3 times with 1 mL of toluene. The white solid 0.20 g (28%) was pure 1b. Mp. 122 °C.

**Compound 2b and [2b]$_2$**

To a suspension of 1b (27 mg, 0.038 mmol) in 1 mL of toluene was added 1% sodium amalgam (113 g, 0.049 mmol) and the reaction stirred vigorously for 24 hours. The stirring was stopped and an hour later the dark brown solution was carefully decanted onto a glass filter. After the filtration and washing with 1 more mL of toluene, the solution was let to stand for 24 hours and checked for the presence of grey mercury particles, if these formed the solution was filtered once more. The solvent was concentrated by half and the solution layered with 2 mL of pentanes to yield 11 mg (46%) of the product as beige-orange microcrystals (suitable for a single crystal x-ray diffraction study).
EPR data

**Figure S1**: Experimental and simulated ESR spectra of 2a and associated data

Experimental EPR parameters:

- Temperature: 295 K
- g-value: 2.0026
- Compound: 2a
- Solvent: Toluene
- MWFQ: 9.525384 GHz
- Experiment name: 14mm1527

**Simulated spectrum**: simulations were performed with the EasySpin package in Matlab.iii

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EPR spectra were recorded with the same settings at different temperature. Above are depicted the integrals of signals measured between 295 and 322 K. The area of these signals was calculated.

Formulas used:

\[ K = \frac{[D]}{[M]^2} \]

\[ \ln(K) = -\frac{\Delta G}{RT} \]

\[ \text{integral} = c \times [M] \]

\[ [D_0] = [D] + 0.5 \times [M] \]

Combined:

\[ \ln\left(\frac{[D_0]}{[M]^2} - \frac{1}{2[M]}\right) = -\frac{\Delta G}{RT} \]

\[ \ln\left(\frac{[D_0]}{\text{integral}} - \frac{1}{2\times\text{integral}}\right) = -\frac{\Delta G}{RT} \]

Using the integral and temperature data to fit \([D_0]\), \(c\) and \(\Delta G\), the following values were obtained. \([D_0] = 0.626 \text{ mol/L}, c = 4.89 \times 10^{-6} \text{ L/mol} \) and \(\Delta G = -38 \text{ kJ/mol}\)
**Figure S3**: Experimental and simulated ESR spectra of 2b

**Experimental EPR parameters:**

- **Temperature**: 293 K
- **g-value**: 2.0024
- **compound**: 2b
- **Solvent**: Toluene
- **MWFQ**: 9.528071 GHz
- **experiment name**: 15mm0236

**Simulated spectrum**: simulations were performed with the EasySpin package in Matlab.

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NMR SPECTRA

Figure S4: $^1$H NMR of 1a (400 MHz, 253 K) in CD$_2$Cl$_2$

Figure S5: $^1$H NMR of 1a (400 MHz, 253 K) in CD$_2$Cl$_2$: aliphatic region

Figure S6: $^1$H NMR of 1a (400 MHz, 253 K) in CD$_2$Cl$_2$: aromatic region
Figure S7: $^1$H-$^{31}$P NMR of 1a (400 MHz, 253 K) in CD$_2$Cl$_2$: aliphatic region

Figure S8: $^1$H-$^{31}$P NMR of 1a (400 MHz, 253 K) in CD$_2$Cl$_2$: aromatic region

Figure S9: $^{13}$C-$^1$H NMR of 1a (100.6 MHz, 253 K, CD$_2$Cl$_2$/C$_6$D$_6$)
Figure S10: $^{13}$C ($^1$H) NMR of 1a (100.6 MHz, 253 K) CD$_2$Cl$_2$ / C$_6$D$_6$ : aliphatic region

Figure S11: $^{13}$C ($^1$H) NMR of 1a (100.6 MHz, 253 K) CD$_2$Cl$_2$ / C$_6$D$_6$ : aromatic region

Figure S12: $^{13}$C ($^{31}$P,$^1$H) NMR of 1a (100.6 MHz, 253 K) CD$_2$Cl$_2$ / C$_6$D$_6$

Figure S13: $^{13}$C ($^{31}$P,$^1$H) NMR of 1a (100.6 MHz, 253 K) CD$_2$Cl$_2$ / C$_6$D$_6$ : aliphatic region

S12
Figure S14: $^{13}$C ($^{31}$P, $^1$H) NMR of 1a (100.6 MHz, 253 K) CD$_2$Cl$_2$ / C$_6$D$_6$ : aromatic region

Figure S15: $^{31}$P($^1$H) NMR of 1a (162 MHz, 253 K) in CD$_2$Cl$_2$ / C$_6$D$_6$

Figure S16: $^{11}$B ($^1$H) NMR of 1a (96.3 MHz, 298 K) CD$_2$Cl$_2$/C$_6$D$_6$
**Figure S17**: $^{31}$P $\{^1\text{H}\}$ NMR of [2a]$_2$ (96.3 MHz, 298 K) CD$_2$Cl$_2$/C$_6$D$_6$

**Figure S18**: $^{11}$B $\{^1\text{H}\}$ NMR of [2a]$_2$ (96.3 MHz, 298 K) CD$_2$Cl$_2$/C$_6$D$_6$
Figure S19: $^1$H NMR of 3 (500 MHz, 283 K) in C$_6$D$_6$

Figure S20: $^1$H NMR of 3 (500 MHz, 283 K) in C$_6$D$_6$; aromatic region

Figure S21: $^1$H NMR of 3 (500 MHz, 283 K) in C$_6$D$_6$; aliphatic region

* Signals attributed to pentane
Figure S22: $^{13}$C{$^1$H} NMR of 3 (125.8 MHz, 283 K) in C$_6$D$_6$

Figure S23: $^{13}$C{$^1$H} NMR of 3 (125.8 MHz, 283 K) in C$_6$D$_6$; aromatic region

Figure S24: $^{13}$C{$^1$H} NMR of 3 (125.8 MHz, 283 K) in C$_6$D$_6$; aliphatic region

* Signals attributed to pentane
Figure S25: $^{31}$P$^1$H NMR of 3 (202.4 MHz, 283 K) in C$_6$D$_6$

Figure S26: $^{11}$B$^1$H NMR of 3 (160.5 MHz, 283 K) in C$_6$D$_6$

Figure S27: $^1$H NMR of 4 (500.3 MHz, 253 K) in CD$_2$Cl$_2$
Figure S28: $^1$H NMR of 4 (500.3 MHz, 253 K) in CD$_2$Cl$_2$; aromatic region

Figure S29: $^1$H NMR of 4 (500.3 MHz, 253 K) in CD$_2$Cl$_2$; aliphatic region

Figure S30: $^{13}$C($^1$H) NMR of 4 (125.8 MHz, 253 K) in CD$_2$Cl$_2$
**Figure S31** : $^{13}$C($^1$H) NMR of 4 (125.8 MHz, 253 K) in C$_2$D$_2$Cl$_2$; quaternary carbon region

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* unidentified product.

**Figure S32** : $^{13}$C($^1$H) NMR of 4 (125.8 MHz, 253 K) in C$_2$D$_2$Cl$_2$; aromatic region

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**Figure S33** : $^{13}$C($^1$H,$^{31}$P) NMR of 4 (125.8 MHz, 253 K) in C$_2$D$_2$Cl$_2$; aromatic region

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**Figure S34**: $^{13}$C($^1$H) NMR of 4 (125.8 MHz, 253 K) in CD$_2$Cl$_2$; aliphatic region

**Figure S35**: $^{31}$P($^1$H) NMR of 4 (202.4 MHz, 298 K) in CD$_2$Cl$_2$

**Figure S36**: $^{11}$B NMR of 4 (96.3 MHz, 298 K) in CD$_2$Cl$_2$
Figure S37: $^1$H NMR of 1b (500.3 MHz, 273 K) in CD$_2$Cl$_2$

Figure S38: $^1$H NMR of 1b (500.3 MHz, 273 K) in CD$_2$Cl$_2$; aromatic region

Figure S39: $^1$H($^{31}$P) NMR of 1b (500.3 MHz, 273 K) in CD$_2$Cl$_2$; aromatic region

Figure S40: $^{13}$C($^1$H) NMR of 1b (125.8 MHz, 273 K) in CD$_2$Cl$_2$
**Figure S41**: $^{13}$C($^1$H) NMR of 1b (125.8 MHz, 273 K) in CD$_2$Cl$_2$; aliphatic region

![Aliphatic Region](image)

**Figure S42**: $^{13}$C($^1$H) NMR of 1b (125.8 MHz, 273 K) in CD$_2$Cl$_2$; aromatic region

![Aromatic Region](image)

**Figure S43**: $^{13}$C($^1$H,$^{31}$P) NMR of 1b (125.8 MHz, 273 K) in CD$_2$Cl$_2$; aromatic region

![Aromatic Region with Phosphorus](image)
Figure S44: $^{13}$C($^1$H) NMR of 1b (125.8 MHz, 273 K) in CD$_2$Cl$_2$; aromatic region

Figure S45: $^{13}$C($^1$H, $^{31}$P) NMR of 1b (125.8 MHz, 273 K) in CD$_2$Cl$_2$; aromatic region

Figure S46: $^{31}$P($^1$H) NMR of 1b (202.4 MHz, 273 K) in CD$_2$Cl$_2$
**Figure S47:** $^{11}$B NMR of $1b$ (96.3 MHz, 298 K) in CD$_2$Cl$_2$

![NMR Spectrum](image1)

**Figure S48:** $^{11}$B ($^1$H) NMR of [2b]$_2$ (128.2 MHz, 298 K, MAS NMR, 10 KHz)

![NMR Spectrum](image2)

Experimental spectrum in blue and simulated spectrum in red.
Figure S49: $^{31}$P NMR of [2b]$_2$ (161.8 MHz, 298 K, MAS NMR, 20 KHz)
Crystallographic data

Crystallographic data were collected at low temperature (173(2) K) on a Bruker-AXS APEXII QUAZAR diffractometer equipped with a 30W air-cooled microfocus source (3 and 1b) and on a Bruker-AXS PHOTON100 D8 VENTURE diffractometer (1a, [2a]2, 4 and [2b]2). MoKα radiation (λ = 0.71073 Å) and Phi-omega-scan were used for data collection. An empirical absorption correction was performed with SADABS. The structures were solved by direct methods or by intrinsic phasing method and refined by the least-squares method on F2. All non-hydrogen atoms were refined with anisotropic displacement parameters and the hydrogen atoms were refined isotropically.

1a (CCDC 1833880): C37H30BBP, M = 605.36, monoclinic, P21/c, a = 9.2089(4) Å, b = 13.9378(5) Å, c = 24.6940(11) Å, α = 90°, β = 95.9776(16)°, γ = 90°, V = 3152.3(2) Å3, Z = 4, crystal size 0.50 x 0.50 x 0.50 mm3, crystal habitat colourless cube, 68951 reflections collected (9597 independent, Rint = 0.0607), 367 parameters, R1 [I>2σ(I)] = 0.0379, wR2 [all data] = 0.1036, largest diff. peak and hole: 0.857 and -0.786 eÅ⁻³.

[2a]2 (CCDC 1833883): C62H38B2O2P2, M = 1199.16, monoclinic, P21/c, a = 21.237(13) Å, b = 16.487(8) Å, c = 21.593(10) Å, α = 90°, β = 109.523(13)°, γ = 90°, V = 7126(6) Å³, Z = 4, crystal size 0.19 x 0.13 x 0.04 mm³, crystal habitat red plate, 70677 reflections collected (7707 independent, Rint = 0.0998), 881 parameters, R1 [I>2σ(I)] = 0.0598, wR2 [all data] = 0.1598, largest diff. peak and hole: 0.462 and -0.325 eÅ⁻³.

3 (CCDC 1833881): C66H72BNOP, M = 681.71, orthorhombic, Pna21, a = 15.1607(7) Å, b = 13.7714(7) Å, c = 18.9735(8) Å, α = β = γ = 90°, V = 3961.4(3) Å³, Z = 4, crystal size 0.21 x 0.20 x 0.19 mm³, crystal habitat colourless cube, 60557 reflections collected (10672 independent, Rint = 0.1046), 461 parameters, R1 [I>2σ(I)] = 0.0533, wR2 [all data] = 0.1143, largest diff. peak and hole: 0.326 and -0.291 eÅ⁻³.

4 (CCDC 1833882): C37H39BCIP, M = 560.91, monoclinic, P21/n, a = 9.1955(17) Å, b = 13.889(2) Å, c = 24.546(4) Å, α = 90°, β = 95.995(6)°, γ = 90°, V = 3117.8(9) Å³, Z = 4, crystal size 0.14 x 0.14 x 0.04 mm³, crystal habitat colourless plate, 56781 reflections collected (8797 independent, Rint = 0.0511), 367 parameters, R1 [I>2σ(I)] = 0.0451, wR2 [all data] = 0.1423, largest diff. peak and hole: 0.319 and -0.295 eÅ⁻³.

1b (CCDC 1833884): C46H31BBP, M = 715.47, monoclinic, P21/n, a = 9.2827(14) Å, b = 23.486(5) Å, c = 16.7061(17) Å, α = 90°, β = 97.942(10)°, γ = 90°, V = 3607.2(10) Å³, Z = 4, crystal size 0.127 x 0.077 x 0.041 mm³, crystal habitat colourless plate, 26502 reflections collected (6317 independent, Rint = 0.1118), 484 parameters, R1 [I>2σ(I)] = 0.0694, wR2 [all data] = 0.2711, largest diff. peak and hole: 0.667 and -1.093 eÅ⁻³.

[2b]2 (CCDC 1833885): C79H52B2P2, M = 1351.27, triclinic, P1, a = 11.857(4) Å, b = 17.522(5) Å, c = 20.340(5) Å, α = 66.613(11)°, β = 79.646(14)°, γ = 88.865(11)°, V = 3809(2) Å³, Z = 2, crystal size 0.140 x 0.058 x 0.020 mm³, crystal habitat orange diamond, 38721 reflections collected (10584 independent, Rint = 0.3533), 969 parameters, R1 [I>2σ(I)] = 0.0941, wR2 [all data] = 0.2326, largest diff. peak and hole: 0.248 and -0.284 eÅ⁻³.

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*Bruker, SADABS,Bruker AXS Inc., Madison, Wisconsin, USA.

† G. M. Sheldrick Acta Cryst., 2008, A64, 112.

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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Click on the hyperlinks for more details of the test.
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0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
0 ALERT level G = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: 3

Bond precision:  C-C = 0.0043 A Wavelength=0.71073

Cell:  a=15.1607(7) b=13.7714(7) c=18.9735(8)
       alpha=90 beta=90 gamma=90
Temperature:  173 K

Volume Calculated 3961.4(3) Reported 3961.4(3)
Space group P n a 21 P n a 21
Hall group P 2c -2n P 2c -2n
Moiety formula C46 H57 B N O P C46 H57 B N O P
Sum formula C46 H57 B N O P C46 H57 B N O P
Mr 681.71 681.71
Dx,g cm\(^{-3}\) 1.143 1.143
Z 4 4
Mu (mm\(^{-1}\)) 0.104 0.104
F000 1472.0 1472.0
F000’ 1472.90
h,k,lmax 21,19,26 21,19,26
Nref 11243[ 5781] 10672
Tmin,Tmax 0.978,0.980 0.707,0.793
Tmin’ 0.978

Correction method= # Reported T Limits: Tmin=0.707 Tmax=0.793
AbsCorr = EMPIRICAL

Data completeness= 1.85/0.95 Theta(max)= 29.681
R(reflections)= 0.0533( 7526) wR2(reflections)= 0.1143( 10672)
S = 1.012 Npar= 461
The following ALERTS were generated. Each ALERT has the format test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

**Alert level C**
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ............... 0.0043 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 36 Ang**3

**Alert level G**
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1 121.4 Degree

0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
1 ALERT level G = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

**Datablock: 4**
No errors found in this datablock

<table>
<thead>
<tr>
<th>Bond precision: C-C = 0.0024 A</th>
<th>Wavelength=0.71073</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell:</td>
<td></td>
</tr>
<tr>
<td>a=9.1955(17)</td>
<td>b=13.889(2)</td>
</tr>
<tr>
<td>alpha=90</td>
<td>beta=95.995(6)</td>
</tr>
<tr>
<td>c=24.546(4)</td>
<td>gamma=90</td>
</tr>
<tr>
<td>Temperature:</td>
<td></td>
</tr>
<tr>
<td>173 K</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>3117.8(9)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21/c</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 2ybc</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C37 H39 B Cl P</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C37 H39 B Cl P</td>
</tr>
<tr>
<td>Mr</td>
<td>560.91</td>
</tr>
<tr>
<td>Dx,g cm-3</td>
<td>1.195</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>Mu (mm-1)</td>
<td>0.198</td>
</tr>
<tr>
<td>F000</td>
<td>1192.0</td>
</tr>
<tr>
<td>F000’</td>
<td>1193.36</td>
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<tr>
<td>h,k,lmax</td>
<td>12,19,34</td>
</tr>
<tr>
<td>Nref</td>
<td>8829</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.972,0.992</td>
</tr>
<tr>
<td>Tmin’</td>
<td>0.972</td>
</tr>
</tbody>
</table>
Correction method= # Reported T Limits: Tmin=0.707 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.996       Theta(max) = 29.667
R(reflections)= 0.0451( 6419)   wR2(reflections)= 0.1423( 8797)
S = 0.920
Npar= 367

Datablock: 2a2

Bond precision:      C-C = 0.0073 A      Wavelength=0.71073

                    alpha=90              beta=109.523(13)          gamma=90
Temperature:      173 K

Calculated          Reported
Volume             7126(6)             7126(6)
Space group        P 21/c             P 21/c
Hall group         -P 2ybc            -P 2ybc
Moiety formula     C74 H78 B2 P2, 2(C4 H10 O) C74 H78 B2 P2, 2(C4 H10 O)
Sum formula        C82 H98 B2 O2 P2   C82 H98 B2 O2 P2
Mr                 1199.16            1199.16
Dx,g cm-3          1.118              1.118
Z                   4                  4
Mu (mm-1)           0.107              0.107
F000               2584.0             2584.0
F000’              2585.69           2585.69
h,k,lmax           21,16,21          21,16,21
Nref               7753              7707
Tmin,Tmax          0.983,0.996       0.666,0.745
Tmin’              0.980

Correction method= # Reported T Limits: Tmin=0.666 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.994       Theta(max) = 21.095
R(reflections)= 0.0598( 5575)   wR2(reflections)= 0.1598( 7707)
S = 1.056
Npar= 881
The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

**Alert level A**

**THETM01_ALERT_3_A** The value of sin(\(theta_{\text{max}}\))/wavelength is less than 0.550

Calculated sin(\(theta_{\text{max}}\))/wavelength = 0.5064

**PLAT023_ALERT_3_A** Resolution (too) Low \([\text{sin(\(theta\))/\Lambda} < 0.6]\)........ 21.09 Degree

**Alert level C**

**REFNR01_ALERT_3_C** Ratio of reflections to parameters is < 10 for a

centrosymmetric structure

\[
\text{sin(\(theta\))/\lambda} \quad 0.5064
\]

Proportion of unique data used 1.0000

Ratio reflections to parameters 8.7480

**PLAT088_ALERT_3_C** Poor Data / Parameter Ratio ......................... 8.80 Note

**PLAT220_ALERT_2_C** Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.1 Ratio

**PLAT222_ALERT_3_C** Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 4.9 Ratio

**PLAT230_ALERT_2_C** Hirshfeld Test Diff for C42 --C43 .. 5.5 s.u.

**PLAT241_ALERT_2_C** High ‘MainMol’ Ueq as Compared to Neighbors of C73 Check

**PLAT243_ALERT_4_C** High ‘Solvent’ Ueq as Compared to Neighbors of C81 Check

**PLAT244_ALERT_4_C** Low ‘Solvent’ Ueq as Compared to Neighbors of O2 Check

**PLAT340_ALERT_3_C** Low Bond Precision on C-C Bonds ............... 0.00728 Ang.

**PLAT360_ALERT_2_C** Short C(sp3)-C(sp3) Bond C80 - C81 .. 1.36 Ang.

**Alert level G**

**PLAT002_ALERT_2_G** Number of Distance or Angle Restraints on AtSite 17 Note

**PLAT003_ALERT_2_G** Number of Uiso or Uij Restrained non-H Atoms ... 16 Report

**PLAT083_ALERT_2_G** SHEXL Second Parameter in WGHT Unusually Large 11.74 Why?

**PLAT175_ALERT_4_G** The CIF-Embedded .res File Contains SAME Records 3 Report

**PLAT177_ALERT_4_G** The CIF-Embedded .res File Contains DELU Records 2 Report

**PLAT178_ALERT_4_G** The CIF-Embedded .res File Contains SIMU Records 2 Report

**PLAT301_ALERT_3_G** Main Residue Disorder ..............(Resd 1 ) 4% Note

**PLAT302_ALERT_4_G** Anion/Solvent/Minor-Residue Disorder (Resd 2 ) 100% Note

**PLAT302_ALERT_4_G** Anion/Solvent/Minor-Residue Disorder (Resd 4 ) 100% Note

**PLAT304_ALERT_4_G** Non-Integer Number of Atoms in ...... Resd 2 8.80 Check

**PLAT304_ALERT_4_G** Non-Integer Number of Atoms in ...... Resd 4 6.20 Check

**PLAT398_ALERT_2_G** Deviating C-O-C Angle From 120 for O1 101.8 Degree

**PLAT793_ALERT_4_G** Model has Chirality at C4 (Centro SPGR) S Verify

**PLAT860_ALERT_3_G** Number of Least-Squares Restraints ............. 243 Note

2 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
14 ALERT level G = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
11 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

**Datablock: 1b**
### Structure Information

**Bond precision:** C-C = 0.0109 Å

**Wavelength:** 0.71073 Å

**Cell:**
- a = 9.2827(14) Å
- b = 23.486(5) Å
- c = 16.7061(17) Å
- α = 90°
- β = 97.942(10)°
- γ = 90°

**Temperature:** 173 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>3607.2(10) Å³</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21/n</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 2yn</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C46 H41 B Br P</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C46 H41 B Br P</td>
</tr>
<tr>
<td>Mr</td>
<td>715.47 g/mol</td>
</tr>
<tr>
<td>Dx, g cm⁻³</td>
<td>1.317</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>F₀₀₀</td>
<td>1488.0</td>
</tr>
<tr>
<td>F₀₀₀'</td>
<td>1487.71</td>
</tr>
<tr>
<td>h, k, l max</td>
<td>11, 27, 19</td>
</tr>
<tr>
<td>Nref</td>
<td>6364</td>
</tr>
<tr>
<td>Tmin, Tmax</td>
<td>0.894, 0.951</td>
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<tr>
<td>Tmin'</td>
<td>0.857</td>
</tr>
</tbody>
</table>

**Correction method:** # Reported T Limits: Tmin=0.610 Tmax=0.745

**AbsCorr:** MULTI-SCAN

**Data completeness:** 0.993

**Theta(max):** 25.026

**R(reflections):** 0.0694 (3853)

**wr²(reflections):** 0.2711 (6317)

**S:** 1.065

**Npar:** 448

---

**The following ALERTS were generated. Each ALERT has the format**

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

### Alert level C

- **PLATO84_ALERT_3_C**
  - High wR² Value (i.e. > 0.25) .................. 0.27 Report

- **PLAT220_ALERT_2_C**
  - Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.7 Ratio

- **PLAT341_ALERT_3_C**
  - Low Bond Precision on C-C Bonds .............. 0.01092 Ang.

### Alert level G

- **PLAT072_ALERT_2_G**
  - SHELXL First Parameter in WGHT Unusually Large 0.17 Report

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

1 **ALERT level G** = General information/check it is not something unexpected
Datablock: 2b2

Bond precision: C-C = 0.0131 Å  Wavelength=0.71073

Cell:
\[
\begin{align*}
a &= 11.857(4) \\
b &= 17.522(5) \\
c &= 20.340(5) \\
\alpha &= 66.613(11) \\
\beta &= 79.646(14) \\
\gamma &= 88.865(11)
\end{align*}
\]

Temperature: 173 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>3809(2)</td>
</tr>
<tr>
<td>Space group</td>
<td>P -1</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 1</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C92 H82 B2 P2, C5 H10</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C97 H92 B2 P2</td>
</tr>
<tr>
<td>Mr</td>
<td>1341.27</td>
</tr>
<tr>
<td>Dx, g cm(^{-3})</td>
<td>1.169</td>
</tr>
<tr>
<td>Z</td>
<td>2</td>
</tr>
<tr>
<td>Mu (mm(^{-1}))</td>
<td>0.105</td>
</tr>
<tr>
<td>F000</td>
<td>1428.0</td>
</tr>
<tr>
<td>F000'</td>
<td>1428.88</td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>13,19,22</td>
</tr>
<tr>
<td>Nref</td>
<td>10940</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.993,0.998</td>
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<tr>
<td>Tmin'</td>
<td>0.985</td>
</tr>
</tbody>
</table>

Correction method = # Reported T Limits: Tmin=0.595 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness = 0.967
Theta(max) = 23.256
R(reflections) = 0.0941 (3653)
wR2(reflections) = 0.2326 (10584)
S = 0.948
Npar = 969

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

- **Alert level A**
  - **RINTA01_ALERT_3_A**: The value of Rint is greater than 0.25
    - Rint given: 0.353
  - **PLAT020_ALERT_3_A**: The Value of Rint is Greater Than 0.12
    - 0.353 Report
**Alert level B**

<table>
<thead>
<tr>
<th>Alert Code</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>THETM01_ALERT_3_B</td>
<td>The value of $\sin(\theta_{\text{max}})/\text{wavelength}$ is less than 0.575</td>
</tr>
<tr>
<td></td>
<td>Calculated $\sin(\theta_{\text{max}})/\text{wavelength} = 0.5555$</td>
</tr>
<tr>
<td>PLATO23_ALERT_3_B</td>
<td>Resolution (too) Low [sin(theta)/Lambda &lt; 0.6] .. 23.26 Degree</td>
</tr>
<tr>
<td>PLATO26_ALERT_3_B</td>
<td>Ratio Observed / Unique Reflections (too) Low .. 35% Check</td>
</tr>
<tr>
<td>PLATO34_ALERT_3_B</td>
<td>Low Bond Precision on C-C Bonds ............... 0.01314 Ang.</td>
</tr>
</tbody>
</table>

**Alert level C**

<table>
<thead>
<tr>
<th>Alert Code</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLATO29_ALERT_3_C</td>
<td>_differn_measured_fraction_theta_full value Low . 0.967 Why?</td>
</tr>
<tr>
<td>PLATO23_ALERT_2_C</td>
<td>Atom C34 has ADP max/min Ratio ..... 3.1 prolat</td>
</tr>
<tr>
<td>PLATO22_ALERT_2_C</td>
<td>Non-Solvent Resd 1 C $U_{eq}(\text{max})/U_{eq}(\text{min})$ Range 3.9 Ratio</td>
</tr>
<tr>
<td>PLATO22_ALERT_3_C</td>
<td>Non-Solv. Resd 1 H $U_{iso}(\text{max})/U_{iso}(\text{min})$ Range 4.4 Ratio</td>
</tr>
<tr>
<td>PLATO24_ALERT_4_C</td>
<td>Large Hirshfeld Difference C3 --C4 0.17 Ang.</td>
</tr>
<tr>
<td>PLATO24_ALERT_4_C</td>
<td>Large Hirshfeld Difference C20 --C21 0.16 Ang.</td>
</tr>
<tr>
<td>PLATO24_ALERT_4_C</td>
<td>Large Hirshfeld Difference C26 --C27 0.18 Ang.</td>
</tr>
<tr>
<td>PLATO24_ALERT_4_C</td>
<td>Large Hirshfeld Difference C28 --C29 0.16 Ang.</td>
</tr>
<tr>
<td>PLATO24_ALERT_4_C</td>
<td>Large Hirshfeld Difference C30 --C31 0.16 Ang.</td>
</tr>
<tr>
<td>PLATO24_ALERT_4_C</td>
<td>Large Hirshfeld Difference C65 --C66 0.17 Ang.</td>
</tr>
<tr>
<td>PLATO24_ALERT_4_C</td>
<td>Large Hirshfeld Difference C81 --C82 0.18 Ang.</td>
</tr>
<tr>
<td>PLATO24_ALERT_4_C</td>
<td>Large Hirshfeld Difference C82 --C83 0.17 Ang.</td>
</tr>
<tr>
<td>PLATO24_ALERT_4_C</td>
<td>Low ‘MainMol’ $U_{eq}$ as Compared to Neighbors of C29 Check</td>
</tr>
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</table>

**Alert level G**

<table>
<thead>
<tr>
<th>Alert Code</th>
<th>Description</th>
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<tbody>
<tr>
<td>PLATO2_ALERT_2_G</td>
<td>Number of Distance or Angle Restraints on AtSite 9 Note</td>
</tr>
<tr>
<td>PLATO0_ALERT_2_G</td>
<td>Number of Uiso or Uij Restained non-H Atoms ... 9 Report</td>
</tr>
<tr>
<td>PLATO9_ALERT_4_G</td>
<td>The CIF-Embedded .res File Contains DFIX Records 1 Report</td>
</tr>
<tr>
<td>PLATO1_ALERT_4_G</td>
<td>The CIF-Embedded .res File Contains SAME Records 2 Report</td>
</tr>
<tr>
<td>PLATO2_ALERT_4_G</td>
<td>The CIF-Embedded .res File Contains DELU Records 1 Report</td>
</tr>
<tr>
<td>PLATO4_ALERT_4_G</td>
<td>Anion/Solvent/Minor-Residue Disorder (Resd 2 ) 100% Note</td>
</tr>
<tr>
<td>PLATO0_ALERT_4_G</td>
<td>Anion/Solvent/Minor-Residue Disorder (Resd 3 ) 100% Note</td>
</tr>
<tr>
<td>PLATO0_ALERT_4_G</td>
<td>Non-Integer Number of Atoms in ...... Resd 2 7.80 Check</td>
</tr>
<tr>
<td>PLATO0_ALERT_4_G</td>
<td>Non-Integer Number of Atoms in ...... Resd 3 7.20 Check</td>
</tr>
<tr>
<td>PLATO0_ALERT_4_G</td>
<td>Incorrectly? Oriented X(sp2)–Methyl Moiety ..... C69 Check</td>
</tr>
<tr>
<td>PLATO9_ALERT_4_G</td>
<td>Centre of Gravity not Within Unit Cell: Resd. # 2 Note</td>
</tr>
<tr>
<td>PLATO0_ALERT_4_G</td>
<td>Model has Chirality at C4 (Centro SPGR) S Verify</td>
</tr>
<tr>
<td>PLATO0_ALERT_4_G</td>
<td>Model has Chirality at C47 (Centro SPGR) R Verify</td>
</tr>
<tr>
<td>PLATO0_ALERT_4_G</td>
<td>Model has Chirality at C50 (Centro SPGR) S Verify</td>
</tr>
<tr>
<td>PLATO0_ALERT_4_G</td>
<td>Number of Least-Squares Restraints ............... 134 Note</td>
</tr>
</tbody>
</table>

| ALERT level A | Most likely a serious problem - resolve or explain                          |
| ALERT level B | A potentially serious problem, consider carefully                           |
| ALERT level C | Check. Ensure it is not caused by an omission or oversight                  |
| ALERT level G | General information/check it is not something unexpected                    |

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
9 ALERT type 3 Indicator that the structure quality may be low
21 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

**checkCIF publication errors**
Publication of your CIF

You should attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author’s name and address are missing,
_RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.
Datablock 2a2 - ellipsoid plot

NOMOVE FORCED

Prob = 50
Temp = 173

PLATON-Mo 30 17:11:10 2018 - (70316)

Z -133 2a2 P 21/c R = 0.06 RES = 0 -118 X