

# Supporting Information

For

## **Diboran(4)yl Platinum(II) Complexes**

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## Experimental Section

### General Considerations

All manipulations were conducted either under an atmosphere of dry argon or *in vacuo* using standard Schlenk line or glovebox techniques. Solvents were purified by distillation from CaH<sub>2</sub> under dry argon and stored over molecular sieves. C<sub>6</sub>D<sub>6</sub> and CD<sub>2</sub>Cl<sub>2</sub> was degassed by three freeze-pump-thaw cycles and stored over molecular sieves. *trans*-[Pt(PEt<sub>3</sub>)<sub>4</sub>],<sup>[1]</sup> Cl<sub>2</sub>B<sub>2</sub>mes<sub>2</sub>,<sup>[2]</sup> Cl<sub>2</sub>B<sub>2</sub>dur<sub>2</sub><sup>[2]</sup> and I<sub>2</sub>B<sub>2</sub>mes<sub>2</sub><sup>[3]</sup> (mes = mesityl, dur = duryl) were prepared according to published procedures. NMR spectra were acquired on a Bruker Avance 400 (<sup>1</sup>H: 400.1 MHz, <sup>11</sup>B: 128.3 MHz, <sup>13</sup>C: 100.6 MHz; <sup>31</sup>P{<sup>1</sup>H}: 161.9 MHz) and Avance 500 (<sup>1</sup>H: 500.1 MHz, <sup>11</sup>B: 160.4 MHz, <sup>13</sup>C: 125.7 MHz; <sup>31</sup>P{<sup>1</sup>H}: 202.2 MHz) FT-NMR spectrometer. <sup>1</sup>H, <sup>13</sup>C and <sup>13</sup>C{<sup>1</sup>H} NMR spectra were referenced to external TMS *via* the residual protons of the solvent (<sup>1</sup>H) or the solvent itself (<sup>13</sup>C). <sup>11</sup>B{<sup>1</sup>H} NMR spectra were referenced to external BF<sub>3</sub>·OEt<sub>2</sub>. <sup>31</sup>P{<sup>1</sup>H} NMR spectra were referenced to external 85% H<sub>3</sub>PO<sub>4</sub>. Microanalyses (C, H, N) were performed on a Leco Instruments elemental analyzer, type CHNS 932.

**Preparation of 1:** [Pt(PEt<sub>3</sub>)<sub>4</sub>] (150 mg, 0.22 mmol) was placed in a Schlenk flask and heated at 55 °C over a period of one hour under high vacuum to remove one PEt<sub>3</sub> ligand. Orange oily [Pt(PEt<sub>3</sub>)<sub>3</sub>] was subsequently dissolved in pentane (2 mL) and treated with Cl<sub>2</sub>B<sub>2</sub>mes<sub>2</sub> (148 mg, 0.44 mmol). After 15 minutes, the colorless precipitate was filtered off and all volatiles were removed *in vacuo*. The remaining solid was recrystallized from dichloromethane/pentane at −25 °C to afford *trans*-[(Et<sub>3</sub>P)<sub>2</sub>Pt(Cl)]{B(mes)B(mes)(Cl)} (1; 41.0 mg, 0.05 mmol, 24%) as a crystalline material.

**<sup>1</sup>H NMR** (400.1 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 300 K): δ = 7.01 (s, 1H; CH), 6.98 (s, 1H; CH), 6.94–6.60 (br m, 2H; CH), 3.42 (s, 3H; CH<sub>3</sub>), 3.09 (br s, 3H; CH<sub>3</sub>), 2.54 (s, 3H; CH<sub>3</sub>), 2.25 (s, 3H; CH<sub>3</sub>), 2.24 (s, 3H; CH<sub>3</sub>), 2.20–1.96 (m, 3H; P<sup>2</sup>CH<sub>2</sub>), 1.80–1.58 (m, 3H; P<sup>2</sup>CH<sub>2</sub>), 1.55–1.23 (m, 6H; P<sup>1</sup>CH<sub>2</sub>), 1.09–0.96 (br m, 9H; P<sup>2</sup>(CH<sub>2</sub>CH<sub>3</sub>)<sub>3</sub>), 0.95–0.79 ppm (br m, 9H; P<sup>1</sup>(CH<sub>2</sub>CH<sub>3</sub>)<sub>3</sub>); **<sup>11</sup>B{<sup>1</sup>H} NMR** (128.3 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 300 K): δ = 105 (vbr s; FWHM = 1646 Hz), 59.9 ppm (br s; FWHM =

1735 Hz);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100.6 MHz,  $\text{CD}_2\text{Cl}_2$ , 300 K):  $\delta$  = 146.3 (s;  $\text{C}_i$ ), 144.7 (s;  $\text{C}_i$ ), 142.9 (s;  $\text{C}_i$ ), 140.2 (s;  $\text{C}_i$ ), 139.8 (s;  $\text{C}_i$ ), 139.0 (s;  $\text{C}_i$ ), 129.8 (s; CH), 129.7 (s; CH), 128.3 (br s; CH), 29.8 (sv  $\text{CH}_3$ ), 28.4 (s;  $\text{CH}_3$ ), 26.1 (br s;  $\text{CH}_3$ ), 23.3 (br s;  $\text{CH}_3$ ), 21.6 (s;  $\text{CH}_3$ ), 21.1 (s;  $\text{CH}_3$ ), 17.1–16.1 (m;  $\text{PCH}_2$ ), 9.24–8.57 ppm (m;  $\text{PCH}_2\text{CH}_3$ );  $^{31}\text{P}\{^1\text{H}\}$  NMR (161.9 MHz,  $\text{CD}_2\text{Cl}_2$ , 300 K):  $\delta$  = 11.42 (d,  $^1J_{\text{P-Pt}}$  = 2916 Hz,  $^2J_{\text{P-P}}$  = 327 Hz), 8.06 ppm (d,  $^1J_{\text{P-Pt}}$  = 2972 Hz,  $^2J_{\text{P-P}}$  = 327 Hz); **El. Anal.** (%) calc. for  $\text{C}_{30}\text{H}_{52}\text{B}_2\text{Cl}_2\text{P}_2\text{Pt}$  (762.28  $\text{g}\cdot\text{mol}^{-1}$ ): C 47.27, H 6.88; found: C 47.57, H 7.02.

**Preparation of 2:**  $[\text{Pt}(\text{PEt}_3)_4]$  (148 mg, 0.22 mmol) was placed in a Schlenk flask and heated at 55 °C over a period of one hour under high vacuum to remove one  $\text{PEt}_3$  ligand. Orange oily  $[\text{Pt}(\text{PEt}_3)_3]$  was subsequently dissolved in pentane (5 mL) and reacted with  $\text{Cl}_2\text{B}_2\text{dur}_2$  (160 mg, 0.44 mmol). After 15 minutes, the colorless precipitate was filtered off and all volatiles were removed in vacuo. The remaining orange-red solid was taken up into  $\text{CH}_2\text{Cl}_2$  and layered with pentane until a colorless precipitate formed, which was again removed by filtration. The filtrate was stored at –25 °C to afford *trans*- $[(\text{Et}_3\text{P})_2\text{Pt}(\text{Cl})\{\text{B}(\text{dur})\text{B}(\text{dur})(\text{Cl})\}]$  (**2**; 87.0 mg, 0.11 mmol, 49%) as a orange-red material.

$^1\text{H}$  NMR (400.1 MHz,  $\text{CD}_2\text{Cl}_2$ , 300 K):  $\delta$  = 7.28 (s, 1H;  $\text{Dur}^1$ , CH), 6.94 (s, 1H;  $\text{Dur}^2$ , CH), 3.44 (br s, 3H;  $\text{Dur}^1$ ,  $\text{CH}_3$ ), 3.08 (s, 3H;  $\text{Dur}^2$ ,  $\text{CH}_3$ ), 2.54 (br s, 3H;  $\text{Dur}^1$ ,  $\text{CH}_3$ ), 2.31 (s, 3H;  $\text{Dur}^1$ ,  $\text{CH}_3$ ), 2.25 (s, 3H;  $\text{Dur}^2$ ,  $\text{CH}_3$ ), 2.09 (s, 3H;  $\text{Dur}^1$ ,  $\text{CH}_3$ ), 2.09 (s, 3H;  $\text{Dur}^2$ ,  $\text{CH}_3$ ), 2.20–2.06 (m, 3H;  $\text{P}^2\text{CH}_2$ ), 2.05 (s, 3H;  $\text{Dur}^2$ ,  $\text{CH}_3$ ), 1.80–1.56 (m, 3H;  $\text{P}^2\text{CH}_2$ ), 1.55–1.23 (m, 6H;  $\text{P}^1\text{CH}_2$ ), 1.15–0.95 (br m, 9H;  $\text{P}^2(\text{CH}_2\text{CH}_3)_3$ ), 0.94–0.66 (br m, 9H;  $\text{P}^1(\text{CH}_2\text{CH}_3)_3$ );  $^{11}\text{B}\{^1\text{H}\}$  NMR (128.3 MHz,  $\text{CD}_2\text{Cl}_2$ , 300 K):  $\delta$  = 109 (vbr s; FWHM = 1830 Hz), 57.7 ppm (br s; FWHM = 1739 Hz);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100.6 MHz,  $\text{CD}_2\text{Cl}_2$ , 300 K):  $\delta$  = 143.9 (s;  $\text{C}_i$ ), 143.0 (s;  $\text{C}_i$ ), 139.6 (s;  $\text{C}_i$ ), 136.3 (s, 1C; CH), 135.1 (s;  $\text{C}_i$ ), 134.9 (s;  $\text{C}_i$ ), 134.7 (s;  $\text{C}_i$ ), 133.6 (s;  $\text{C}_i$ ), 132.4 (s; CH), 27.7 (br s;  $\text{CH}_3$ ), 27.7 (br s;  $\text{CH}_3$ ), 23.4 (br s;  $\text{CH}_3$ ), 21.3 (s;  $\text{CH}_3$ ), 20.6 (s;  $\text{CH}_3$ ), 20.5 (s;  $\text{CH}_3$ ), 20.4 (s;  $\text{CH}_3$ ), 20.3 (s;  $\text{CH}_3$ ), 17.3–15.9 (m;  $\text{PCH}_2$ ), 8.86 ppm (s;  $\text{PCH}_2\text{CH}_3$ );  $^{31}\text{P}\{^1\text{H}\}$  NMR (161.9 MHz,  $\text{CD}_2\text{Cl}_2$ , 300 K):  $\delta$  = 11.21 (d,  $^1J_{\text{P-Pt}}$  = 2929 Hz,  $^2J_{\text{P-P}}$  = 326 Hz), 7.69 ppm (d,  $^1J_{\text{P-Pt}}$  = 2984 Hz,  $^2J_{\text{P-P}}$  = 326 Hz); **El. Anal.** (%) calc. for  $\text{C}_{32}\text{H}_{56}\text{B}_2\text{Cl}_2\text{P}_2\text{Pt}$  (790.33  $\text{g}\cdot\text{mol}^{-1}$ ): C 48.63, H 7.14; found: C 48.85, H 7.02.

**Preparation of 3:**  $[\text{Pt}(\text{PEt}_3)_4]$  (102 mg, 0.15 mmol) was placed in a Schlenk flask and heated at 55 °C over a period of one hour under high vacuum to remove one  $\text{PEt}_3$  ligand. Orange oily

[Pt(PEt<sub>3</sub>)<sub>3</sub>] was subsequently dissolved in pentane (1 mL) and reacted with I<sub>2</sub>B<sub>2</sub>mes<sub>2</sub> (160 mg, 0.31 mmol). After 15 minutes, the colorless precipitate was filtered off and all volatiles were removed in vacuo. The remaining orange-red solid was dissolved in CH<sub>2</sub>Cl<sub>2</sub> and layered with pentane until a colorless precipitate formed, which was again removed by filtration. The filtrate was stored at –25 °C to afford *trans*-[(Et<sub>3</sub>P)<sub>2</sub>Pt(I){B(mes)B(mes)(I)}] (**3**; (42.0 mg, 0.04 mmol, 28%) as a red material.

**<sup>1</sup>H NMR** (400.1 MHz, C<sub>6</sub>D<sub>6</sub>, 300 K):  $\delta$  = 6.94 (s, 2H; *m*-CH), 6.86 (s, 1H; *m*-CH), 6.59 (s, 1H; *m*-CH), 3.57 (s, 3H; CH<sub>3</sub>), 3.42 (s, 3H; CH<sub>3</sub>), 3.03 (s, 3H; CH<sub>3</sub>), 2.31 (s, 3H; CH<sub>3</sub>), 2.12 (s, 3H; CH<sub>3</sub>), 2.05 (s, 3H; CH<sub>3</sub>), 2.31 (m, <sup>1</sup>J<sub>H-P</sub> = 304 Hz, 6H; PCH<sub>2</sub>), 2.01–1.14 (br m, 6H; PCH<sub>2</sub>), 0.97–0.82 (m, 9H; PCH<sub>2</sub>CH<sub>3</sub>), 0.69 ppm (m, 9H; PCH<sub>2</sub>CH<sub>3</sub>); **<sup>11</sup>B{<sup>1</sup>H} NMR** (128.3 MHz, C<sub>6</sub>D<sub>6</sub>, 300 K):  $\delta$  = 106 (vbr s; FWHM = 1772 Hz), 50.0 ppm (br s; FWHM = 1567 Hz). **<sup>13</sup>C{<sup>1</sup>H} NMR** (100.6 MHz, C<sub>6</sub>D<sub>6</sub>, 300 K):  $\delta$  = 147.4 (s; C<sub>i</sub>), 145.0 (s; C<sub>i</sub>), 143.1 (s; C<sub>i</sub>), 140.7 (s; C<sub>i</sub>), 138.8 (s; C<sub>i</sub>), 138.3 (s; C<sub>i</sub>), 135.0 (s; C<sub>i</sub>), 130.8 (s; *m*-CH), 130.1 (s; *m*-CH), 129.8 (s; *m*-CH), 127.8 (s; *m*-CH), 32.1 (s; CH<sub>3</sub>), 29.9 (s; CH<sub>3</sub>), 28.7 (s; CH<sub>3</sub>), 24.1 (s; CH<sub>3</sub>), 21.4 (s; CH<sub>3</sub>), 21.0 (s; CH<sub>3</sub>), 19.7–18.3 (m; PCH<sub>2</sub>), 10.2–9.27 ppm (m; PCH<sub>2</sub>CH<sub>3</sub>). **<sup>31</sup>P{<sup>1</sup>H} NMR** (161.9 MHz, C<sub>6</sub>D<sub>6</sub>, 300 K):  $\delta$  = 2.48 (d, <sup>1</sup>J<sub>P-Pt</sub> = 2812 Hz, <sup>2</sup>J<sub>P-P</sub> = 335 Hz), 1.82 ppm (d, <sup>1</sup>J<sub>P-Pt</sub> = 2837 Hz, <sup>2</sup>J<sub>P-P</sub> = 335 Hz); **El. Anal.** (%) calc. for C<sub>30</sub>H<sub>52</sub>B<sub>2</sub>I<sub>2</sub>P<sub>2</sub>Pt (945.19 g·mol<sup>–1</sup>): C 38.12, H 5.55; found: C 38.61, H 5.66.

## Crystal structure determination

The crystal data of **1-3** and  $\text{Cl}_2\text{B}_2\text{dur}_2$  were collected on a Bruker X8APEX diffractometer with a CCD area detector and multi-layer mirror monochromated  $\text{Mo}_{K\alpha}$  radiation. The structure were solved using direct methods, refined with the ShelX software package and expanded using Fourier techniques.<sup>[4]</sup> All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were assigned to idealized positions and were included in structure factors calculations.

The crystals of **1** were racemic twins [TWIN -1 0 0, 0 -1 0, 0 0 -1 ]. The BASF parameter was refined to 51.9%. The crystals of  **$\text{Cl}_2\text{B}_2\text{dur}_2$**  were pseudo-merohedral twins with domains rotated by 180° around reciprocal axis [0.000, 0.000, 1.000]. The BASF parameter was refined to 13%.

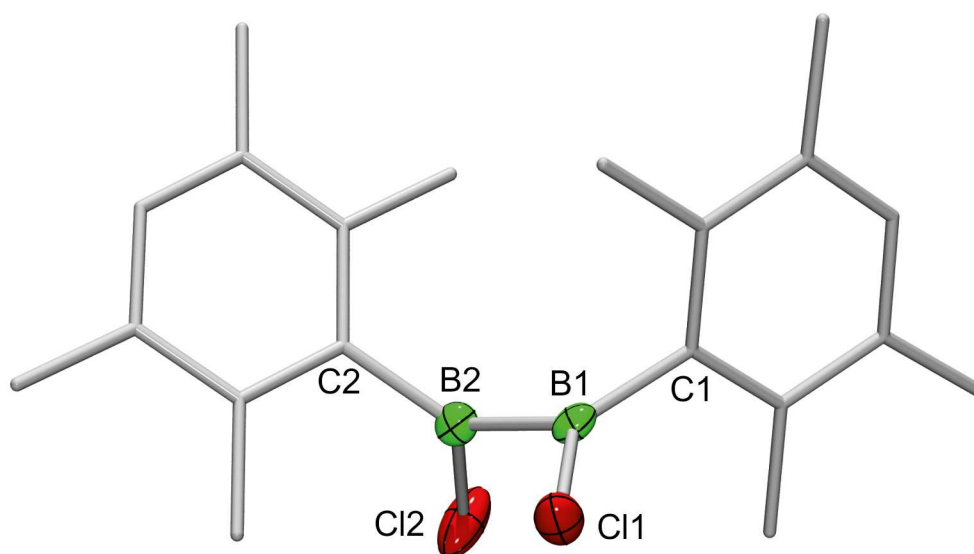
Crystal data for **1**:  $\text{C}_{30}\text{H}_{52}\text{B}_2\text{Cl}_2\text{P}_2\text{Pt}$ ,  $M_r = 762.27$ , yellow block,  $0.40 \times 0.30 \times 0.20 \text{ mm}^3$ , Monoclinic space group  $P2_1$ ,  $a = 9.9318(8) \text{ \AA}$ ,  $b = 14.4156(13) \text{ \AA}$ ,  $c = 11.6055(11) \text{ \AA}$ ,  $\beta = 94.726(3)^\circ$ ,  $V = 1655.9(3) \text{ \AA}^3$ ,  $Z = 2$ ,  $\rho_{\text{calcd}} = 1.529 \text{ g}\cdot\text{cm}^{-3}$ ,  $\mu = 4.513 \text{ mm}^{-1}$ ,  $F(000) = 768$ ,  $T = 100(2) \text{ K}$ ,  $R_I = 0.0112$ ,  $wR^2 = 0.0254$ , 6345 independent reflections [ $2\theta \leq 52.12^\circ$ ] and 346 parameters.

Crystal data for **2**:  $\text{C}_{32}\text{H}_{56}\text{B}_2\text{Cl}_2\text{P}_2\text{Pt}$ ,  $M_r = 790.32$ , orange block,  $0.349 \times 0.295 \times 0.245 \text{ mm}^3$ , Monoclinic space group  $P2_1/n$ ,  $a = 12.4828(9) \text{ \AA}$ ,  $b = 19.9323(15) \text{ \AA}$ ,  $c = 14.2861(11) \text{ \AA}$ ,  $\beta = 99.094(2)^\circ$ ,  $V = 3509.9(5) \text{ \AA}^3$ ,  $Z = 4$ ,  $\rho_{\text{calcd}} = 1.496 \text{ g}\cdot\text{cm}^{-3}$ ,  $\mu = 4.261 \text{ mm}^{-1}$ ,  $F(000) = 1600$ ,  $T = 100(2) \text{ K}$ ,  $R_I = 0.0223$ ,  $wR^2 = 0.0511$ , 7454 independent reflections [ $2\theta \leq 53.54^\circ$ ] and 360 parameters.

Crystal data for **3**:  $\text{C}_{30}\text{H}_{52}\text{B}_2\text{I}_2\text{P}_2\text{Pt}$ ,  $M_r = 945.17$ , yellow block,  $0.044 \times 0.124 \times 0.197 \text{ mm}^3$ , Monoclinic space group  $P2_1$ ,  $a = 10.2358(8) \text{ \AA}$ ,  $b = 14.2110(12) \text{ \AA}$ ,  $c = 11.9534(10) \text{ \AA}$ ,  $\beta = 90.376(4)^\circ$ ,  $V = 1738.7(2) \text{ \AA}^3$ ,  $Z = 2$ ,  $\rho_{\text{calcd}} = 1.805 \text{ g}\cdot\text{cm}^{-3}$ ,  $\mu = 5.921 \text{ mm}^{-1}$ ,  $F(000) = 912$ ,  $T = 100(2) \text{ K}$ ,  $R_I = 0.0185$ ,  $wR^2 = 0.0455$ , 6852 independent reflections [ $2\theta \leq 52.2^\circ$ ] and 347 parameters.

Crystal data for **Cl<sub>2</sub>B<sub>2</sub>dur<sub>2</sub>**: C<sub>20</sub>H<sub>26</sub>B<sub>2</sub>Cl<sub>2</sub>,  $M_r = 358.93$ , colourless block, 0.92×0.45×0.30 mm<sup>3</sup>, Monoclinic space group  $P2_1/c$ ,  $a = 9.1831(7)$  Å,  $b = 15.2072(12)$  Å,  $c = 14.8233(12)$  Å,  $\beta = 105.077(3)^\circ$ ,  $V = 1998.8(3)$  Å<sup>3</sup>,  $Z = 4$ ,  $\rho_{\text{calcd}} = 1.193$  g·cm<sup>-3</sup>,  $\mu = 0.323$  mm<sup>-1</sup>,  $F(000) = 760$ ,  $T = 100(2)$  K,  $R_1 = 0.0602$ ,  $wR^2 = 0.1419$ , 4015 independent reflections [ $2\theta \leq 52.22^\circ$ ] and 226 parameters.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC 928667 (1), CCDC 928668 (2), 928669 (3), and CCDC 928691 (Cl<sub>2</sub>B<sub>2</sub>dur<sub>2</sub>). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif)



**Figure S1.** Molecular structure of the Cl<sub>2</sub>B<sub>2</sub>dur<sub>2</sub> in the solid state. Thermal ellipsoids are displayed at the 50% probability level. For clarity, hydrogen atoms and thermal ellipsoids of the carbon atoms have been omitted. Selected bond lengths (Å) and angles (deg): B1–C1 1.561(4), B1–B2 1.690(4), B1–Cl1 1.777(3), B2–C2 1.564(3), B2–Cl2 1.761(3), C1–B1–B2 127.4(2), C1–B1–Cl1 118.30(18), B2–B1–Cl1 114.25(19), C2–B2–B1 126.5(2), C2–B2–Cl2 117.19(18), B1–B2–Cl2 116.29(18), C1–B1–B2–C2 -97.4(3), Cl1–B1–B2–C2 80.5(3), C1–B1–B2–Cl2 82.6(3).

**Table S1.** Crystallographic data of **1** and **2**.

Data	<b>1</b>	<b>2</b>
Empirical formula	C <sub>30</sub> H <sub>52</sub> B <sub>2</sub> Cl <sub>2</sub> P <sub>2</sub> Pt	C <sub>32</sub> H <sub>56</sub> B <sub>2</sub> Cl <sub>2</sub> P <sub>2</sub> Pt
Formula weight (g·mol <sup>-1</sup> )	762.27	790.32
Temperature (K)	100(2)	100(2)
Radiation, $\lambda$ (Å)	MoK $\alpha$ 0.71073	MoK $\alpha$ 0.71073
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub>	<i>P</i> 2 <sub>1</sub> / <i>n</i>
<i>Unit cell dimensions</i>		
<i>a</i> (Å)	9.9318(8)	12.4828(9)
<i>b</i> (Å)	14.4156(13)	19.9323(15)
<i>c</i> (Å)	11.6055(11)	14.2861(11)
$\alpha$ (°)	90.00	90.00
$\beta$ (°)	94.726(3)	99.094(2)
$\gamma$ (°)	90.00	90.00
Volume (Å <sup>3</sup> )	1655.9(3)	3509.9(5)
<i>Z</i>	2	4
Calculated density (Mg·m <sup>-3</sup> )	1.529	1.496
Absorbtion coefficient (mm <sup>-1</sup> )	4.513	4.261
<i>F</i> (000)	768	1600
Theta range for collection	1.76 to 26.06°	1.77 to 26.77°
Reflections collected	51179	57289
Independent reflections	6345	7454
Minimum/maximum transmission	0.5833/0.7453	0.5169/0.7454
Refinement method	Full-matrix least-squares on <i>F</i> <sup>2</sup>	Full-matrix least-squares on <i>F</i> <sup>2</sup>
Data / parameters / restrains	6345 / 346 / 1	7454 / 360 / 0
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.005	1.086
Final R indices [ <i>I</i> >2 $\sigma$ ( <i>I</i> )]	R <sub>1</sub> = 0.0108, <i>w</i> R <sup>2</sup> = 0.0253	R <sub>1</sub> = 0.0200, <i>w</i> R <sup>2</sup> = 0.0500
R indices (all data)	R <sub>1</sub> = 0.0112, <i>w</i> R <sup>2</sup> = 0.0254	R <sub>1</sub> = 0.0223, <i>w</i> R <sup>2</sup> = 0.0511
Maximum/minimum residual electron density (e·Å <sup>-3</sup> )	0.550 / -0.281	1.159 / -0.557

**Table S2.** Crystallographic data of **3** and **Cl<sub>2</sub>B<sub>2</sub>dur<sub>2</sub>**.

Data	<b>3</b>	<b>Cl<sub>2</sub>B<sub>2</sub>dur<sub>2</sub></b>
Empirical formula	C <sub>30</sub> H <sub>52</sub> B <sub>2</sub> I <sub>2</sub> P <sub>2</sub> Pt	C <sub>20</sub> H <sub>26</sub> B <sub>2</sub> Cl <sub>2</sub>
Formula weight (g·mol <sup>-1</sup> )	945.17	358.93
Temperature (K)	100(2)	100(2)
Radiation, λ (Å)	MoK <sub>α</sub> 0.71073	MoK <sub>α</sub> 0.71073
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub>	<i>P</i> 2 <sub>1</sub> / <i>c</i>
<i>Unit cell dimensions</i>		
<i>a</i> (Å)	10.2358(8)	9.1831(7)
<i>b</i> (Å)	14.2110(12)	15.2072(12)
<i>c</i> (Å)	11.9534(10)	14.8233(12)
α (°)	90.00	90.00
β (°)	90.376(4)	105.077(3)
γ (°)	90.00	90.00
Volume (Å <sup>3</sup> )	1738.7(2)	1998.8(3)
<i>Z</i>	2	4
Calculated density (Mg·m <sup>-3</sup> )	1.805	1.193
Absorbtion coefficient (mm <sup>-1</sup> )	5.921	0.323
<i>F</i> (000)	912	760
Theta range for collection	1.70 to 26.10°	1.95 to 26.11°
Reflections collected	95789	3955
Independent reflections	6852	4015
Minimum/maximum transmission	0.5798/0.7453	0.400285/0.745318
Refinement method	Full-matrix least-squares on <i>F</i> <sup>2</sup>	Full-matrix least-squares on <i>F</i> <sup>2</sup>
Data / parameters / restraints	6852 / 347 / 1	4015 / 226 / 0
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.118	1.081
Final R indices [ <i>I</i> >2σ( <i>I</i> )]	R <sub>1</sub> = 0.0171, wR <sup>2</sup> = 0.0439	R <sub>1</sub> = 0.0502, wR <sup>2</sup> = 0.1368
R indices (all data)	R <sub>1</sub> = 0.0185, wR <sup>2</sup> = 0.0455	R <sub>1</sub> = 0.0602, wR <sup>2</sup> = 0.1419
Maximum/minimum residual electron density (e·Å <sup>-3</sup> )	1.625 / -1.156	0.641 / -0.551



## References

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