

## Electronic Supplementary Information

### **Pt(II)-Coordinated Tricomponent Self-Assemblies of Tetrapyrridyl Porphyrin and Dicarboxylate Ligands: Are They 3D Prisms or 2D Bow Ties?†**

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## General Materials and Methods

Reagents, starting materials, and solvents were purchased from Sigma-Aldrich, Acros Organic and TCI America. *cis*-Pt(PET<sub>3</sub>)<sub>2</sub>(OTf)<sub>2</sub> and ZnTPP were prepared following reported procedures.<sup>1,2</sup>

The <sup>1</sup>H, COSY, and ROESY NMR spectra were recorded on a Bruker NEO 500 MHz NMR spectrometers. For ROESY, a mixing time of 491 ms was employed for all samples. The <sup>31</sup>P NMR spectra was recorded at 122 MHz using the same instrument. The DOSY NMR spectra were recorded using a gradient duration of 1 ms and a diffusion delay of 0.1 s. Diffusion coefficient values (D) were calculated from the TOPSPIN software and the hydrodynamic radii (r<sub>H</sub>) was calculated using Stokes-Einstein equation at *T* = 298 K.

The electrochemical measurements were conducted on a Princeton Applied Research VersaStat-3-450 instrument using a glassy carbon working electrode, Ag/AgCl reference electrode, Pt counter electrode, and a 0.1 M of Bu<sub>4</sub>N<sup>+</sup>TfO<sup>-</sup>/CH<sub>2</sub>Cl<sub>2</sub> solution as supporting electrolyte.

UV-vis absorption spectra were recorded in a Shimadzu UV-2600 spectrophotometer equipped with an integrated sphere (200–1100 nm range).

Electrospray ionization mass spectra (ESIMS) were recorded on a Bruker BioTOF II ESI/TOF-MS instrument at the Waters Center for Innovation in Mass Spectrometry of the Department of Chemistry at the University of Minnesota, Twin Cities.

The single crystal X-ray diffraction (SXRD) data were collected on a Bruker D8 Venture dual source diffractometer equipped with Cu and Mo radiation sources and CMOS detector. The crystal structures of bow tie complexes were solved and refined by using Bruker SHELXTL software package. The crystals of some bow tie complexes diffracted poorly, and the ethyl groups on Et<sub>3</sub>P ligands were highly disordered due to thermal motions. These disordered ethyl groups were fixed by using the DFIX, DANG commands. In addition, the coordination of bridging XDC linkers with two Pt(II) corners also created strain and made them slightly bend and disordered in **BT3**, **BT3'**, and **BT4**. AFIX and DFIX commands were applied to fix these issues. The highly disordered triflate anions were hard to assign and omitted by PLATON/SQUEEZE in some cases, while in other cases they were assigned fully/partially using SAME/SIMU commands. ISOR and RIGU commands were applied for the atoms that were not behaving well isothermally. A SHEL cut-off was applied to remove the weak reflections in most of the structures. The disordered solvent molecules were also removed by PLATON/SQUEEZE model. The significant amount of disorder and weak diffraction of some crystals resulted in several A- and B-alerts, which have been addressed properly in the corresponding checkCIFs, while the commands applied to fix the disordered atoms and groups caused large R-values in those cases. Nevertheless, the basic bow tie skeletons of all complexes were well resolved and the disordered Et<sub>3</sub>P groups, counter anions, and solvent molecules had practically no impact on the overall shape and geometry of these complexes.

The geometry optimized structures were calculated with semi-empirical methods using PM6 model on Gaussian software version 09.

## Synthesis and Characterization

**Dicarboxylate (XDC) Ligands.** In general, aqueous solutions of 2.5 equiv. of KOH was added to respective dicarboxylic acids (i.e., hexane-, 4,4'-biphenyl, 1,4-benzene-, and 2,6-naphthalene dicarboxylic acids) and the resulting mixtures were stirred until the solids were fully solubilized due to salt formation. At this point, MeOH was added to the solution mixtures, which led to the precipitation of dipotassium dicarboxylate salts. The resulting solids were filtrated, washed thoroughly with cold MeOH, and recrystallized from MeOH, to remove excess of KOH and obtain pure products.

**General Protocol of Tricomponent Self-Assembly of *cis*-Pt(Et<sub>3</sub>P)<sub>2</sub>(TfO)<sub>2</sub>, M'TPP, and XDC.** The supramolecular coordination complexes were prepared following previously reported procedures.<sup>3</sup> Briefly, to a mixture of *cis*-Pt(PET<sub>3</sub>)<sub>2</sub>(OTf)<sub>2</sub> (4 equiv.), M'TPP (M' = Zn or H<sub>2</sub>, 1 equiv.), and XDC (XDC = HDC, BPDC, BDC, and NDC, 2 equiv.) placed in a 20 mL screw-capped glass was added a 1:1:1

CH<sub>2</sub>Cl<sub>2</sub>/MeNO<sub>2</sub>/MeCN (or 1:1 (CH<sub>3</sub>)<sub>2</sub>CO/H<sub>2</sub>O) solvent mixture (5mL). The reaction mixtures were then stirred at 60 °C overnight. After allowing the reaction mixtures to cool down to room temperature, Et<sub>2</sub>O was added to the filtrates and the resulting precipitates were collected by centrifugation. This washing process was repeated three times to obtain pure tricomponent bow tie complexes **BT1–BT4** containing ZnTPP and **BT1'–BT4'** containing H<sub>2</sub>TPP cores.

**BT1.** *cis*-Pt(PEt<sub>3</sub>)<sub>2</sub>(OTf)<sub>2</sub> (4.49 mg, 0.0059 mmol), ZnTPP (1.0 mg, 0.00147 mmol), and HDC (0.64 mg, 0.0029 mmol) in a 1:1:1 DCM/MeNO<sub>2</sub>/MeCN solvent mixture (1 mL). Yield = 4.5 mg (93%). <sup>1</sup>H NMR (500 MHz, acetone-*d*<sub>6</sub>) δ = 9.28 (br s, 8H, H<sub>a</sub>), 9.18 (s, 4H, H<sub>c'</sub>), 8.50 (d, *J* = 5.8 Hz, 8H, H<sub>b</sub>), 8.38 (s, 4H, H<sub>c</sub>), 2.33 – 2.15 (m, 56H, H<sub>s</sub> and H<sub>CH<sub>2</sub></sub>), 1.65 (br s, 8H, H<sub>i</sub>), 1.51 – 1.36 (m, 72H, H<sub>CH<sub>3</sub></sub>) ppm. <sup>31</sup>P NMR (202 MHz, acetone-*d*<sub>6</sub>) δ 6.23 (d, *J* = 20.5 Hz), 0.23 (d, *J* = 21.0 Hz). ESI-MS (*m/z*) Calculated for C<sub>102</sub>H<sub>160</sub>F<sub>6</sub>N<sub>8</sub>O<sub>14</sub>P<sub>8</sub>Pt<sub>4</sub>S<sub>2</sub>Zn [M–2TfO]<sup>2+</sup>: 1497.14. Found: 1497.09.

**BT2.** *cis*-Pt(PEt<sub>3</sub>)<sub>2</sub>(OTf)<sub>2</sub> (14.10 mg, 0.019 mmol), ZnTPP (3.30 mg, 0.0048 mmol), and BPDC (3.08 mg, 0.0096 mmol) in a 1:1:1 DCM/MeNO<sub>2</sub>/MeCN (or 1:1 (CH<sub>3</sub>)<sub>2</sub>CO/H<sub>2</sub>O) solvent mixture (5 mL). Yield = 16.02 mg (95%). <sup>1</sup>H NMR (500 MHz, acetone-*d*<sub>6</sub>) δ = 9.28 (br s, 8H, H<sub>a</sub>), 8.58 (s, 4H, H<sub>c'</sub>), 8.38 (d, *J* = 5.6 Hz, 8H, H<sub>b</sub>), 8.10 (d, *J* = 8.1 Hz, 8H, H<sub>u</sub>), 7.98 (d, *J* = 8.2 Hz, 8H, H<sub>v</sub>), 7.74 (s, 4H, H<sub>c</sub>), 2.44 – 2.18 (m, 48H, H<sub>CH<sub>2</sub></sub>), 1.58 – 1.42 (m, 72H, H<sub>CH<sub>3</sub></sub>). <sup>31</sup>P NMR (122 MHz, acetone-*d*<sub>6</sub>) δ 6.83 (d, *J* = 20.6 Hz), 1.78 (d, *J* = 21.2 Hz). ESI-MS (*m/z*) Calculated for C<sub>118</sub>H<sub>160</sub>F<sub>6</sub>N<sub>8</sub>O<sub>14</sub>P<sub>8</sub>Pt<sub>4</sub>S<sub>2</sub>Zn [M–2TfO]<sup>2+</sup> 1593.23, Found: 1593.58.

**BT3.** *cis*-Pt(PEt<sub>3</sub>)<sub>2</sub>(OTf)<sub>2</sub> (14.10 mg, 0.019 mmol), BDC (2.34 mg, 0.0096 mmol) and ZnTPP (3.30 mg, 0.0048 mmol) in a 1:1:1 DCM/MeNO<sub>2</sub>/MeCN (or 1:1 (CH<sub>3</sub>)<sub>2</sub>CO/H<sub>2</sub>O) solvent mixture (5 mL). Yield = 14.83 mg (92%). <sup>1</sup>H NMR (500 MHz, acetone-*d*<sub>6</sub>) δ = 9.35 (br s, 8H, H<sub>a</sub>), 9.16 (s, 4H, H<sub>c'</sub>), 8.36 (d, *J* = 6.3 Hz, 8H, H<sub>b</sub>), 8.09 (s, 8H, H<sub>w</sub>), 7.13 (s, 4H, H<sub>c</sub>), 2.40 – 2.19 (m, 48H, H<sub>CH<sub>2</sub></sub>), 1.57 – 1.41 (m, 72H, H<sub>CH<sub>3</sub></sub>) ppm. <sup>31</sup>P NMR (203 MHz, acetone-*d*<sub>6</sub>) δ = 6.02 (d, *J* = 20.5 Hz), 1.01 (d, *J* = 21.4 Hz) ppm. ESI-MS (*m/z*) Calculated for C<sub>106</sub>H<sub>152</sub>F<sub>6</sub>N<sub>8</sub>O<sub>14</sub>P<sub>8</sub>Pt<sub>4</sub>S<sub>2</sub>Zn [M–2TfO]<sup>2+</sup>: 1517.13. Found: 1517.01.

**BT4.** *cis*-Pt(PEt<sub>3</sub>)<sub>2</sub>(OTf)<sub>2</sub> (14.10 mg, 0.019 mmol), BDC (2.83 mg, 0.0096 mmol) and ZnTPP (3.30 mg, 0.0048 mmol) in a 1:1:1 DCM/MeNO<sub>2</sub>/MeCN (or 1:1 (CH<sub>3</sub>)<sub>2</sub>CO/H<sub>2</sub>O) solvent mixture (5 mL). Yield = 15.78 mg (95%). <sup>1</sup>H NMR (500 MHz, acetone-*d*<sub>6</sub>) δ = 9.37 (br s, 8H, H<sub>a</sub>), 8.86 (s, 4H, H<sub>c'</sub>), 8.71 (s, 4H, H<sub>x</sub>), 8.26 (d, *J* = 5.6 Hz, 8H, H<sub>b</sub>), 8.16 (d, *J* = 8.3 Hz, 4H, H<sub>y</sub>), 8.09 (d, *J* = 8.4 Hz, 4H, H<sub>z</sub>), 6.79 (s, 4H, H<sub>c</sub>), 2.35 – 2.24 (m, 48H, H<sub>CH<sub>2</sub></sub>), 1.49 (m, 72H, H<sub>CH<sub>3</sub></sub>) ppm. <sup>31</sup>P NMR (203 MHz, acetone-*d*<sub>6</sub>) δ = 6.13 (d, *J* = 21.0 Hz), 1.09 (d, *J* = 20.8 Hz) ppm. ESI-MS (*m/z*) Calculated for C<sub>114</sub>H<sub>156</sub>F<sub>6</sub>N<sub>8</sub>O<sub>14</sub>P<sub>8</sub>Pt<sub>4</sub>S<sub>2</sub>Zn [M–2TfO]<sup>2+</sup>: 1567.19. Found: 1567.05.

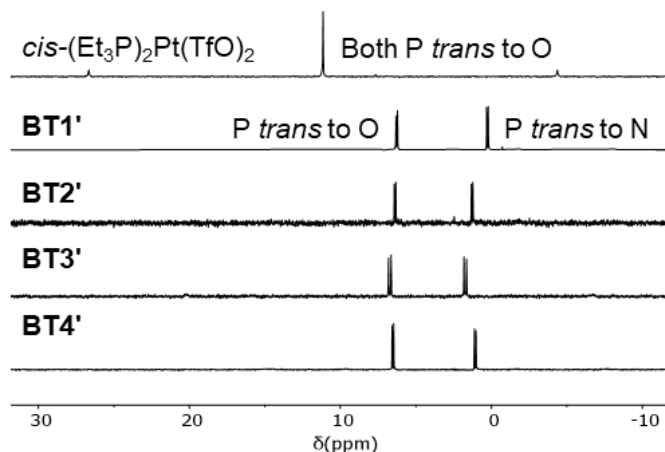
**BT1'.** *cis*-Pt(PEt<sub>3</sub>)<sub>2</sub>(OTf)<sub>2</sub> (4.47 mg, 0.0064 mmol), HDC (0.72 mg, 0.0032 mmol) and TPP (1.0 mg, 0.00162 mmol) in a 1:1:1 DCM/MeNO<sub>2</sub>/MeCN solvent mixture (1 mL). Yield = 4.7 mg (91%). <sup>1</sup>H NMR (500 MHz, acetone-*d*<sub>6</sub>) δ = 9.39 (br s, 4H, H<sub>c'</sub>), 9.37 – 9.31 (m, 8H, H<sub>a</sub>), 8.59 (d, *J* = 6.4 Hz, 8H, H<sub>b</sub>), 8.37 (s, 4H, H<sub>c</sub>), 2.40 – 2.16 (m, 56H, H<sub>s</sub> and H<sub>CH<sub>2</sub></sub>), 1.66 (br s, 8H, H<sub>i</sub>), 1.55 – 1.36 (m, 72H, H<sub>CH<sub>3</sub></sub>), –2.97 (s, 2H, H<sub>d</sub>). <sup>31</sup>P NMR (203 MHz, acetone-*d*<sub>6</sub>) δ = 6.27 (d, *J* = 21.1 Hz), 0.26 (d, *J* = 21.2 Hz) ppm.

**BT2'.** *cis*-Pt(PEt<sub>3</sub>)<sub>2</sub>(OTf)<sub>2</sub> (14.1 mg, 0.019 mmol), BPDC (3.08 mg, 0.0096 mmol) and TPP (3.0 mg, 0.0048 mmol) in a 1:1:1 DCM/MeNO<sub>2</sub>/MeCN (or 1:1 (CH<sub>3</sub>)<sub>2</sub>CO/H<sub>2</sub>O) solvent mixture (5 mL). Yield = 14.94 mg (90%). <sup>1</sup>H NMR (500 MHz, acetone-*d*<sub>6</sub>) δ = 9.34 (brs, 8H, H<sub>a</sub>), 8.58 (s, 4H, H<sub>c'</sub>), 8.38 (d, *J* = 5.6 Hz, 8H, H<sub>b</sub>), 8.10 (d, *J* = 8.1 Hz, 8H, H<sub>u</sub>), 7.98 (d, *J* = 8.2 Hz, 8H, H<sub>v</sub>), 7.74 (s, 4H, H<sub>c</sub>), 2.44 – 2.18 (m, 48H, H<sub>CH<sub>2</sub></sub>), 1.58 – 1.42 (m, 72H, H<sub>CH<sub>3</sub></sub>), –3.31 (s, 2H, H<sub>d</sub>). <sup>31</sup>P NMR (202 MHz, acetone-*d*<sub>6</sub>) δ = 6.37 (d, *J* = 21.0 Hz), 1.28 (d, *J* = 21.2 Hz) ppm. ESI-MS (*m/z*) Calculated for C<sub>118</sub>H<sub>162</sub>F<sub>6</sub>N<sub>8</sub>O<sub>14</sub>P<sub>8</sub>Pt<sub>4</sub>S<sub>2</sub> [M–2TfO]<sup>2+</sup>: 1561.55. Found: 1561.60.

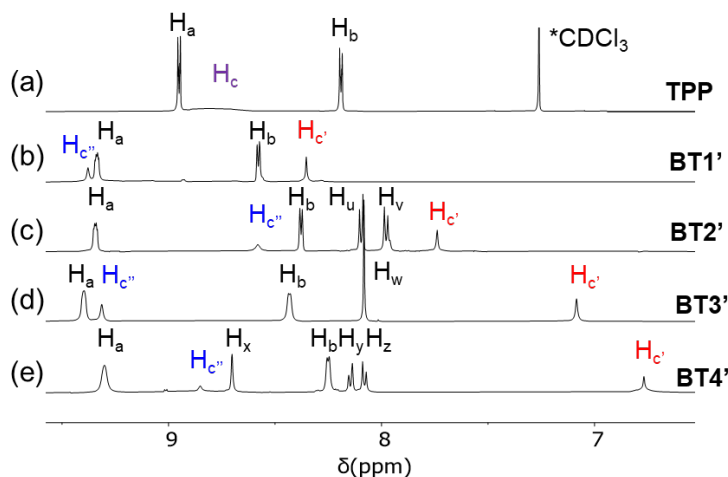
**BT3'.** *cis*-Pt(PEt<sub>3</sub>)<sub>2</sub>(OTf)<sub>2</sub> (14.10 mg, 0.019 mmol), BDC (2.34 mg, 0.0096 mmol) and TPP (3.0 mg, 0.0048 mmol) in a 1:1:1 DCM/MeNO<sub>2</sub>/MeCN (or 1:1 (CH<sub>3</sub>)<sub>2</sub>CO/H<sub>2</sub>O) solvent mixture (5 mL). Yield = 14.75 mg (93%). <sup>1</sup>H NMR (500 MHz, acetone-*d*<sub>6</sub>) δ = 9.40 (d, *J* = 6.1 Hz, 8H, H<sub>a</sub>), 9.31 (s, 4H, H<sub>c'</sub>), 8.43 (d, *J* = 5.5

Hz, 8H, H<sub>b</sub>), 8.08 (s, 8H, H<sub>w</sub>), 7.08 (s, 4H, H<sub>c'</sub>), 2.40 – 2.18 (m, 48H, H<sub>CH2-</sub>), 1.61 – 1.38 (m, 72H, H<sub>CH3</sub>), –3.27 (s, 2H, H<sub>d</sub>) ppm. <sup>31</sup>P NMR (122 MHz, acetone-*d*<sub>6</sub>) δ = 6.73 (d, *J* = 20.6 Hz), 1.73 (d, *J* = 21.2 Hz) ppm. ESI-MS (*m/z*) Calculated for C<sub>106</sub>H<sub>154</sub>F<sub>6</sub>N<sub>8</sub>O<sub>14</sub>P<sub>8</sub>Pt<sub>4</sub>S<sub>2</sub> [M–2TfO]<sup>2+</sup>: 1485.45. Found: 1485.52.

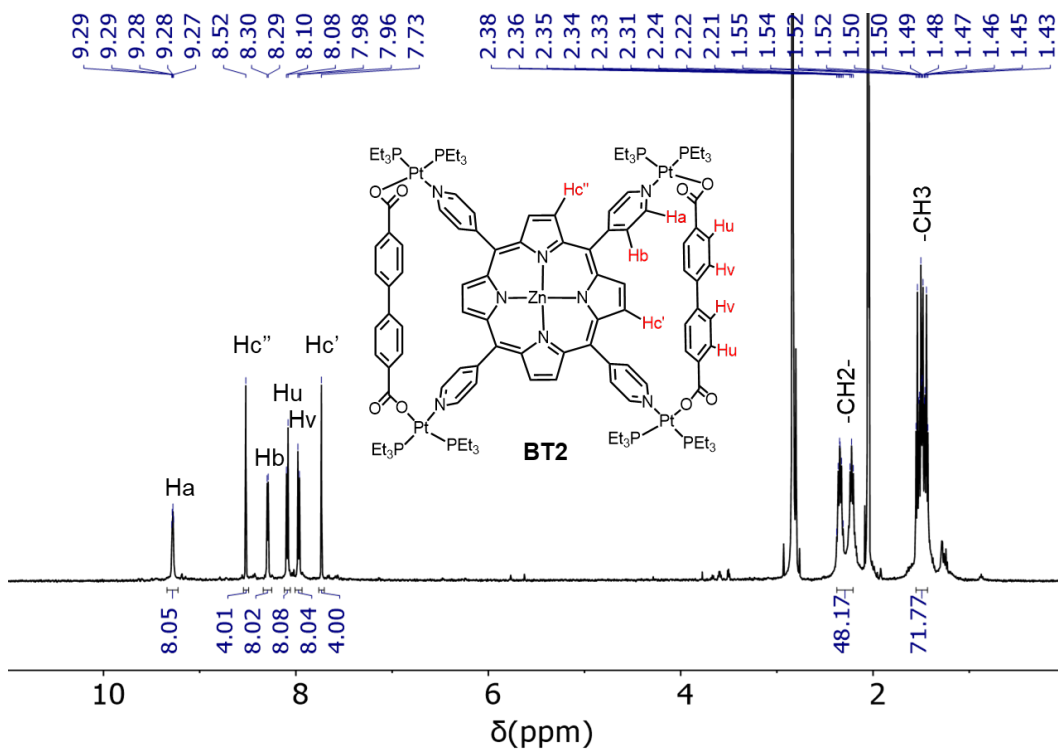
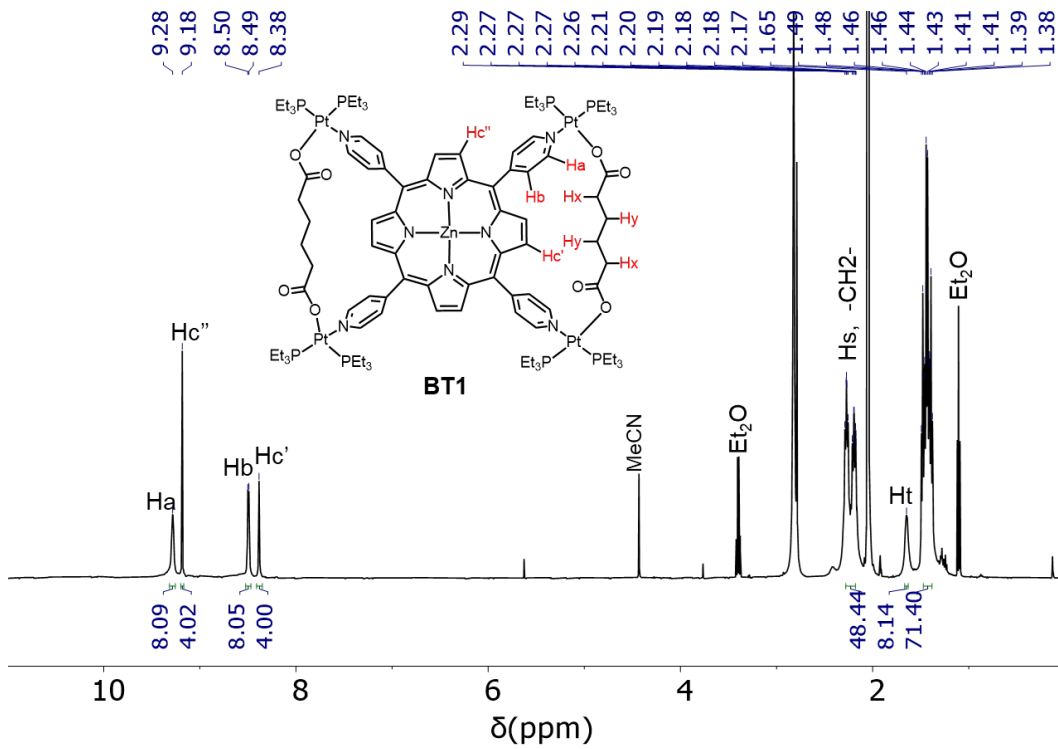
**BT4'**. *cis*-Pt(PEt<sub>3</sub>)<sub>2</sub>(OTf)<sub>2</sub> (14.10 mg, 0.019 mmol), BDC (2.83 mg, 0.0096 mmol) and TPP (3.0 mg, 0.0048 mmol) in a 1:1:1 DCM/MeNO<sub>2</sub>/MeCN (or 1:1 (CH<sub>3</sub>)<sub>2</sub>CO/H<sub>2</sub>O) solvent mixture (5 mL). Yield = 14.70 mg (90%). <sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>NO<sub>2</sub>) δ = 9.33 (br s, 8H, H<sub>a</sub>), 8.88 (s, 4H, H<sub>c''</sub>), 8.73 (d, *J* = 1.6 Hz, 4H, H<sub>x</sub>), 8.28 (d, *J* = 5.5 Hz, 8H, H<sub>b</sub>), 8.18 (d, *J* = 8.3 Hz, 4H, H<sub>y</sub>), 8.11 (d, *J* = 8.4 Hz, 4H, H<sub>z</sub>), 6.80 (s, 4H, H<sub>c'</sub>), 2.29 (m, 48H, H<sub>CH2-</sub>), 1.53 (m, 72H, H<sub>CH3</sub>), –3.42 (s, 2H, H<sub>d</sub>) ppm. <sup>31</sup>P NMR (203 MHz, CD<sub>3</sub>NO<sub>2</sub>) δ = 6.52 (d, *J* = 21.2 Hz), 1.07 (d, *J* = 21.1 Hz) ppm. ESI-MS (*m/z*) Calculated for C<sub>114</sub>H<sub>158</sub>F<sub>6</sub>N<sub>8</sub>O<sub>14</sub>P<sub>8</sub>Pt<sub>4</sub>S<sub>2</sub> [M–2TfO]<sup>2+</sup>: 1535.51. Found: 1535.60.

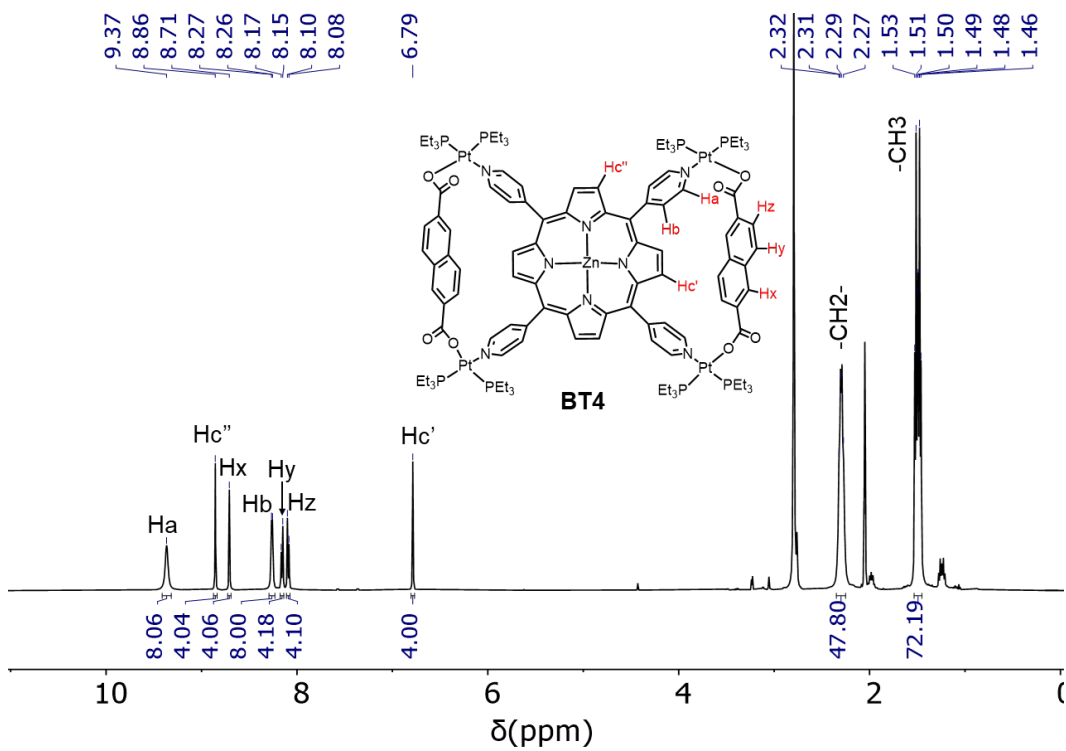
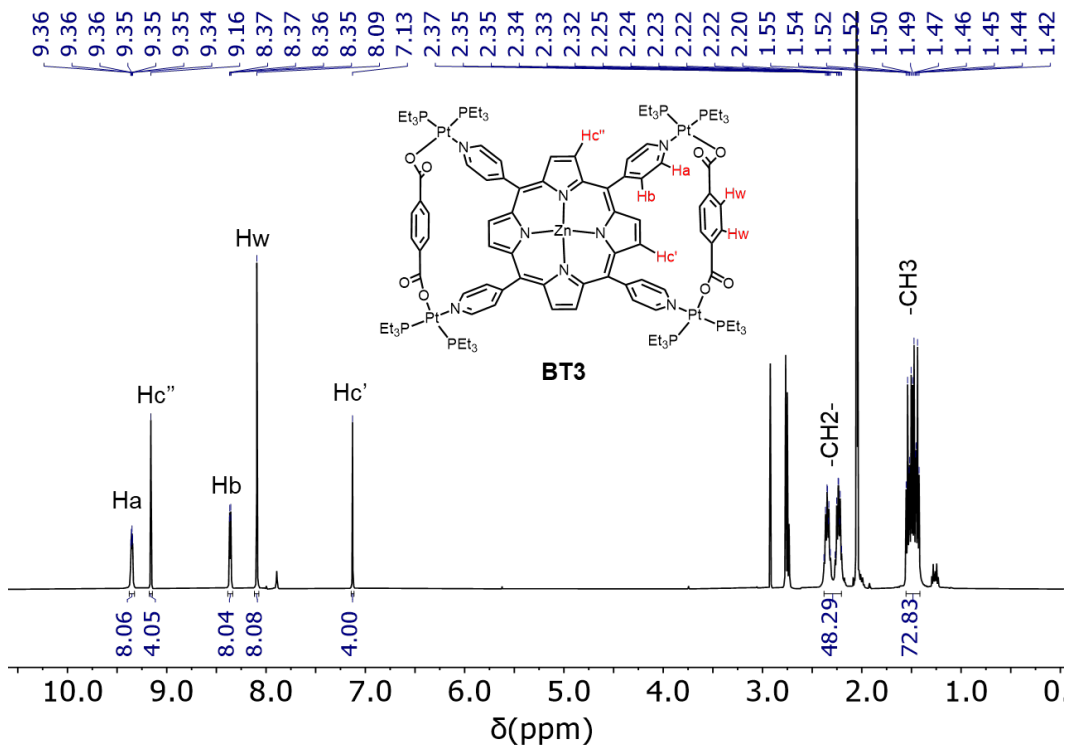


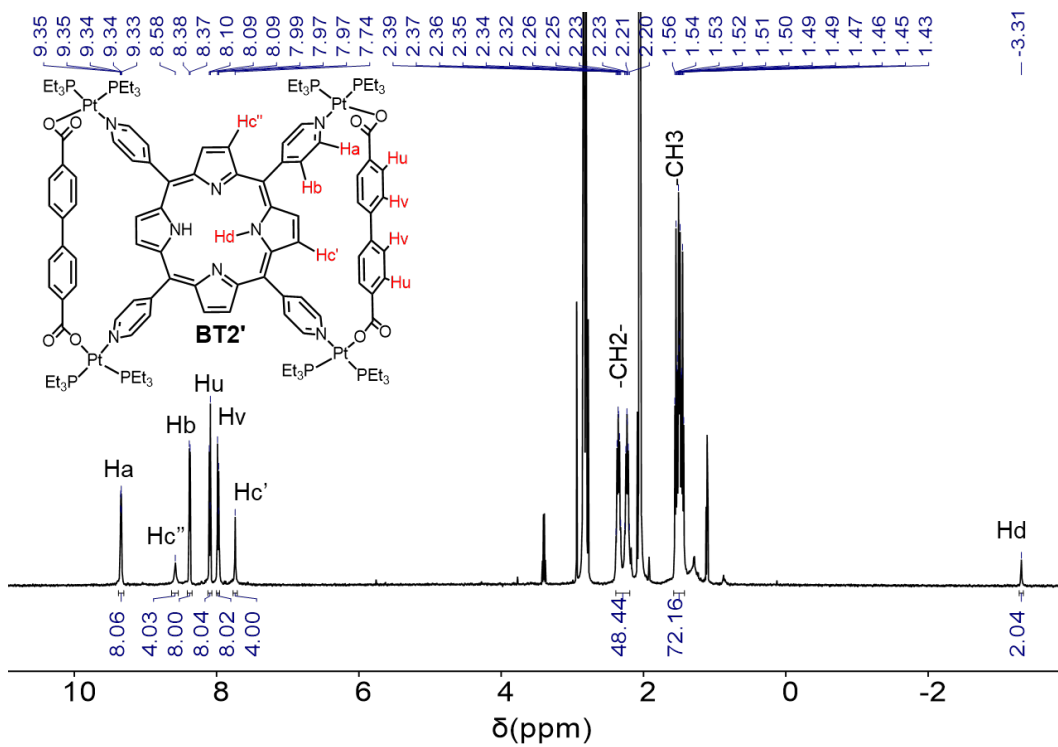
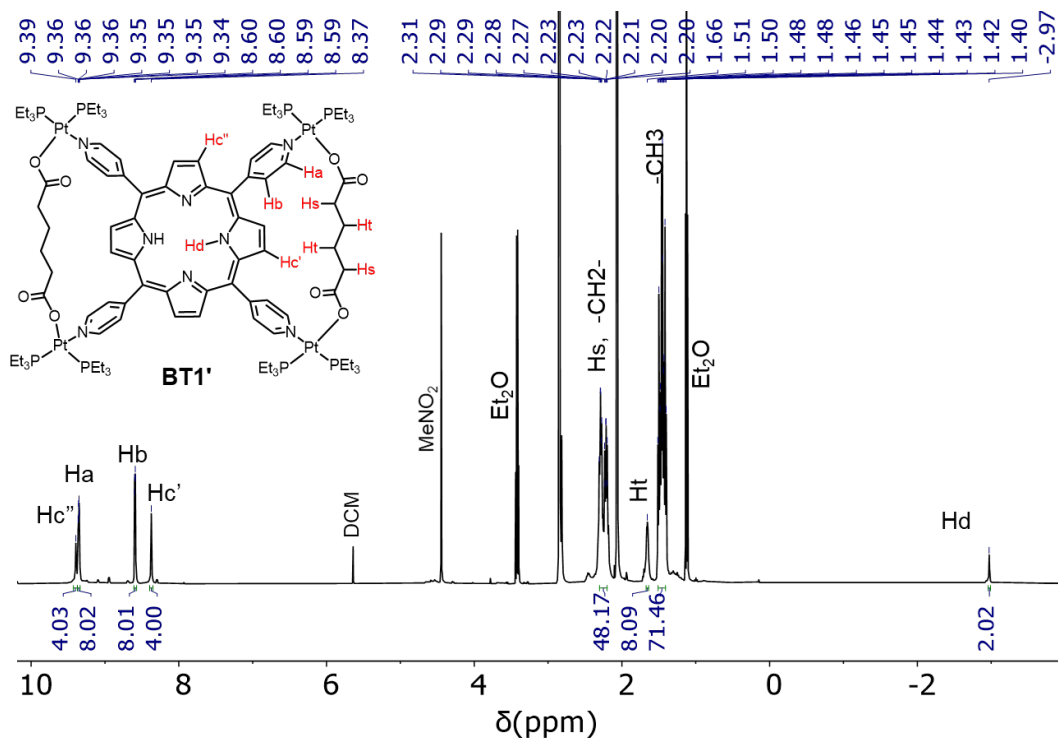
**Fig. S1.** The <sup>31</sup>P NMR spectra (122 MHz, acetone-*d*<sub>6</sub>) of *cis*-(Et<sub>3</sub>P)<sub>2</sub>Pt(TfO), BT1', BT2', BT3', and BT4' complexes reveal simultaneous coordination of carboxylate and pyridyl groups with heteroligated Pt(N,O) corners in the bow tie complexes.



**Fig. S2.** The partial <sup>1</sup>H NMR spectra (500 MHz) of (a) free H<sub>2</sub>TPP ligand (in CDCl<sub>3</sub>), (b) BT1', (c) BT2', (d) BT3', and (e) BT4' complexes (in acetone-*d*<sub>6</sub>) show that the enclosed H<sub>c'</sub> pyrrole protons (highlighted in red) of bow tie complexes are shifted up-field commensurately with the shielding effect of the adjacent XDC linkers, whereas the chemical shifts of exposed H<sub>c''</sub> pyrrole protons (highlighted in blue) vary depending on the length of XDC linkers that dictate their distances from the adjacent pyridyl rings.







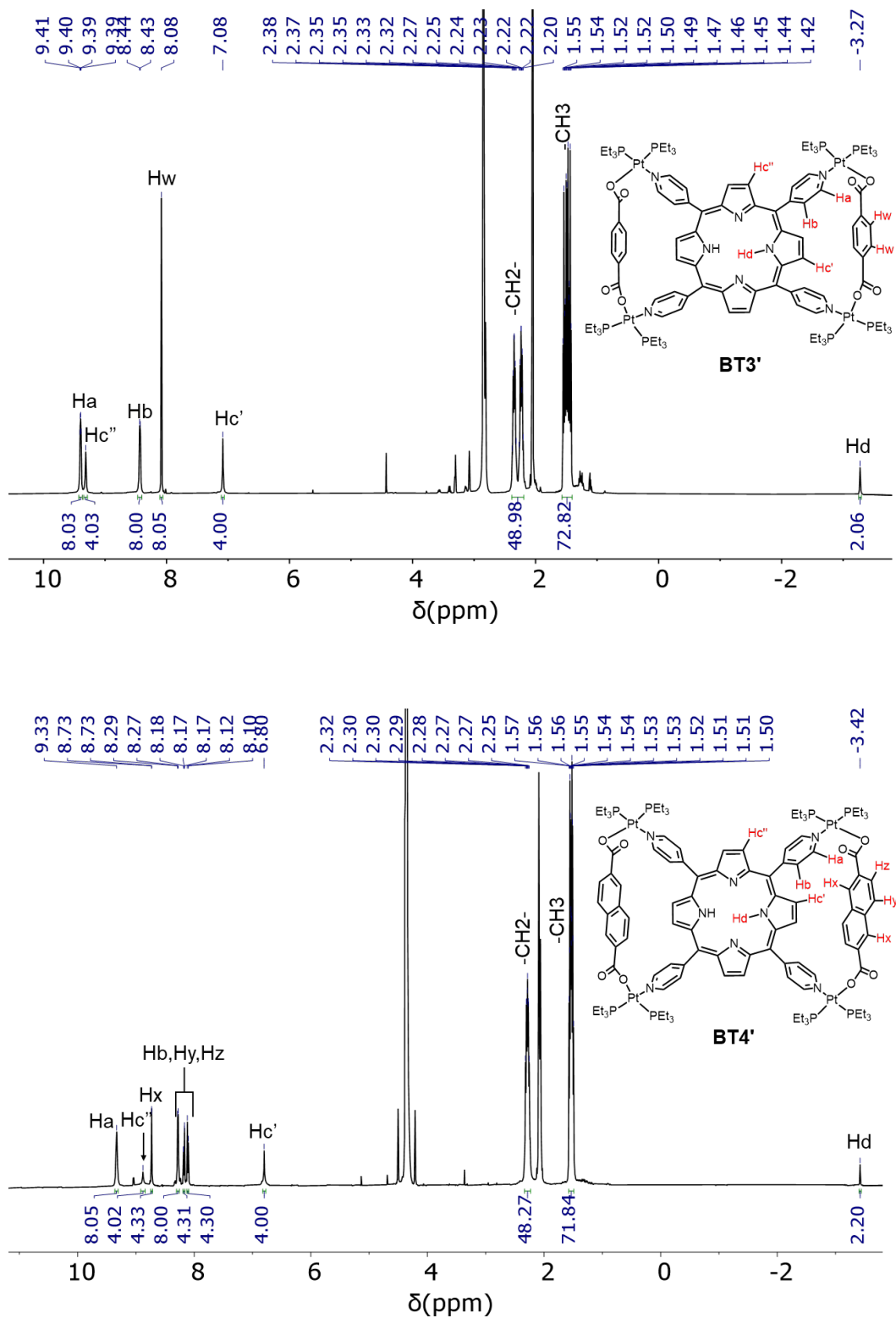
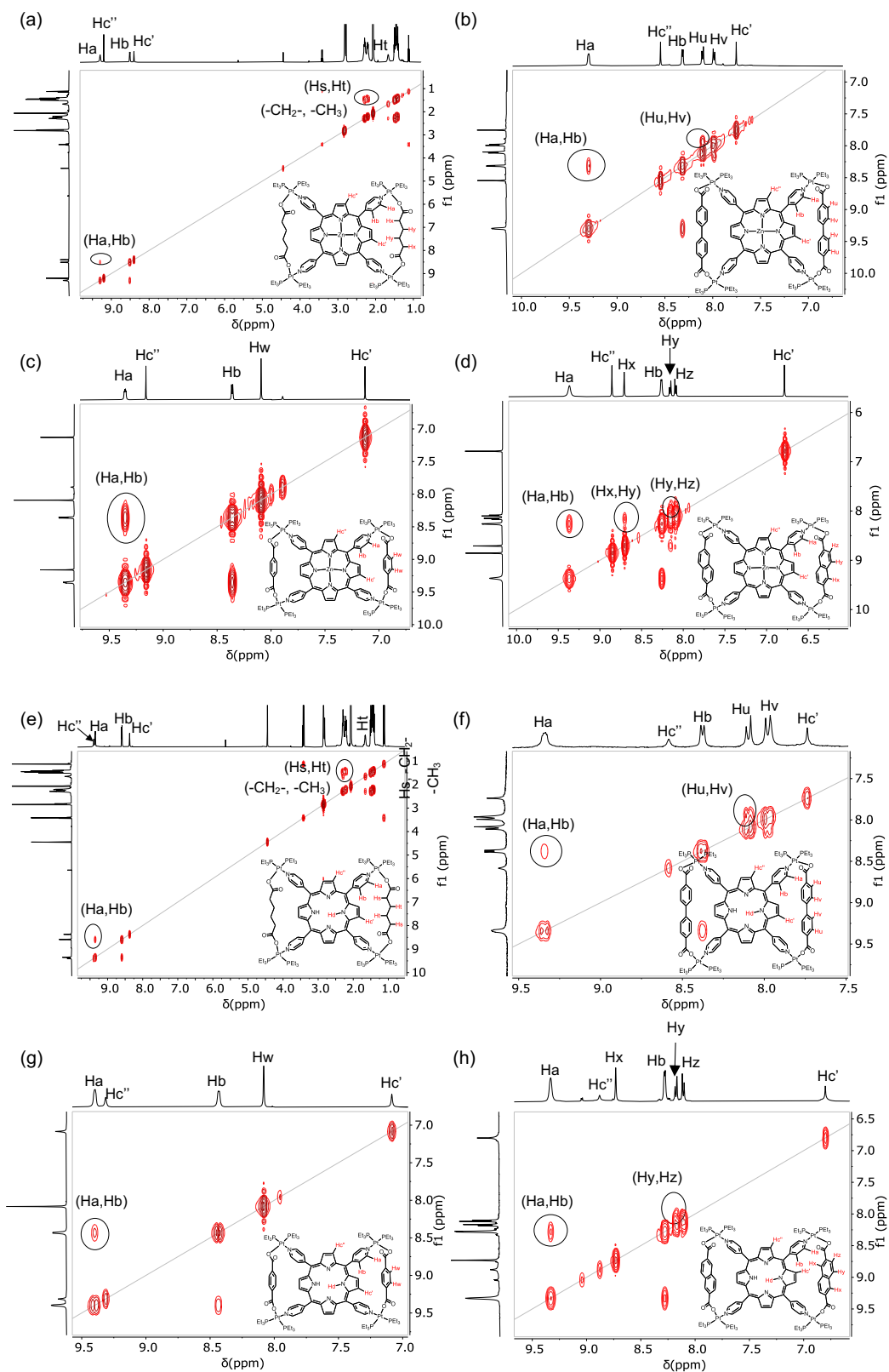
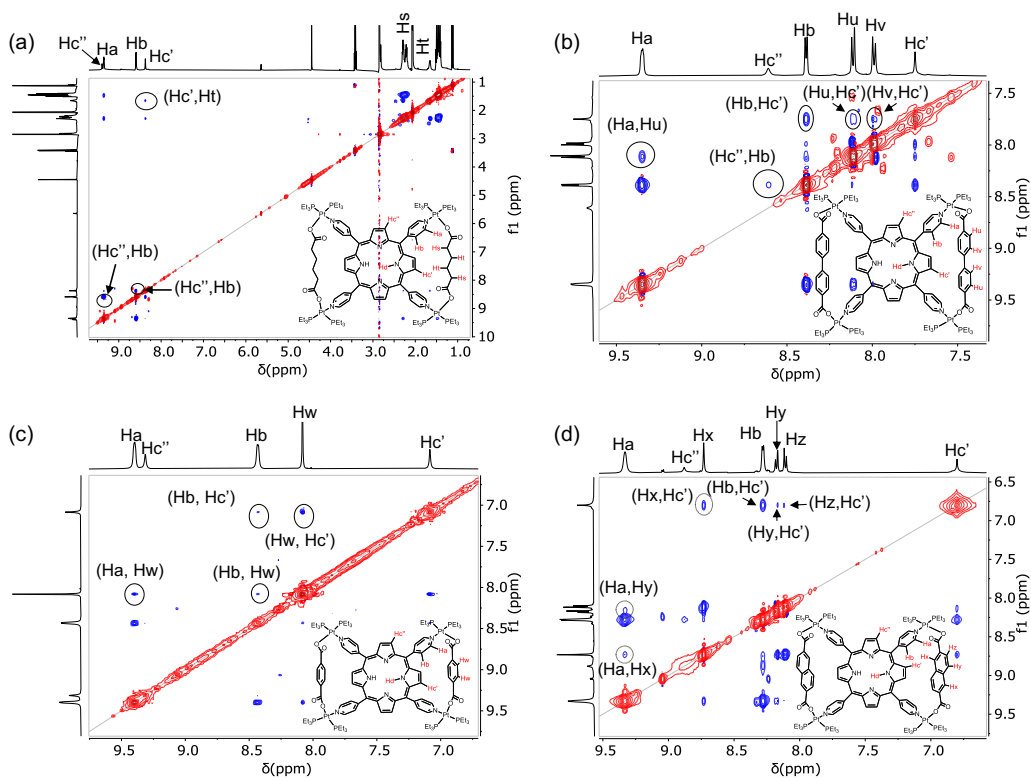


Fig. S3. <sup>1</sup>H NMR spectra (500 MHz, acetone-*d*<sub>6</sub>) of BT1–BT4 and BT1'–BT4' complexes.

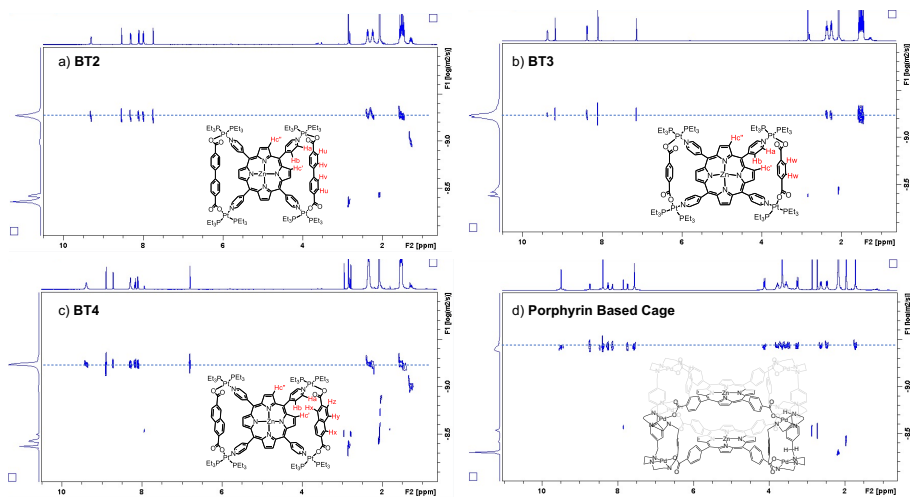




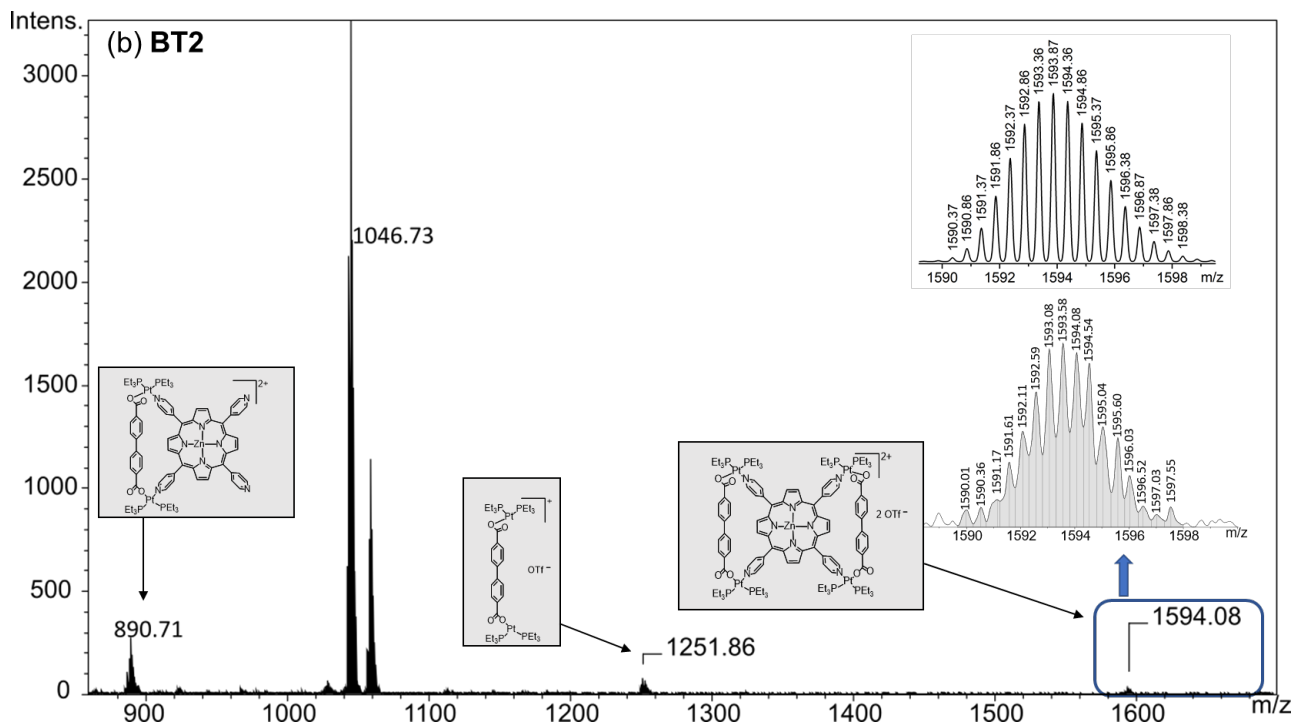
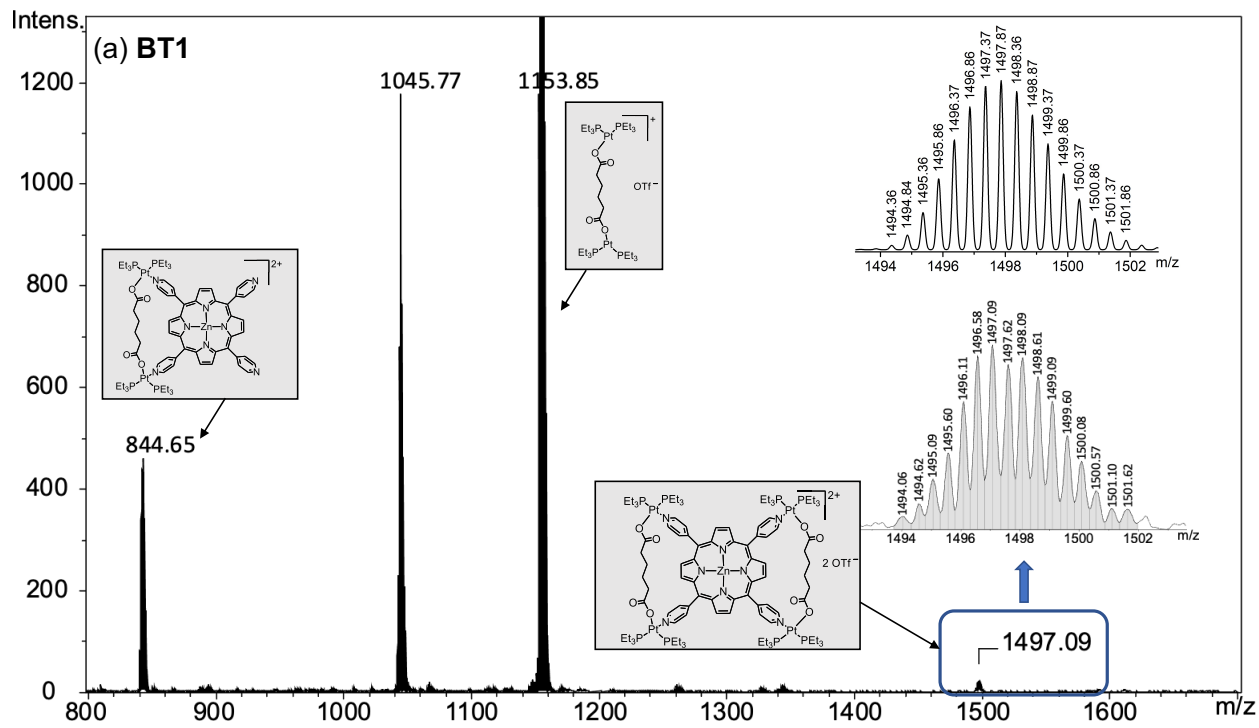
**Fig. S4.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectra (500 MHz, acetone- $d_6$ ) of (a-d) BT1-BT4 and (e-h) BT1'-BT4' complexes.

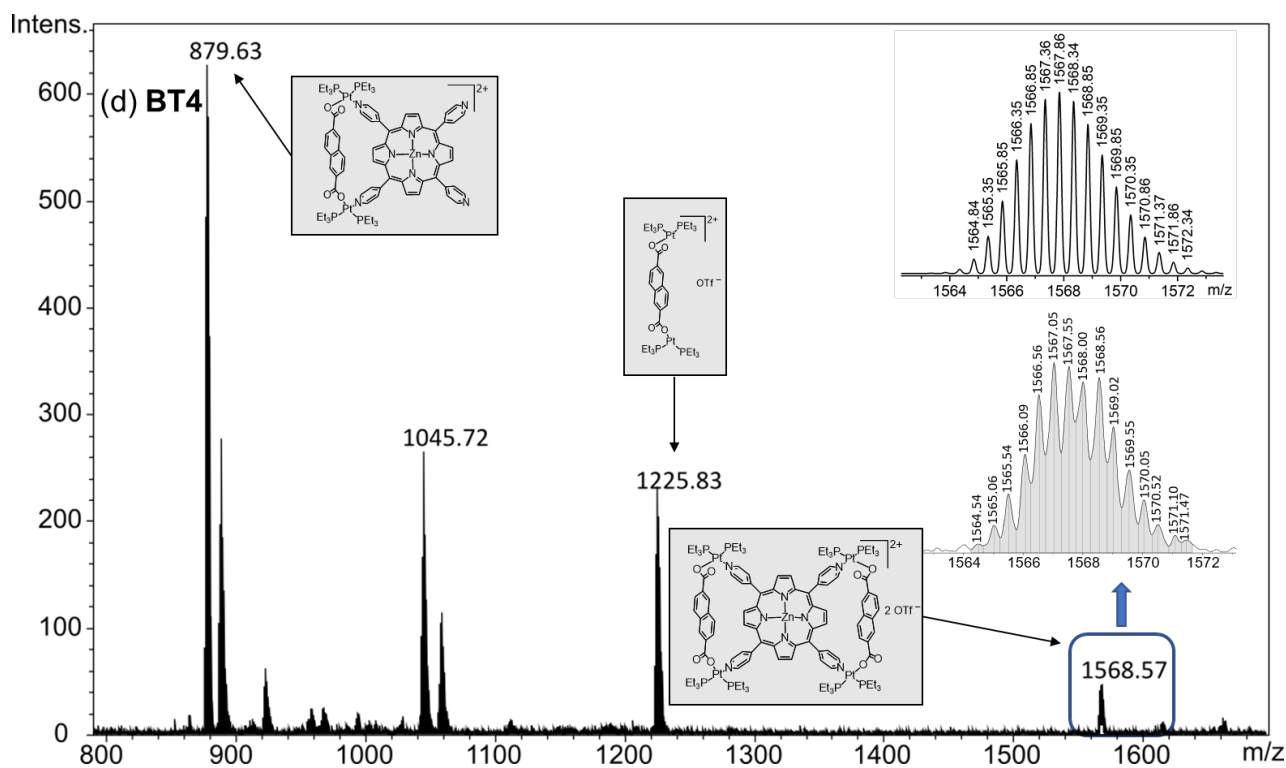
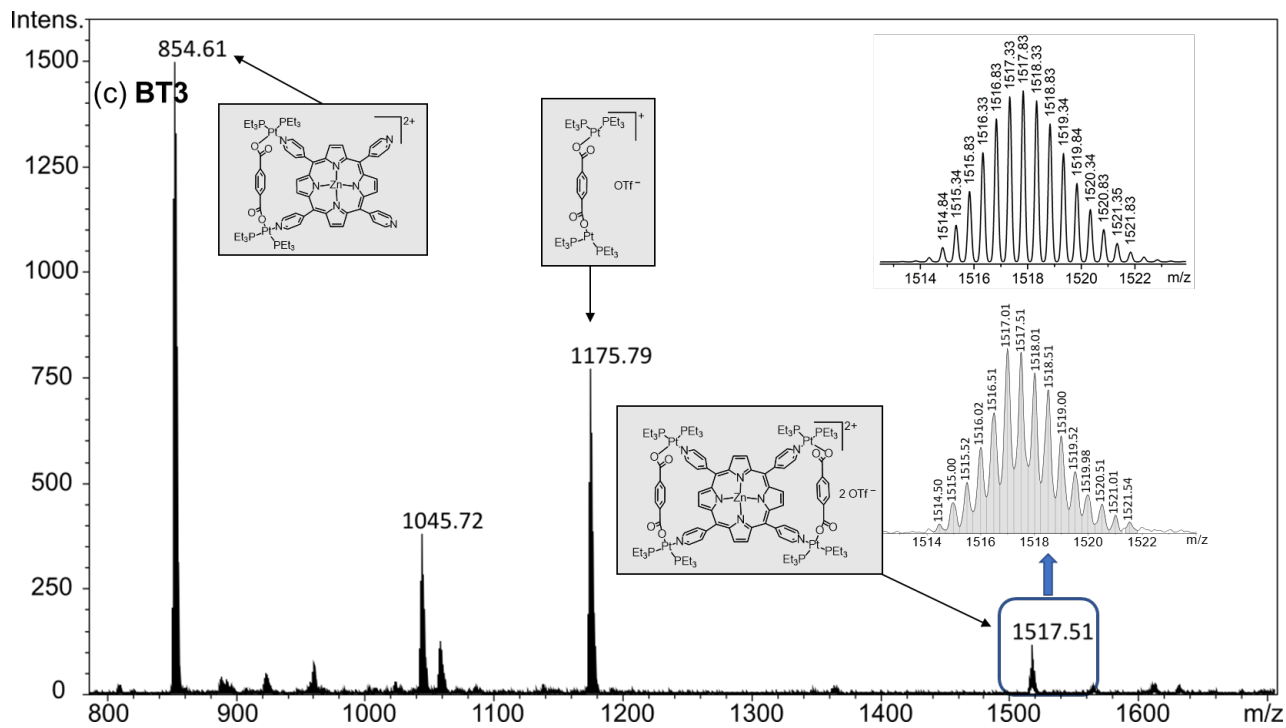


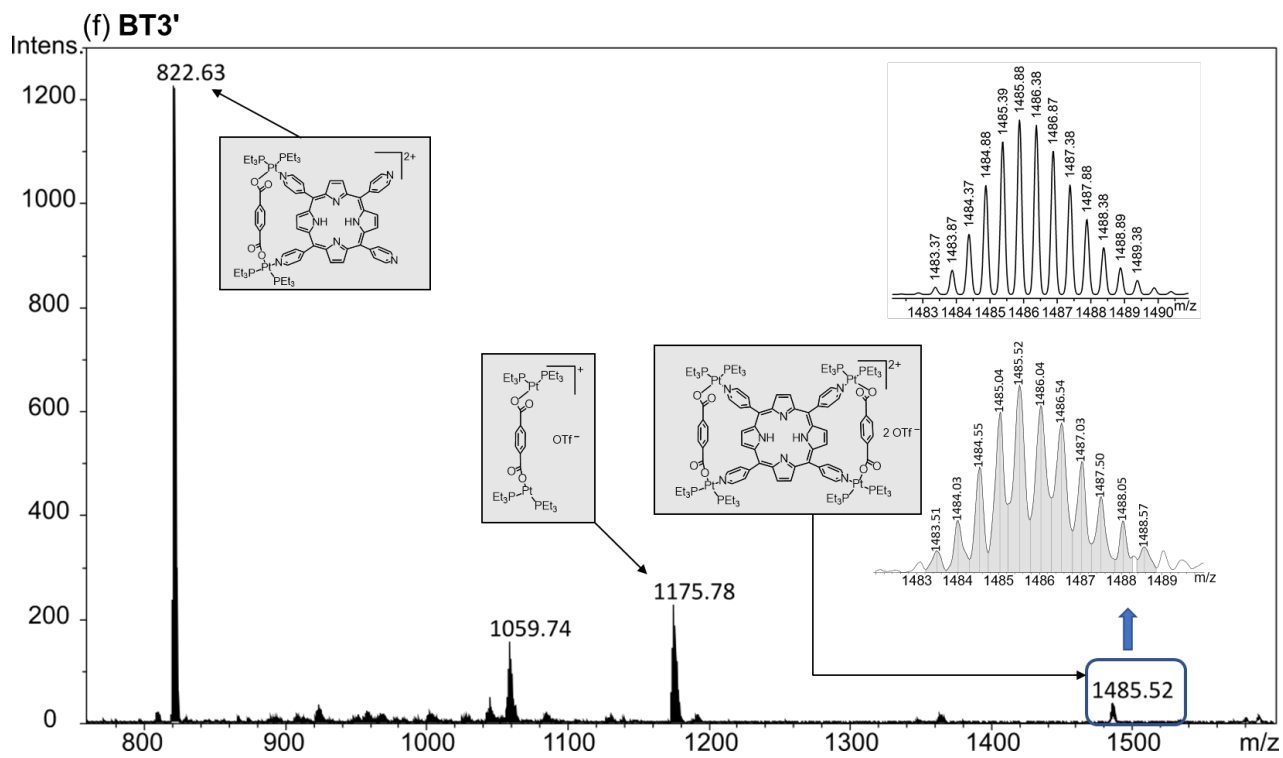
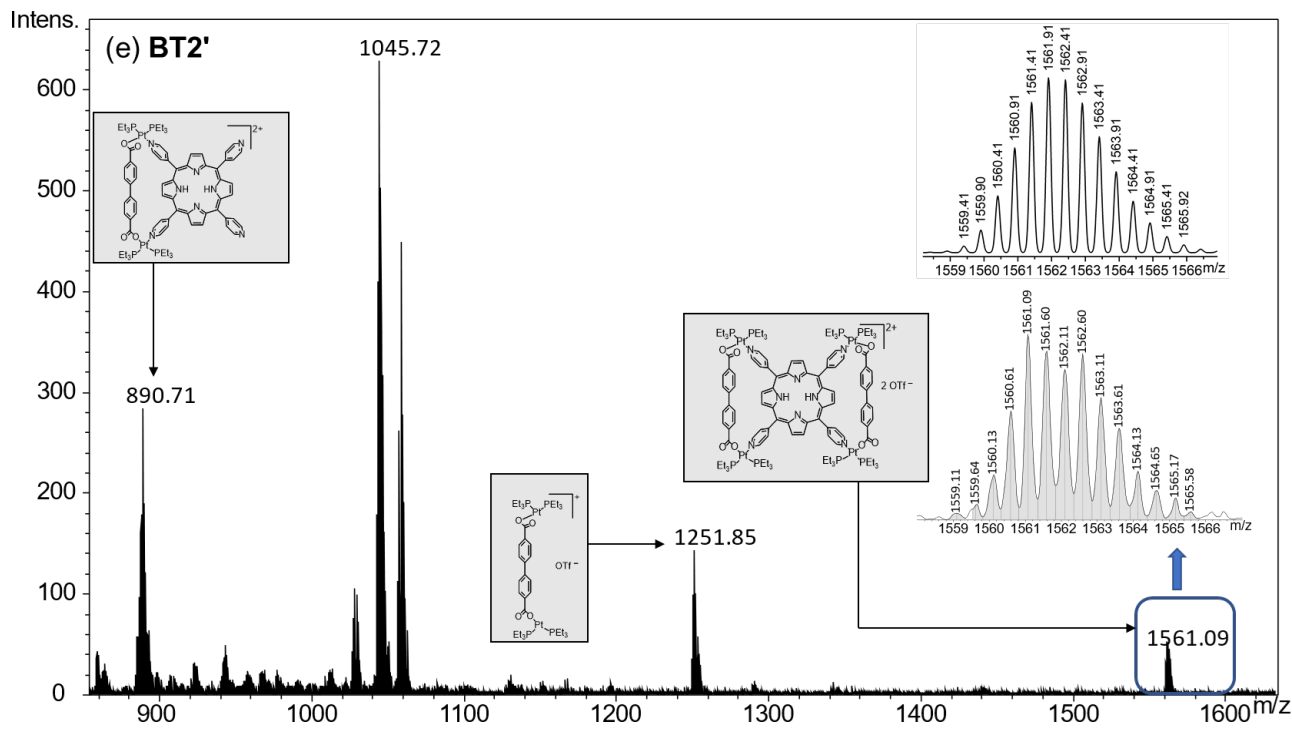
**Fig. S5.**  $^1\text{H}$ - $^1\text{H}$  ROESY NMR spectra (500 MHz, acetone- $d_6$ ) of (a) **BT1'**, (b) **BT2'**, (c) **BT3'**, and (d) **BT4'** complexes.

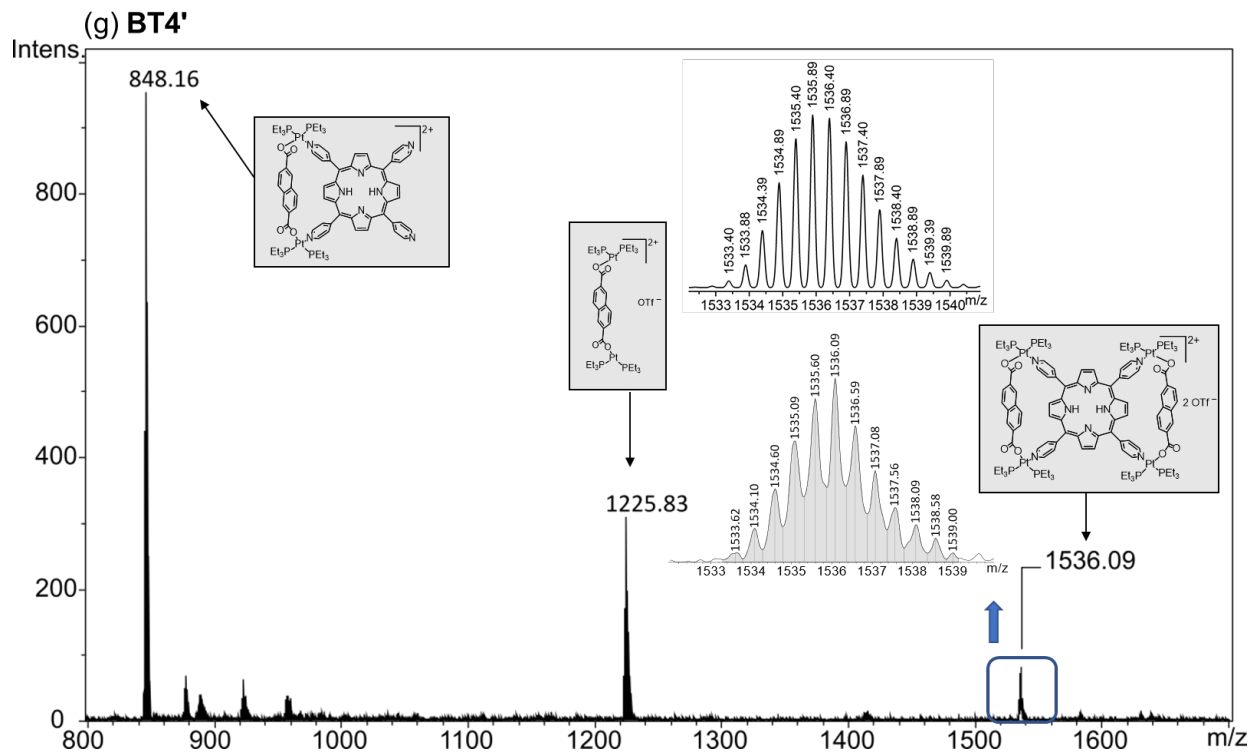


**Fig. S6.** DOSY NMR spectra (500 MHz) of **BT2** ( $D = 5.40 \times 10^{-10} \text{ m}^2/\text{s}$ ), **BT3** ( $D = 5.63 \times 10^{-10} \text{ m}^2/\text{s}$ ), **BT4** ( $D = 5.67 \times 10^{-10} \text{ m}^2/\text{s}$ ) in acetone- $d_6$  and a porphyrin-based cage ( $D = 3.76 \times 10^{-10} \text{ m}^2/\text{s}$ ) in  $\text{CD}_3\text{CN}$ .

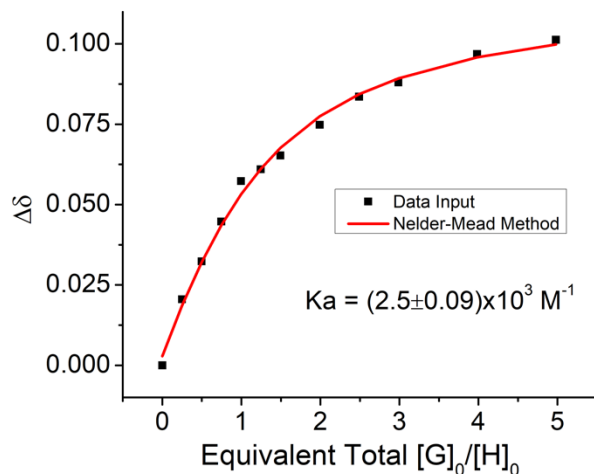




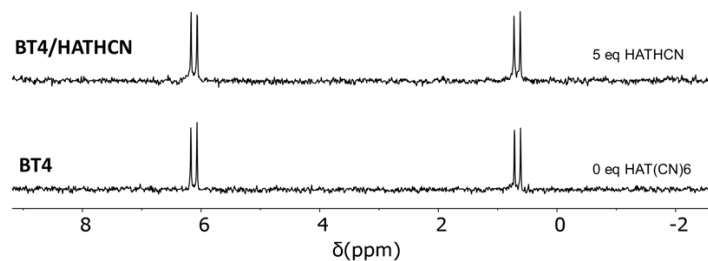




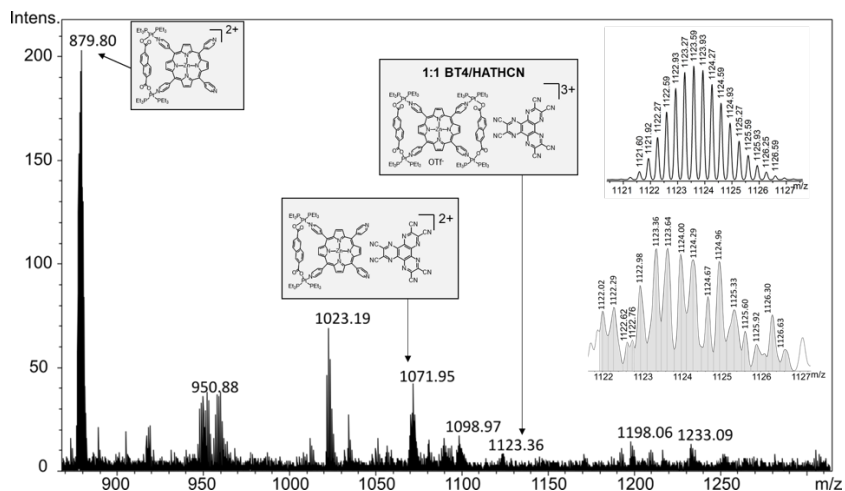
**Fig. S7.** ESI-MS data of (a) **BT1**, (b) **BT2**, (c) **BT3**, (d) **BT4**, (e) **BT2'**, (f) **BT3'**, and (g) **BT4'** complexes. The insets show the calculated (top) and experimental (bottom) isotopic distributions of respective  $[M - 2TfO]^{2+}$  species.



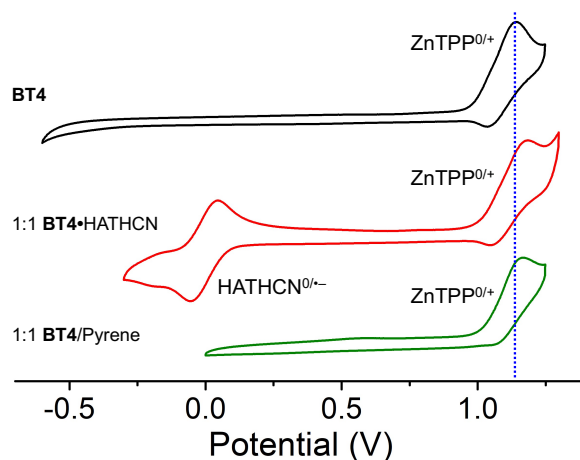
**Fig. S8.** To determine the association constant corresponding to the formation of the **BT4/HATHCN** complex  $^1\text{H}$  NMR titration was carried by adding a solution of **HATHCN** (0 – 5 eq) to a solution of **BT4** ( $[\text{BT4}] = 5.8 \times 10^{-4} \text{ M}$ ) in 3:7  $\text{CD}_2\text{Cl}_2/\text{CD}_3\text{NO}_2$ . The association constant ( $K_a$ ) was calculated by a global fitting analysis to a 1:1 binding model using Nelder-Mead fit method from [www.supramolecular.org](http://www.supramolecular.org) web applet.<sup>4</sup>



**Fig. S9.** The  $^{31}\text{P}$  NMR spectrum (122 MHz,  $\text{CD}_2\text{Cl}_2/\text{CD}_3\text{NO}_2$  4:1) of the **BT4** complex reveals that the simultaneous coordination of carboxylate and pyridyl groups with heteroligated Pt(N,O) corners in the bow tie complexes remains after the formation of the **BT4**•HATHCN.



**Fig. S10.** ESI-MS data of 1:1 **BT4**•HATHCN complex. The inset shows the calculated (top) and experimental (bottom) isotopic distribution for  $[\text{M} - \text{TfO}]^{3+}$ .



**Fig. S11.** Cyclic voltammograms of the **BT4** (black), 1:1 **BT4**•HATHCN complex (red), and 1:1 **BT4**/Pyrene mixture (green) (vs. Ag/AgCl in 0.1 M of  $\text{Bu}_4\text{N} \cdot \text{TfO}/\text{CH}_2\text{Cl}_2$ ).

## Crystallographic Data.

**Table 1.** Crystallographic Data for **BT2**, **BT3** and **BT4**.

Compound	<b>BT2</b>	<b>BT3</b>	<b>BT4</b>
Empirical formula	C120 H160 F12 N8 O20 P8 Pt4 S4 Zn	C108 H152 F12 N8 O20 P8 Pt4 S4 Zn	C116 H156 F12 N8 O11 P8 Pt4 S4 Zn
Formula weight	3484.28	3332.1	3278.21
Temperature	173(2) K	100(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	P -1	C 2/c	P 21/c
Unit cell dimensions	a = 14.177(3) Å    α = 100.941(5)°. b = 15.762(3) Å    β = 104.110(5)°. c = 20.164(4) Å    γ = 95.391(6)°.	a = 30.647(10) Å    α = 90°. b = 15.376(5) Å    β = 104.412(8)°. c = 31.873(11) Å    γ = 90°.	a = 23.980(2) Å    α = 90°. b = 33.628(3) Å    β = 109.469(2)°. c = 22.415(2) Å    γ = 90°.
Volume	4243.8(16) Å <sup>3</sup>	14547(9) Å <sup>3</sup>	17042(3) Å <sup>3</sup>
Z	1	4	4
Density (calculated)	1.363 Mg/m <sup>3</sup>	1.521 Mg/m <sup>3</sup>	1.278 Mg/m <sup>3</sup>
Absorption coefficient	3.614 mm <sup>-1</sup>	4.213 mm <sup>-1</sup>	3.592 mm <sup>-1</sup>
F(000)	1730	6600	6504
Crystal size	0.164 x 0.132 x 0.112 mm <sup>3</sup>	0.350 x 0.260 x 0.020 mm <sup>3</sup>	0.330 x 0.080 x 0.060 mm <sup>3</sup>
Theta range for data collection	2.688 to 25.250°.	4.116 to 16.974°.	4.076 to 19.082°.
Index ranges	-17<=h<=17, -18<=k<=18, -24<=l<=24	-25<=h<=24, -12<=k<=12, -26<=l<=24	-21<=h<=21, -30<=k<=30, -20<=l<=20
Reflections collected	40383	15135	54937
Independent reflections	15172 [R(int) = 0.0832]	4045 [R(int) = 0.1205]	13508 [R(int) = 0.1416]
Completeness to theta	(25.242°) 98.7%	(16.974°) 95.8%	(19.082°) 97.1%
Absorption correction	Semi-empirical from equivalents	None	None
Refinement method	Full-matrix least-squares on F <sup>2</sup>	Full-matrix least-squares on F <sup>2</sup>	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	15172 / 345 / 655	4045 / 650 / 571	13508 / 3329 / 1507
Goodness-of-fit on F <sup>2</sup>	1.047	2.694	1.022
Final R indices [I>2σ(I)]	R1 = 0.1438, wR2 = 0.3449	R1 = 0.2450, wR2 = 0.5287	R1 = 0.1157, wR2 = 0.2864
R indices (all data)	R1 = 0.2192, wR2 = 0.4222	R1 = 0.2787, wR2 = 0.5508	R1 = 0.1868, wR2 = 0.3442
Largest diff. peak and hole	3.868 and -3.352 e.Å <sup>-3</sup>	4.770 and -1.921 e.Å <sup>-3</sup>	1.948 and -1.323 e.Å <sup>-3</sup>



**Table 2.** Crystallographic Data for **BT2'** and **BT3'**.

Compound	<b>BT2'</b>	<b>BT3'</b>
Empirical formula	C123 H168 F12 N8 O21 P8 Pt4 S4	C108 H152 F12 N8 O20 P8 Pt4 S4
Formula weight	3479	3264.71
Temperature	100(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Tetragonal
Space group	C 2/c	I 41/a
Unit cell dimensions	a = 42.500(3) Å $\alpha = 90^\circ$ . b = 17.5276(14) Å $\beta = 107.338(2)^\circ$ . c = 22.8229(18) Å $\gamma = 90^\circ$ .	a = 34.285(6) Å $\alpha = 90^\circ$ . b = 34.285(6) Å $\beta = 90^\circ$ . c = 23.949(5) Å $\gamma = 90^\circ$ .
Volume	16229(2) Å <sup>3</sup>	28151(11) Å <sup>3</sup>
Z	4	8
Density (calculated)	1.424 Mg/m <sup>3</sup>	1.541 Mg/m <sup>3</sup>
Absorption coefficient	3.638 mm <sup>-1</sup>	4.188 mm <sup>-1</sup>
F(000)	6936	12944
Crystal size	0.160 x 0.120 x 0.030 mm <sup>3</sup>	0.18 x 0.12 x 0.04 mm <sup>3</sup>
Theta range for data collection	2.309 to 25.250°.	2.304 to 17.312°.
Index ranges	-50<=h<=50, -20<=k<=21, -27<=l<=27	-28<=h<=28, -28<=k<=28, -20<=l<=19
Reflections collected	48255	33537
Independent reflections	14608 [R(int) = 0.0829]	4010 [R(int) = 0.1656]
Completeness to theta	(25.242°) 99.4%	(17.312°) 92.7%
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F <sup>2</sup>	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	14608 / 96 / 824	4010 / 1227 / 696
Goodness-of-fit on F2	1.065	1.361
Final R indices [I>2sigma(I)]	R1 = 0.0850, wR2 = 0.1982	R1 = 0.1104, wR2 = 0.2814
R indices (all data)	R1 = 0.1100, wR2 = 0.2126	R1 = 0.1786, wR2 = 0.3603
Largest diff. peak and hole	3.151 and -3.752 e.Å <sup>-3</sup>	2.357 and -0.946 e.Å <sup>-3</sup>

**Table 3.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{Å}^2 \times 10^3$ ) for **BT2**. U(eq) is defined as one third of the trace of the orthogonalized U<sup>ij</sup> tensor.

	x	y	z	U(eq)
Pt(1)	7791(1)	5049(1)	7517(1)	63(1)
Pt(2)	3947(1)	-1436(1)	1101(1)	70(1)
Zn(1)	10000	0	5000	87(2)
P(1)	6998(7)	6182(5)	7805(5)	93(3)

P(2)	9278(5)	5624(5)	8225(4)	62(2)
P(3)	4493(5)	-2410(6)	329(5)	82(2)
P(4)	2484(6)	-1474(6)	334(5)	86(3)
O(1)	6183(15)	3477(13)	7453(10)	81(4)
O(2)	6454(14)	4549(13)	6813(9)	70(4)
O(3)	3596(14)	-445(11)	1769(12)	79(4)
O(4)	2973(15)	-1373(12)	2334(12)	86(5)
N(1)	10534(15)	864(13)	5922(11)	63(5)
N(2)	8687(16)	512(15)	4855(12)	74(6)
N(3)	8275(13)	3898(11)	7029(12)	54(4)
N(4)	5266(14)	-1203(17)	1928(12)	69(5)
C(1)	11409(18)	978(17)	6387(13)	61(6)
C(2)	11493(19)	1613(19)	6990(14)	72(6)
C(3)	10665(18)	1948(19)	6923(14)	72(6)
C(4)	10039(18)	1480(19)	6230(13)	67(6)
C(5)	9068(19)	1630(17)	5941(14)	63(7)
C(6)	8453(18)	1163(18)	5286(14)	66(6)
C(7)	7461(18)	1337(18)	4973(14)	66(6)
C(8)	7080(20)	686(18)	4337(14)	68(6)
C(9)	7884(18)	219(18)	4269(13)	63(6)
C(10)	7800(20)	-453(19)	3724(13)	69(8)
C(11)	8725(16)	2421(17)	6313(13)	58(7)
C(12)	8780(30)	3140(20)	6086(17)	102(13)
C(13)	8484(16)	3931(14)	6503(15)	55(4)
C(14)	8205(16)	3181(14)	7297(15)	55(4)
C(15)	8453(17)	2389(15)	6934(11)	50(6)
C(16)	6896(16)	-677(17)	3078(12)	52(6)
C(17)	6700(20)	-200(20)	2591(16)	92(11)
C(18)	5831(17)	-440(20)	2029(15)	70(5)
C(19)	5407(17)	-1660(20)	2401(15)	69(5)
C(20)	6210(20)	-1450(20)	3002(16)	84(9)
C(21)	6110(20)	3760(20)	6923(15)	71(4)
C(22)	5520(30)	3115(16)	6249(16)	92(4)
C(23)	5470(30)	2225(15)	6229(16)	91(4)
C(24)	5090(30)	1650(20)	5586(12)	91(4)
C(25)	4740(30)	1890(16)	4957(15)	91(4)
C(26)	4770(30)	2781(15)	4991(16)	93(4)
C(27)	5180(30)	3380(20)	5627(12)	93(4)
C(28)	4289(19)	1324(17)	4297(15)	89(4)
C(29)	3712(17)	507(15)	4243(15)	89(4)
C(30)	3430(20)	-138(19)	3608(12)	89(4)
C(31)	3670(20)	10(18)	2989(15)	89(4)
C(32)	4300(20)	797(16)	3058(16)	89(4)

C(33)	4570(20)	1450(20)	3687(13)	89(4)
C(34)	3400(20)	-713(17)	2346(19)	81(4)
C(35)	10150(20)	4860(30)	8130(20)	108(9)
C(36)	11190(20)	5250(30)	8580(20)	109(9)
C(37)	9870(30)	6630(30)	8040(20)	110(10)
C(38)	10040(30)	6520(30)	7330(20)	111(10)
C(39)	9450(30)	5850(20)	9170(20)	117(10)
C(40)	8880(30)	5120(20)	9390(20)	118(10)
C(41)	5890(20)	5710(20)	7928(19)	98(8)
C(42)	6110(30)	5420(20)	8611(18)	98(8)
C(43)	7580(30)	7110(20)	8480(20)	130(11)
C(44)	6820(30)	7850(30)	8520(20)	131(11)
C(45)	6620(30)	6610(30)	7048(19)	125(11)
C(46)	7230(30)	6950(30)	6770(20)	126(11)
C(47)	1560(20)	-2430(20)	225(19)	108(10)
C(48)	1450(30)	-2600(20)	927(19)	111(10)
C(49)	1930(30)	-510(20)	620(30)	190(20)
C(50)	980(30)	-480(30)	60(30)	190(20)
C(51)	2440(40)	-1470(30)	-582(17)	184(18)
C(52)	3030(40)	-640(30)	-650(30)	186(18)
C(53)	3690(40)	-3400(30)	-100(30)	153(13)
C(54)	3170(40)	-3980(30)	270(30)	153(13)
C(56)	5850(30)	-1170(30)	90(20)	134(11)
C(55)	5210(30)	-2060(30)	-240(20)	135(11)
C(57)	5500(40)	-2920(30)	880(20)	140(12)
C(58)	5840(40)	-3660(30)	430(20)	143(12)

**Table 4.** Bond lengths [Å] and angles [°] for **BT2**.

Pt(1)-O(2)	2.052(19)
Pt(1)-N(3)	2.148(17)
Pt(1)-P(2)	2.233(7)
Pt(1)-P(1)	2.258(7)
Pt(2)-O(3)	2.044(19)
Pt(2)-N(4)	2.13(2)
Pt(2)-P(4)	2.253(8)
Pt(2)-P(3)	2.298(9)
Zn(1)-N(1)#1	2.011(18)
Zn(1)-N(1)	2.011(18)
Zn(1)-N(2)#1	2.08(2)

Zn(1)-N(2)	2.08(2)
P(1)-C(41)	1.77(3)
P(1)-C(45)	1.77(3)
P(1)-C(43)	1.77(3)
P(2)-C(39)	1.81(4)
P(2)-C(35)	1.82(4)
P(2)-C(37)	1.87(3)
P(3)-C(53)	1.78(5)
P(3)-C(55)	1.83(4)
P(3)-C(57)	1.92(5)
P(4)-C(51)	1.83(3)
P(4)-C(49)	1.83(3)
P(4)-C(47)	1.84(2)
O(1)-C(21)	1.22(3)
O(2)-C(21)	1.37(4)
O(3)-C(34)	1.39(4)
O(4)-C(34)	1.15(3)
N(1)-C(1)	1.33(3)
N(1)-C(4)	1.39(3)
N(2)-C(6)	1.34(3)
N(2)-C(9)	1.39(3)
N(3)-C(13)	1.18(3)
N(3)-C(14)	1.35(3)
N(4)-C(19)	1.29(4)
N(4)-C(18)	1.33(4)
C(1)-C(2)	1.39(3)
C(1)-C(10)#1	1.49(3)
C(2)-C(3)	1.32(3)
C(2)-H(2)	0.95
C(3)-C(4)	1.47(3)
C(3)-H(3)	0.95
C(4)-C(5)	1.42(3)
C(5)-C(6)	1.41(4)
C(5)-C(11)	1.51(3)
C(6)-C(7)	1.47(4)
C(7)-C(8)	1.43(3)
C(7)-H(7)	0.95
C(8)-C(9)	1.44(4)
C(8)-H(8)	0.95
C(9)-C(10)	1.35(3)
C(10)-C(16)	1.55(3)
C(11)-C(12)	1.31(4)
C(11)-C(15)	1.40(3)

C(12)-C(13)	1.52(3)
C(12)-H(12)	0.95
C(13)-H(13)	0.95
C(14)-C(15)	1.44(3)
C(14)-H(14)	0.95
C(15)-H(15)	0.95
C(16)-C(17)	1.34(4)
C(16)-C(20)	1.45(4)
C(17)-C(18)	1.42(4)
C(17)-H(17)	0.95
C(18)-H(18)	0.95
C(19)-C(20)	1.40(4)
C(19)-H(19)	0.95
C(20)-H(20)	0.95
C(21)-C(22)	1.53(4)
C(22)-C(27)	1.388(18)
C(22)-C(23)	1.389(18)
C(23)-C(24)	1.386(18)
C(23)-H(23)	0.95
C(24)-C(25)	1.384(18)
C(24)-H(24)	0.95
C(25)-C(26)	1.389(18)
C(25)-C(28)	1.42(4)
C(26)-C(27)	1.398(18)
C(26)-H(26)	0.95
C(27)-H(27)	0.95
C(28)-C(33)	1.425(18)
C(28)-C(29)	1.431(18)
C(29)-C(30)	1.418(18)
C(29)-H(29)	0.95
C(30)-C(31)	1.424(18)
C(30)-H(30)	0.95
C(31)-C(32)	1.421(18)
C(31)-C(34)	1.50(4)
C(32)-C(33)	1.417(18)
C(32)-H(32)	0.95
C(33)-H(33)	0.95
C(35)-C(36)	1.52(5)
C(35)-H(35A)	0.99
C(35)-H(35B)	0.99
C(36)-H(36A)	0.98
C(36)-H(36B)	0.98
C(36)-H(36C)	0.98

C(37)-C(38)	1.49(5)
C(37)-H(37A)	0.99
C(37)-H(37B)	0.99
C(38)-H(38A)	0.98
C(38)-H(38B)	0.98
C(38)-H(38C)	0.98
C(39)-C(40)	1.53(5)
C(39)-H(39A)	0.99
C(39)-H(39B)	0.99
C(40)-H(40A)	0.98
C(40)-H(40B)	0.98
C(40)-H(40C)	0.98
C(41)-C(42)	1.50(5)
C(41)-H(41A)	0.99
C(41)-H(41B)	0.99
C(42)-H(42A)	0.98
C(42)-H(42B)	0.98
C(42)-H(42C)	0.98
C(43)-C(44)	1.66(5)
C(43)-H(43A)	0.99
C(43)-H(43B)	0.99
C(44)-H(44A)	0.98
C(44)-H(44B)	0.98
C(44)-H(44C)	0.98
C(45)-C(46)	1.27(5)
C(45)-H(45A)	0.99
C(45)-H(45B)	0.99
C(46)-H(46A)	0.98
C(46)-H(46B)	0.98
C(46)-H(46C)	0.98
C(47)-C(48)	1.532(10)
C(47)-H(47A)	0.99
C(47)-H(47B)	0.99
C(48)-H(48A)	0.98
C(48)-H(48B)	0.98
C(48)-H(48C)	0.98
C(49)-C(50)	1.534(10)
C(49)-H(49A)	0.99
C(49)-H(49B)	0.99
C(50)-H(50A)	0.98
C(50)-H(50B)	0.98
C(50)-H(50C)	0.98
C(51)-C(52)	1.531(10)

C(51)-H(51A)	0.99
C(51)-H(51B)	0.99
C(52)-H(52A)	0.98
C(52)-H(52B)	0.98
C(52)-H(52C)	0.98
C(53)-C(54)	1.529(10)
C(53)-H(53A)	0.99
C(53)-H(53B)	0.99
C(54)-H(54A)	0.98
C(54)-H(54B)	0.98
C(54)-H(54C)	0.98
C(56)-C(55)	1.530(10)
C(56)-H(56A)	0.98
C(56)-H(56B)	0.98
C(56)-H(56C)	0.98
C(55)-H(55A)	0.99
C(55)-H(55B)	0.99
C(57)-C(58)	1.531(10)
C(57)-H(57A)	0.99
C(57)-H(57B)	0.99
C(58)-H(58A)	0.98
C(58)-H(58B)	0.98
C(58)-H(58C)	0.98
O(2)-Pt(1)-N(3)	84.8(7)
O(2)-Pt(1)-P(2)	176.2(6)
N(3)-Pt(1)-P(2)	94.5(6)
O(2)-Pt(1)-P(1)	82.8(5)
N(3)-Pt(1)-P(1)	167.0(6)
P(2)-Pt(1)-P(1)	97.6(3)
O(3)-Pt(2)-N(4)	81.6(8)
O(3)-Pt(2)-P(4)	88.4(6)
N(4)-Pt(2)-P(4)	170.0(6)
O(3)-Pt(2)-P(3)	172.3(5)
N(4)-Pt(2)-P(3)	95.7(6)
P(4)-Pt(2)-P(3)	94.0(3)
N(1)#1-Zn(1)-N(1)	180
N(1)#1-Zn(1)-N(2)#1	89.8(8)
N(1)-Zn(1)-N(2)#1	90.2(8)
N(1)#1-Zn(1)-N(2)	90.2(8)
N(1)-Zn(1)-N(2)	89.8(8)
N(2)#1-Zn(1)-N(2)	180
C(41)-P(1)-C(45)	104(2)

C(41)-P(1)-C(43)	112(2)
C(45)-P(1)-C(43)	104(2)
C(41)-P(1)-Pt(1)	105.1(13)
C(45)-P(1)-Pt(1)	107.3(15)
C(43)-P(1)-Pt(1)	122.1(15)
C(39)-P(2)-C(35)	101(2)
C(39)-P(2)-C(37)	105.9(19)
C(35)-P(2)-C(37)	103.1(18)
C(39)-P(2)-Pt(1)	119.1(15)
C(35)-P(2)-Pt(1)	110.2(13)
C(37)-P(2)-Pt(1)	115.8(13)
C(53)-P(3)-C(55)	111(2)
C(53)-P(3)-C(57)	97(2)
C(55)-P(3)-C(57)	97(2)
C(53)-P(3)-Pt(2)	116.9(17)
C(55)-P(3)-Pt(2)	122.5(14)
C(57)-P(3)-Pt(2)	107.2(12)
C(51)-P(4)-C(49)	104(3)
C(51)-P(4)-C(47)	101.3(18)
C(49)-P(4)-C(47)	106(2)
C(51)-P(4)-Pt(2)	119(2)
C(49)-P(4)-Pt(2)	109.7(11)
C(47)-P(4)-Pt(2)	115.6(13)
C(21)-O(2)-Pt(1)	110.0(18)
C(34)-O(3)-Pt(2)	111.9(16)
C(1)-N(1)-C(4)	103.6(18)
C(1)-N(1)-Zn(1)	129.8(15)
C(4)-N(1)-Zn(1)	126.6(17)
C(6)-N(2)-C(9)	108(2)
C(6)-N(2)-Zn(1)	127.6(18)
C(9)-N(2)-Zn(1)	124.3(16)
C(13)-N(3)-C(14)	126(2)
C(13)-N(3)-Pt(1)	115.5(16)
C(14)-N(3)-Pt(1)	118.2(16)
C(19)-N(4)-C(18)	120(2)
C(19)-N(4)-Pt(2)	122.1(19)
C(18)-N(4)-Pt(2)	116(2)
N(1)-C(1)-C(2)	113(2)
N(1)-C(1)-C(10)#1	123(2)
C(2)-C(1)-C(10)#1	124(2)
C(3)-C(2)-C(1)	109(2)
C(3)-C(2)-H(2)	125.7
C(1)-C(2)-H(2)	125.7



C(2)-C(3)-C(4)	105(2)
C(2)-C(3)-H(3)	127.6
C(4)-C(3)-H(3)	127.6
N(1)-C(4)-C(5)	126(2)
N(1)-C(4)-C(3)	110(2)
C(5)-C(4)-C(3)	124(2)
C(6)-C(5)-C(4)	124(2)
C(6)-C(5)-C(11)	118(2)
C(4)-C(5)-C(11)	117(2)
N(2)-C(6)-C(5)	125(2)
N(2)-C(6)-C(7)	110(2)
C(5)-C(6)-C(7)	125(2)
C(8)-C(7)-C(6)	106(2)
C(8)-C(7)-H(7)	126.9
C(6)-C(7)-H(7)	126.9
C(7)-C(8)-C(9)	105(2)
C(7)-C(8)-H(8)	127.7
C(9)-C(8)-H(8)	127.7
C(10)-C(9)-N(2)	127(2)
C(10)-C(9)-C(8)	122(2)
N(2)-C(9)-C(8)	111(2)
C(9)-C(10)-C(1)#1	125(2)
C(9)-C(10)-C(16)	122(2)
C(1)#1-C(10)-C(16)	111.6(19)
C(12)-C(11)-C(15)	122(2)
C(12)-C(11)-C(5)	119(3)
C(15)-C(11)-C(5)	119(3)
C(11)-C(12)-C(13)	117(3)
C(11)-C(12)-H(12)	121.7
C(13)-C(12)-H(12)	121.7
N(3)-C(13)-C(12)	121(3)
N(3)-C(13)-H(13)	119.7
C(12)-C(13)-H(13)	119.7
N(3)-C(14)-C(15)	118(2)
N(3)-C(14)-H(14)	121
C(15)-C(14)-H(14)	121
C(11)-C(15)-C(14)	117(2)
C(11)-C(15)-H(15)	121.5
C(14)-C(15)-H(15)	121.5
C(17)-C(16)-C(20)	118(2)
C(17)-C(16)-C(10)	124(2)
C(20)-C(16)-C(10)	117(2)
C(16)-C(17)-C(18)	120(3)

C(16)-C(17)-H(17)	120
C(18)-C(17)-H(17)	120
N(4)-C(18)-C(17)	121(3)
N(4)-C(18)-H(18)	119.7
C(17)-C(18)-H(18)	119.7
N(4)-C(19)-C(20)	123(3)
N(4)-C(19)-H(19)	118.3
C(20)-C(19)-H(19)	118.3
C(19)-C(20)-C(16)	117(3)
C(19)-C(20)-H(20)	121.7
C(16)-C(20)-H(20)	121.7
O(1)-C(21)-O(2)	132(3)
O(1)-C(21)-C(22)	114(3)
O(2)-C(21)-C(22)	113(3)
C(27)-C(22)-C(23)	119(3)
C(27)-C(22)-C(21)	122(2)
C(23)-C(22)-C(21)	119(2)
C(24)-C(23)-C(22)	118(3)
C(24)-C(23)-H(23)	120.9
C(22)-C(23)-H(23)	120.9
C(25)-C(24)-C(23)	125(3)
C(25)-C(24)-H(24)	117.7
C(23)-C(24)-H(24)	117.7
C(24)-C(25)-C(26)	116(3)
C(24)-C(25)-C(28)	127(2)
C(26)-C(25)-C(28)	117(2)
C(25)-C(26)-C(27)	120(3)
C(25)-C(26)-H(26)	119.8
C(27)-C(26)-H(26)	119.8
C(22)-C(27)-C(26)	122(3)
C(22)-C(27)-H(27)	119.2
C(26)-C(27)-H(27)	119.2
C(25)-C(28)-C(33)	121(2)
C(25)-C(28)-C(29)	121(2)
C(33)-C(28)-C(29)	117(3)
C(30)-C(29)-C(28)	121(3)
C(30)-C(29)-H(29)	119.4
C(28)-C(29)-H(29)	119.4
C(29)-C(30)-C(31)	122(3)
C(29)-C(30)-H(30)	119.1
C(31)-C(30)-H(30)	119.1
C(32)-C(31)-C(30)	117(3)
C(32)-C(31)-C(34)	123(2)

C(30)-C(31)-C(34)	119(2)
C(33)-C(32)-C(31)	121(3)
C(33)-C(32)-H(32)	119.3
C(31)-C(32)-H(32)	119.3
C(32)-C(33)-C(28)	122(3)
C(32)-C(33)-H(33)	119.1
C(28)-C(33)-H(33)	119.1
O(4)-C(34)-O(3)	126(3)
O(4)-C(34)-C(31)	121(3)
O(3)-C(34)-C(31)	113(2)
C(36)-C(35)-P(2)	112(3)
C(36)-C(35)-H(35A)	109.3
P(2)-C(35)-H(35A)	109.3
C(36)-C(35)-H(35B)	109.3
P(2)-C(35)-H(35B)	109.3
H(35A)-C(35)-H(35B)	108
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(38)-C(37)-P(2)	115(3)
C(38)-C(37)-H(37A)	108.6
P(2)-C(37)-H(37A)	108.6
C(38)-C(37)-H(37B)	108.6
P(2)-C(37)-H(37B)	108.6
H(37A)-C(37)-H(37B)	107.6
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(40)-C(39)-P(2)	112(2)
C(40)-C(39)-H(39A)	109.3
P(2)-C(39)-H(39A)	109.3
C(40)-C(39)-H(39B)	109.3
P(2)-C(39)-H(39B)	109.3
H(39A)-C(39)-H(39B)	107.9
C(39)-C(40)-H(40A)	109.5
C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5

C(39)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(42)-C(41)-P(1)	109(2)
C(42)-C(41)-H(41A)	109.8
P(1)-C(41)-H(41A)	109.8
C(42)-C(41)-H(41B)	109.8
P(1)-C(41)-H(41B)	109.8
H(41A)-C(41)-H(41B)	108.3
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(44)-C(43)-P(1)	110(3)
C(44)-C(43)-H(43A)	109.7
P(1)-C(43)-H(43A)	109.7
C(44)-C(43)-H(43B)	109.7
P(1)-C(43)-H(43B)	109.7
H(43A)-C(43)-H(43B)	108.2
C(43)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(46)-C(45)-P(1)	122(4)
C(46)-C(45)-H(45A)	106.8
P(1)-C(45)-H(45A)	106.8
C(46)-C(45)-H(45B)	106.8
P(1)-C(45)-H(45B)	106.8
H(45A)-C(45)-H(45B)	106.6
C(45)-C(46)-H(46A)	109.5
C(45)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(45)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(48)-C(47)-P(4)	113(2)
C(48)-C(47)-H(47A)	109.1
P(4)-C(47)-H(47A)	109.1
C(48)-C(47)-H(47B)	109.1

P(4)-C(47)-H(47B)	109.1
H(47A)-C(47)-H(47B)	107.8
C(47)-C(48)-H(48A)	109.5
C(47)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(47)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(50)-C(49)-P(4)	110(3)
C(50)-C(49)-H(49A)	109.6
P(4)-C(49)-H(49A)	109.6
C(50)-C(49)-H(49B)	109.6
P(4)-C(49)-H(49B)	109.6
H(49A)-C(49)-H(49B)	108.1
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(52)-C(51)-P(4)	112(3)
C(52)-C(51)-H(51A)	109.2
P(4)-C(51)-H(51A)	109.2
C(52)-C(51)-H(51B)	109.2
P(4)-C(51)-H(51B)	109.2
H(51A)-C(51)-H(51B)	107.9
C(51)-C(52)-H(52A)	109.5
C(51)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(51)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(54)-C(53)-P(3)	124(4)
C(54)-C(53)-H(53A)	106.3
P(3)-C(53)-H(53A)	106.3
C(54)-C(53)-H(53B)	106.3
P(3)-C(53)-H(53B)	106.3
H(53A)-C(53)-H(53B)	106.4
C(53)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5

H(54B)-C(54)-H(54C)	109.5
C(55)-C(56)-H(56A)	109.5
C(55)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5
C(55)-C(56)-H(56C)	109.5
H(56A)-C(56)-H(56C)	109.5
H(56B)-C(56)-H(56C)	109.5
C(56)-C(55)-P(3)	113(3)
C(56)-C(55)-H(55A)	109
P(3)-C(55)-H(55A)	109
C(56)-C(55)-H(55B)	109
P(3)-C(55)-H(55B)	109
H(55A)-C(55)-H(55B)	107.8
C(58)-C(57)-P(3)	113(3)
C(58)-C(57)-H(57A)	109.1
P(3)-C(57)-H(57A)	109.1
C(58)-C(57)-H(57B)	109.1
P(3)-C(57)-H(57B)	109.1
H(57A)-C(57)-H(57B)	107.8
C(57)-C(58)-H(58A)	109.5
C(57)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(57)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+1

**Table 5.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **BT3**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
Pt(1)	6023(1)	5750(2)	4546(1)	92(2)
O(1)	4438(16)	2350(40)	2539(18)	90(14)
O(2)	3772(14)	2770(30)	2624(17)	108(12)
C(23)	4860(20)	4450(30)	3644(15)	87(13)
C(24)	5107(14)	4030(40)	3390(20)	89(14)
C(25)	4890(20)	3490(30)	3055(18)	90(14)
C(26)	4430(20)	3370(30)	2970(16)	87(13)
C(27)	4180(15)	3790(40)	3220(20)	92(14)
C(28)	4400(20)	4330(30)	3559(18)	88(14)

P(1)	6486(9)	6353(17)	5153(10)	103(7)
Pt(2)	3342(2)	1949(4)	2203(2)	141(3)
P(2)	6004(9)	6885(14)	4089(9)	91(7)
Zn(03)	5000	0	5000	82(5)
O(3)	5615(18)	5070(30)	4027(17)	81(9)
C(2)	5586(12)	4390(30)	5084(15)	67(12)
N(5)	5949(12)	4570(20)	4908(13)	47(8)
C(3)	6177(11)	3890(30)	4767(13)	34(8)
C(4)	6043(14)	3040(20)	4803(15)	55(12)
C(5)	5681(15)	2860(20)	4979(16)	67(11)
C(6)	5453(13)	3540(30)	5120(16)	72(13)
O(4)	4957(18)	5350(40)	4230(20)	100(15)
P(3)	3184(10)	2970(20)	1691(9)	124(7)
P(4)	2867(11)	990(30)	1891(13)	171(13)
C(7)	5530(20)	2030(50)	5030(30)	66(12)
C(8)	5628(18)	1590(30)	5365(14)	69(12)
C(9)	5949(18)	1840(30)	5750(17)	71(15)
C(10)	5968(17)	1170(40)	6062(13)	74(15)
C(11)	5659(18)	510(30)	5870(17)	74(14)
N(3)	5449(15)	770(30)	5439(15)	65(11)
C(12)	5208(18)	1790(40)	4631(16)	80(13)
C(13)	5100(20)	2270(30)	4240(20)	84(15)
C(14)	4760(20)	1820(40)	3935(15)	81(15)
C(15)	4655(17)	1060(30)	4139(19)	79(13)
N(2)	4931(18)	1040(30)	4569(17)	75(7)
C(16)	4430(30)	360(60)	3980(30)	77(9)
C(17)	4180(30)	450(60)	3560(30)	75(14)
C(18)	4180(30)	300(60)	3180(30)	85(14)
C(19)	3990(30)	580(70)	2800(30)	96(15)
N(4)	3640(30)	1130(60)	2740(30)	118(15)
C(21)	3470(30)	1290(60)	3080(30)	98(16)
C(20)	3760(30)	940(50)	3510(30)	76(14)
C(1A)	5710(30)	7640(50)	4100(30)	105(14)
C(2A)	5190(30)	7550(60)	3970(40)	140(30)
C(38)	5910(30)	6620(50)	3500(30)	110(14)
C(39)	6150(30)	5760(50)	3430(30)	120(20)
C(3A)	6650(30)	7160(50)	4170(30)	118(16)
C(49)	2940(30)	-160(70)	2110(40)	170(20)
C(52)	5090(30)	5050(40)	3980(20)	86(12)
C(53)	4161(17)	2750(50)	2650(20)	90(13)
C(9A)	3390(20)	2420(50)	1260(20)	125(9)
C(12A)	6440(30)	5740(70)	5680(20)	128(17)
C(13A)	3880(20)	2320(70)	1230(30)	136(12)

C(14A)	6983(18)	6420(70)	4340(40)	160(30)
C(15A)	5820(20)	7440(60)	5270(30)	110(16)
C(16A)	6700(30)	6050(60)	6130(30)	130(30)
C(17A)	6320(20)	7450(30)	5270(30)	96(13)
C(19A)	2570(40)	-850(50)	1930(40)	200(40)
C(22A)	1980(30)	1010(100)	2120(50)	240(40)
C(23A)	2360(30)	730(90)	1910(40)	200(20)
C(25A)	7054(17)	6250(40)	5080(30)	119(15)
C(28A)	7330(20)	5410(60)	5130(40)	170(40)
C(29A)	2400(40)	710(80)	950(20)	210(40)
C(31A)	2800(30)	570(70)	1348(19)	174(19)
C(32A)	2890(30)	3870(50)	1360(30)	136(17)
C(33A)	3060(40)	4330(70)	1000(30)	190(40)
C(34A)	3530(20)	3940(30)	1720(30)	136(16)
C(35A)	3420(30)	4870(30)	1830(30)	150(20)

**Table 6.** Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **BT3**.

Pt(1)-O(3)	2.09(6)
Pt(1)-N(5)	2.19(3)
Pt(1)-P(2)	2.26(2)
Pt(1)-P(1)	2.29(3)
O(1)-C(53)	1.17(2)
O(2)-C(53)	1.18(2)
O(2)-Pt(2)	2.06(2)
C(23)-C(24)	1.39
C(23)-C(28)	1.39
C(23)-C(52)	1.46(2)
C(24)-C(25)	1.39
C(24)-H(24)	0.95
C(25)-C(26)	1.39
C(25)-H(25)	0.95
C(26)-C(27)	1.39
C(26)-C(53)	1.48(2)
C(27)-C(28)	1.39
C(27)-H(27)	0.95
C(28)-H(28)	0.95
P(1)-C(25A)	1.82(2)
P(1)-C(17A)	1.83(2)
P(1)-C(12A)	1.96(7)
Pt(2)-N(4)	2.13(9)
Pt(2)-P(4)	2.13(3)
Pt(2)-P(3)	2.23(3)



P(2)-C(1A)	1.48(8)
P(2)-C(38)	1.87(9)
P(2)-C(3A)	1.96(9)
Zn(03)-N(3)#1	2.07(4)
Zn(03)-N(3)	2.07(4)
Zn(03)-N(2)	2.08(4)
Zn(03)-N(2)#1	2.08(4)
O(3)-C(52)	1.58(10)
C(2)-N(5)	1.39
C(2)-C(6)	1.39
C(2)-H(2)	0.95
N(5)-C(3)	1.39
C(3)-C(4)	1.39
C(3)-H(3)	0.95
C(4)-C(5)	1.39
C(4)-H(4)	0.95
C(5)-C(7)	1.37(8)
C(5)-C(6)	1.39
C(6)-H(6)	0.95
O(4)-C(52)	1.07(8)
P(3)-C(34A)	1.83(2)
P(3)-C(9A)	1.85(2)
P(3)-C(32A)	1.83(7)
P(4)-C(23A)	1.63(9)
P(4)-C(31A)	1.81(2)
P(4)-C(49)	1.90(10)
C(7)-C(8)	1.23(8)
C(7)-C(12)	1.46(8)
C(8)-N(3)	1.42
C(8)-C(9)	1.42
C(9)-C(10)	1.42
C(9)-H(9)	0.95
C(10)-C(11)	1.42
C(10)-H(10)	0.95
C(11)-N(3)	1.42
C(11)-C(16)#1	1.46(9)
C(12)-C(13)	1.42
C(12)-N(2)	1.42
C(13)-C(14)	1.42
C(13)-H(13)	0.95
C(14)-C(15)	1.42
C(14)-H(14)	0.95
C(15)-C(16)	1.31(9)

C(15)-N(2)	1.42
C(16)-C(17)	1.38(10)
C(17)-C(18)	1.22(10)
C(17)-C(20)	1.46(10)
C(18)-C(19)	1.28(10)
C(18)-H(18)	0.95
C(19)-N(4)	1.35(11)
C(19)-H(19)	0.95
N(4)-C(21)	1.33(11)
C(21)-C(20)	1.54(10)
C(21)-H(21)	0.95
C(20)-H(20)	0.95
C(1A)-C(2A)	1.54(2)
C(1A)-H(1A1)	0.99
C(1A)-H(1A2)	0.99
C(2A)-H(2A1)	0.989
C(2A)-H(2A2)	0.9894
C(2A)-H(2A3)	0.9893
C(38)-C(39)	1.54(2)
C(38)-H(38A)	0.99
C(38)-H(38B)	0.99
C(39)-C(35A)#2	2.20(11)
C(39)-H(39A)	1.0085
C(39)-H(39B)	1.0091
C(39)-H(39C)	1.0095
C(3A)-C(14A)	1.54(2)
C(3A)-H(3A1)	0.99
C(3A)-H(3A2)	0.99
C(49)-C(19A)	1.54(2)
C(49)-H(49A)	0.99
C(49)-H(49B)	0.99
C(9A)-C(13A)	1.55(2)
C(9A)-H(9A1)	0.99
C(9A)-H(9A2)	0.99
C(12A)-C(16A)	1.54(2)
C(12A)-H(12A)	0.99
C(12A)-H(12B)	0.99
C(13A)-H(13A)	0.999
C(13A)-H(13B)	0.9967
C(13A)-H(13C)	0.996
C(14A)-H(14A)	0.9801
C(14A)-H(14B)	0.9801
C(14A)-H(14C)	0.9801

C(15A)-C(17A)	1.53(2)
C(15A)-H(15A)	0.98
C(15A)-H(15B)	0.98
C(15A)-H(15C)	0.98
C(16A)-H(16A)	0.9802
C(16A)-H(16B)	0.9802
C(16A)-H(16C)	0.9802
C(17A)-H(17A)	0.99
C(17A)-H(17B)	0.99
C(19A)-H(19A)	1.0149
C(19A)-H(19B)	1.0127
C(19A)-H(19C)	1.0131
C(22A)-C(23A)	1.54(2)
C(22A)-H(22A)	1.1408
C(22A)-H(22B)	1.1551
C(22A)-H(22C)	1.1401
C(23A)-H(23A)	0.99
C(23A)-H(23B)	0.99
C(25A)-C(28A)	1.53(2)
C(25A)-H(25A)	0.99
C(25A)-H(25B)	0.99
C(28A)-H(28A)	1.0135
C(28A)-H(28B)	1.0125
C(28A)-H(28C)	1.0124
C(29A)-C(31A)	1.54(2)
C(29A)-H(29A)	1.0091
C(29A)-H(29B)	1.0093
C(29A)-H(29C)	1.0078
C(31A)-H(31A)	0.99
C(31A)-H(31B)	0.99
C(32A)-C(33A)	1.55(2)
C(32A)-H(32A)	0.99
C(32A)-H(32B)	0.99
C(33A)-H(33A)	1.0001
C(33A)-H(33B)	1.0009
C(33A)-H(33C)	0.9989
C(34A)-C(35A)	1.53(2)
C(34A)-H(34A)	0.99
C(34A)-H(34B)	0.99
C(35A)-H(35A)	0.9801
C(35A)-H(35B)	0.9801
C(35A)-H(35C)	0.9801

O(3)-Pt(1)-N(5)	83.3(16)
O(3)-Pt(1)-P(2)	87.9(15)
N(5)-Pt(1)-P(2)	170.8(13)
O(3)-Pt(1)-P(1)	173.8(15)
N(5)-Pt(1)-P(1)	90.8(12)
P(2)-Pt(1)-P(1)	98.1(10)
C(53)-O(2)-Pt(2)	120(3)
C(24)-C(23)-C(28)	120
C(24)-C(23)-C(52)	120(6)
C(28)-C(23)-C(52)	120(6)
C(25)-C(24)-C(23)	120
C(25)-C(24)-H(24)	120
C(23)-C(24)-H(24)	120
C(24)-C(25)-C(26)	120
C(24)-C(25)-H(25)	120
C(26)-C(25)-H(25)	120
C(25)-C(26)-C(27)	120
C(25)-C(26)-C(53)	125(5)
C(27)-C(26)-C(53)	115(5)
C(28)-C(27)-C(26)	120
C(28)-C(27)-H(27)	120
C(26)-C(27)-H(27)	120
C(27)-C(28)-C(23)	120
C(27)-C(28)-H(28)	120
C(23)-C(28)-H(28)	120
C(25A)-P(1)-C(17A)	116(3)
C(25A)-P(1)-C(12A)	110(3)
C(17A)-P(1)-C(12A)	101(4)
C(25A)-P(1)-Pt(1)	106(4)
C(17A)-P(1)-Pt(1)	113(3)
C(12A)-P(1)-Pt(1)	111(3)
O(2)-Pt(2)-N(4)	76(3)
O(2)-Pt(2)-P(4)	168(2)
N(4)-Pt(2)-P(4)	94(2)
O(2)-Pt(2)-P(3)	91.9(19)
N(4)-Pt(2)-P(3)	167(2)
P(4)-Pt(2)-P(3)	98.3(13)
C(1A)-P(2)-C(38)	105(5)
C(1A)-P(2)-C(3A)	116(4)
C(38)-P(2)-C(3A)	94(5)
C(1A)-P(2)-Pt(1)	120(4)
C(38)-P(2)-Pt(1)	117(3)
C(3A)-P(2)-Pt(1)	103(2)

N(3)#1-Zn(03)-N(3)	180(5)
N(3)#1-Zn(03)-N(2)	93(5)
N(3)-Zn(03)-N(2)	87(2)
N(3)#1-Zn(03)-N(2)#1	87(7)
N(3)-Zn(03)-N(2)#1	93(6)
N(2)-Zn(03)-N(2)#1	180(6)
C(52)-O(3)-Pt(1)	118(3)
N(5)-C(2)-C(6)	120
N(5)-C(2)-H(2)	120
C(6)-C(2)-H(2)	120
C(2)-N(5)-C(3)	120
C(2)-N(5)-Pt(1)	125(2)
C(3)-N(5)-Pt(1)	109(2)
N(5)-C(3)-C(4)	120
N(5)-C(3)-H(3)	120
C(4)-C(3)-H(3)	120
C(5)-C(4)-C(3)	120
C(5)-C(4)-H(4)	120
C(3)-C(4)-H(4)	120
C(7)-C(5)-C(4)	123(5)
C(7)-C(5)-C(6)	117(5)
C(4)-C(5)-C(6)	120
C(5)-C(6)-C(2)	120
C(5)-C(6)-H(6)	120
C(2)-C(6)-H(6)	120
C(34A)-P(3)-C(9A)	96(2)
C(34A)-P(3)-C(32A)	67(4)
C(9A)-P(3)-C(32A)	97(3)
C(34A)-P(3)-Pt(2)	121(3)
C(9A)-P(3)-Pt(2)	100(3)
C(32A)-P(3)-Pt(2)	160(3)
C(23A)-P(4)-C(31A)	94(5)
C(23A)-P(4)-C(49)	77(6)
C(31A)-P(4)-C(49)	89(6)
C(23A)-P(4)-Pt(2)	135(4)
C(31A)-P(4)-Pt(2)	126(4)
C(49)-P(4)-Pt(2)	118(3)
C(8)-C(7)-C(5)	127(7)
C(8)-C(7)-C(12)	125(7)
C(5)-C(7)-C(12)	108(6)
C(7)-C(8)-N(3)	128(6)
C(7)-C(8)-C(9)	124(6)
N(3)-C(8)-C(9)	108

C(8)-C(9)-C(10)	108
C(8)-C(9)-H(9)	126
C(10)-C(9)-H(9)	126
C(9)-C(10)-C(11)	108
C(9)-C(10)-H(10)	126
C(11)-C(10)-H(10)	126
N(3)-C(11)-C(10)	108
N(3)-C(11)-C(16)#1	119(5)
C(10)-C(11)-C(16)#1	132(5)
C(8)-N(3)-C(11)	108
C(8)-N(3)-Zn(03)	128(3)
C(11)-N(3)-Zn(03)	124(3)
C(13)-C(12)-N(2)	108
C(13)-C(12)-C(7)	126(5)
N(2)-C(12)-C(7)	126(5)
C(12)-C(13)-C(14)	108
C(12)-C(13)-H(13)	126
C(14)-C(13)-H(13)	126
C(15)-C(14)-C(13)	108
C(15)-C(14)-H(14)	126
C(13)-C(14)-H(14)	126
C(16)-C(15)-C(14)	132(6)
C(16)-C(15)-N(2)	119(6)
C(14)-C(15)-N(2)	108
C(15)-N(2)-C(12)	108
C(15)-N(2)-Zn(03)	126(4)
C(12)-N(2)-Zn(03)	125(3)
C(15)-C(16)-C(17)	113(8)
C(15)-C(16)-C(11)#1	139(8)
C(17)-C(16)-C(11)#1	108(7)
C(18)-C(17)-C(16)	144(10)
C(18)-C(17)-C(20)	102(9)
C(16)-C(17)-C(20)	114(8)
C(17)-C(18)-C(19)	140(10)
C(17)-C(18)-H(18)	110.4
C(19)-C(18)-H(18)	110.1
C(18)-C(19)-N(4)	120(10)
C(18)-C(19)-H(19)	119.9
N(4)-C(19)-H(19)	120
C(21)-N(4)-C(19)	117(9)
C(21)-N(4)-Pt(2)	112(8)
C(19)-N(4)-Pt(2)	131(8)
N(4)-C(21)-C(20)	114(9)

N(4)-C(21)-H(21)	123.1
C(20)-C(21)-H(21)	123.2
C(17)-C(20)-C(21)	125(9)
C(17)-C(20)-H(20)	117.6
C(21)-C(20)-H(20)	117.4
P(2)-C(1A)-C(2A)	121(6)
P(2)-C(1A)-H(1A1)	107
C(2A)-C(1A)-H(1A1)	106.9
P(2)-C(1A)-H(1A2)	107
C(2A)-C(1A)-H(1A2)	107
H(1A1)-C(1A)-H(1A2)	106.8
C(1A)-C(2A)-H(2A1)	110.1
C(1A)-C(2A)-H(2A2)	110.6
H(2A1)-C(2A)-H(2A2)	108.5
C(1A)-C(2A)-H(2A3)	110.4
H(2A1)-C(2A)-H(2A3)	108.6
H(2A2)-C(2A)-H(2A3)	108.6
C(39)-C(38)-P(2)	112(6)
C(39)-C(38)-H(38A)	109.1
P(2)-C(38)-H(38A)	109.4
C(39)-C(38)-H(38B)	109.3
P(2)-C(38)-H(38B)	109.3
H(38A)-C(38)-H(38B)	107.9
C(38)-C(39)-C(35A)#2	159(7)
C(38)-C(39)-H(39A)	112.1
C(35A)#2-C(39)-H(39A)	61.4
C(38)-C(39)-H(39B)	112.3
C(35A)#2-C(39)-H(39B)	56
H(39A)-C(39)-H(39B)	106.6
C(38)-C(39)-H(39C)	112.5
C(35A)#2-C(39)-H(39C)	88.7
H(39A)-C(39)-H(39C)	106.5
H(39B)-C(39)-H(39C)	106.5
C(14A)-C(3A)-P(2)	117(5)
C(14A)-C(3A)-H(3A1)	108.3
P(2)-C(3A)-H(3A1)	108.2
C(14A)-C(3A)-H(3A2)	108.2
P(2)-C(3A)-H(3A2)	107.9
H(3A1)-C(3A)-H(3A2)	107.3
C(19A)-C(49)-P(4)	120(6)
C(19A)-C(49)-H(49A)	107.5
P(4)-C(49)-H(49A)	107.5
C(19A)-C(49)-H(49B)	106.9

P(4)-C(49)-H(49B)	107.3
H(49A)-C(49)-H(49B)	106.9
O(4)-C(52)-C(23)	128(9)
O(4)-C(52)-O(3)	119(6)
C(23)-C(52)-O(3)	111(7)
O(1)-C(53)-O(2)	142(5)
O(1)-C(53)-C(26)	104(5)
O(2)-C(53)-C(26)	114(4)
C(13A)-C(9A)-P(3)	127(3)
C(13A)-C(9A)-H(9A1)	106.3
P(3)-C(9A)-H(9A1)	105.7
C(13A)-C(9A)-H(9A2)	104.7
P(3)-C(9A)-H(9A2)	105.6
H(9A1)-C(9A)-H(9A2)	106.1
C(16A)-C(12A)-P(1)	121(6)
C(16A)-C(12A)-H(12A)	107.2
P(1)-C(12A)-H(12A)	107.2
C(16A)-C(12A)-H(12B)	106.9
P(1)-C(12A)-H(12B)	107
H(12A)-C(12A)-H(12B)	106.8
C(9A)-C(13A)-H(13A)	112.2
C(9A)-C(13A)-H(13B)	110.9
H(13A)-C(13A)-H(13B)	107.9
C(9A)-C(13A)-H(13C)	110.4
H(13A)-C(13A)-H(13C)	107.5
H(13B)-C(13A)-H(13C)	107.9
C(3A)-C(14A)-H(14A)	109.6
C(3A)-C(14A)-H(14B)	109.3
H(14A)-C(14A)-H(14B)	109.5
C(3A)-C(14A)-H(14C)	109.6
H(14A)-C(14A)-H(14C)	109.5
H(14B)-C(14A)-H(14C)	109.5
C(17A)-C(15A)-H(15A)	109.5
C(17A)-C(15A)-H(15B)	109.5
H(15A)-C(15A)-H(15B)	109.5
C(17A)-C(15A)-H(15C)	109.4
H(15A)-C(15A)-H(15C)	109.5
H(15B)-C(15A)-H(15C)	109.5
C(12A)-C(16A)-H(16A)	109.3
C(12A)-C(16A)-H(16B)	109.6
H(16A)-C(16A)-H(16B)	109.5
C(12A)-C(16A)-H(16C)	109.5
H(16A)-C(16A)-H(16C)	109.4



H(16B)-C(16A)-H(16C)	109.5
C(15A)-C(17A)-P(1)	109(5)
C(15A)-C(17A)-H(17A)	110
P(1)-C(17A)-H(17A)	109.8
C(15A)-C(17A)-H(17B)	109.9
P(1)-C(17A)-H(17B)	110.1
H(17A)-C(17A)-H(17B)	108.3
C(49)-C(19A)-H(19A)	113.2
C(49)-C(19A)-H(19B)	112.5
H(19A)-C(19A)-H(19B)	106.1
C(49)-C(19A)-H(19C)	112.6
H(19A)-C(19A)-H(19C)	105.9
H(19B)-C(19A)-H(19C)	106.1
C(23A)-C(22A)-H(22A)	125.4
C(23A)-C(22A)-H(22B)	127.3
H(22A)-C(22A)-H(22B)	88.7
C(23A)-C(22A)-H(22C)	124.6
H(22A)-C(22A)-H(22C)	89.7
H(22B)-C(22A)-H(22C)	89.3
C(22A)-C(23A)-P(4)	142(10)
C(22A)-C(23A)-H(23A)	101.6
P(4)-C(23A)-H(23A)	102.1
C(22A)-C(23A)-H(23B)	101.5
P(4)-C(23A)-H(23B)	101.1
H(23A)-C(23A)-H(23B)	104.6
C(28A)-C(25A)-P(1)	126(3)
C(28A)-C(25A)-H(25A)	106.1
P(1)-C(25A)-H(25A)	105.9
C(28A)-C(25A)-H(25B)	105.8
P(1)-C(25A)-H(25B)	105.9
H(25A)-C(25A)-H(25B)	106.2
C(25A)-C(28A)-H(28A)	112.9
C(25A)-C(28A)-H(28B)	112.6
H(28A)-C(28A)-H(28B)	106.1
C(25A)-C(28A)-H(28C)	112.6
H(28A)-C(28A)-H(28C)	106
H(28B)-C(28A)-H(28C)	106.1
C(31A)-C(29A)-H(29A)	112.3
C(31A)-C(29A)-H(29B)	112.4
H(29A)-C(29A)-H(29B)	106.5
C(31A)-C(29A)-H(29C)	112.1
H(29A)-C(29A)-H(29C)	106.7
H(29B)-C(29A)-H(29C)	106.5

C(29A)-C(31A)-P(4)	127(4)
C(29A)-C(31A)-H(31A)	105.7
P(4)-C(31A)-H(31A)	105.5
C(29A)-C(31A)-H(31B)	105.5
P(4)-C(31A)-H(31B)	105.6
H(31A)-C(31A)-H(31B)	106.1
C(33A)-C(32A)-P(3)	124(5)
C(33A)-C(32A)-H(32A)	106.8
P(3)-C(32A)-H(32A)	106.2
C(33A)-C(32A)-H(32B)	105.9
P(3)-C(32A)-H(32B)	106.2
H(32A)-C(32A)-H(32B)	106.4
C(32A)-C(33A)-H(33A)	111.5
C(32A)-C(33A)-H(33B)	111.9
H(33A)-C(33A)-H(33B)	107.4
C(32A)-C(33A)-H(33C)	110.8
H(33A)-C(33A)-H(33C)	107.4
H(33B)-C(33A)-H(33C)	107.6
C(35A)-C(34A)-P(3)	128(4)
C(35A)-C(34A)-H(34A)	104.9
P(3)-C(34A)-H(34A)	105.3
C(35A)-C(34A)-H(34B)	105.7
P(3)-C(34A)-H(34B)	105.4
H(34A)-C(34A)-H(34B)	106
C(34A)-C(35A)-C(39)#2	108(6)
C(34A)-C(35A)-H(35A)	109.3
C(39)#2-C(35A)-H(35A)	133.6
C(34A)-C(35A)-H(35B)	109.1
C(39)#2-C(35A)-H(35B)	30.7
H(35A)-C(35A)-H(35B)	109.5
C(34A)-C(35A)-H(35C)	110
C(39)#2-C(35A)-H(35C)	81.8
H(35A)-C(35A)-H(35C)	109.5
H(35B)-C(35A)-H(35C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1 #2 -x+1,y,-z+1/2

**Table 7.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **BT4**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	$U(\text{eq})$
Pt(1)	11311(1)	5735(1)	5811(1)	95(1)

Pt(2)	7728(1)	7226(1)	636(1)	127(1)
Pt(3)	2824(1)	6741(1)	3123(1)	203(1)
Pt(4)	6519(1)	5208(1)	8238(1)	172(1)
Zn(1)	7006(1)	6042(1)	4265(2)	83(1)
P(4)	6875(7)	7432(6)	-16(7)	196(6)
P(5)	2678(7)	7130(8)	2258(11)	270(12)
P(6)	1911(7)	6815(10)	3164(12)	349(17)
P(7)	6053(8)	5041(7)	8926(8)	220(8)
P(8)	7423(9)	5218(10)	8884(10)	311(15)
O(1)	11074(9)	5931(6)	4915(11)	96(5)
O(2)	10664(9)	5368(7)	4489(10)	98(6)
O(3)	8509(10)	7020(8)	1324(13)	123(7)
O(4)	8572(12)	7579(9)	1931(14)	143(9)
O(5)	3110(11)	6473(12)	4045(15)	164(10)
O(6)	3109(16)	5833(13)	3583(19)	197(13)
O(8)	5735(12)	4709(9)	7128(15)	148(9)
O(9W)	6813(10)	5532(6)	3685(14)	134(8)
N(5)	10369(10)	5770(5)	5630(12)	79(6)
C(29)	7265(11)	6464(5)	1929(12)	118(9)
C(26)	7189(10)	6720(7)	2383(9)	101(7)
C(27)	7199(10)	7129(6)	2297(10)	109(8)
C(28)	7284(10)	7282(5)	1757(12)	118(9)
N(6)	7360(9)	7025(7)	1304(9)	112(7)
C(30)	7350(10)	6616(7)	1390(10)	118(9)
P(1)	11480(4)	5553(3)	6803(6)	118(3)
N(8)	6769(10)	5365(8)	7456(9)	131(8)
C(36)	6914(10)	5087(6)	7073(12)	133(10)
C(37)	6976(10)	5206(7)	6504(11)	120(9)
C(38)	6892(10)	5602(8)	6318(10)	113(8)
C(39)	6747(10)	5880(6)	6702(13)	124(9)
C(40)	6685(10)	5761(7)	7271(11)	134(9)
C(34)	4679(16)	6780(13)	3820(20)	151(12)
C(31)	4895(14)	6427(11)	3566(19)	105(8)
C(32)	4492(15)	6219(12)	3203(19)	118(9)
C(33)	3891(15)	6298(13)	3047(19)	121(10)
N(7)	3724(13)	6654(12)	3245(17)	133(9)
C(35)	4153(17)	6884(14)	3650(20)	153(12)
P(2)	12265(4)	5759(3)	5846(6)	118(4)
N(1)	7590(7)	5853(6)	5128(8)	92(6)
C(1)	7465(6)	5726(6)	5673(10)	85(7)
C(2)	8009(8)	5627(6)	6147(8)	76(6)
C(4)	8470(6)	5693(6)	5894(10)	83(7)
C(4')	8212(8)	5833(6)	5264(9)	82(6)

P(3)	8330(7)	7402(4)	65(7)	156(5)
C(13)	5808(7)	6451(6)	3392(9)	76(6)
C(3)	5593(6)	6646(7)	2798(10)	95(8)
C(11)	6080(9)	6714(7)	2584(8)	94(8)
C(3')	6596(7)	6560(6)	3047(10)	79(6)
N(3)	6427(7)	6397(5)	3546(8)	73(5)
C(5)	8552(12)	5945(8)	4904(16)	81(6)
N(2)	7717(7)	6223(6)	3999(9)	79(5)
C(6)	8320(8)	6119(7)	4300(9)	91(7)
C(7)	8642(6)	6242(7)	3903(11)	99(8)
C(8)	8237(8)	6422(6)	3356(9)	86(7)
C(9)	7666(7)	6410(6)	3415(9)	81(7)
C(10)	7149(13)	6555(9)	2988(16)	91(7)
C(14)	5528(12)	6340(9)	3760(15)	82(7)
N(4)	6333(7)	6041(6)	4657(9)	85(6)
C(16)	5732(8)	6151(6)	4362(8)	83(7)
C(17)	5416(6)	6041(6)	4772(10)	80(7)
C(18)	5822(8)	5864(6)	5320(8)	76(7)
C(19)	6389(7)	5864(6)	5249(9)	82(7)
C(21)	9180(12)	5890(8)	5118(15)	76(7)
C(22)	9434(13)	5513(8)	5232(15)	83(8)
C(23)	10027(11)	5454(7)	5472(13)	61(7)
C(24)	10169(12)	6134(7)	5516(14)	67(7)
C(25)	9561(12)	6201(9)	5268(15)	83(7)
C(41)	10723(15)	5746(12)	4433(19)	92(8)
C(42)	10358(14)	5954(11)	3887(18)	90(7)
C(43)	10256(12)	6374(10)	3935(16)	90(7)
C(44)	9597(10)	6379(5)	2847(12)	93(7)
C(45)	9869(8)	6578(7)	3413(10)	92(7)
C(48)	9762(9)	6981(7)	3463(9)	88(7)
C(49)	9382(10)	7184(5)	2947(12)	119(9)
C(51)	9110(9)	6985(7)	2381(10)	102(8)
C(52)	9218(9)	6583(7)	2331(9)	103(8)
C(46)	9652(14)	5960(10)	2799(17)	95(7)
C(47)	10059(16)	5748(12)	3337(19)	113(9)
C(55)	3886(18)	5607(15)	4740(20)	139(10)
C(57)	3190(20)	6070(20)	4010(30)	146(11)
C(58)	3887(19)	6255(16)	5190(20)	148(11)
C(59)	3675(17)	5986(16)	4710(20)	130(9)
C(60)	4285(10)	5464(10)	5327(11)	128(9)
C(61)	4482(12)	5072(9)	5406(12)	142(10)
C(62)	4888(12)	4951(6)	5980(14)	132(10)
C(63)	5097(9)	5221(9)	6473(10)	105(8)

C(56)	4900(11)	5613(8)	6394(12)	106(8)
C(56')	4494(11)	5734(7)	5821(15)	123(9)
C(65)	11822(17)	5084(12)	7020(20)	128(10)
C(66)	11570(20)	4771(14)	6640(20)	168(17)
C(67)	10812(14)	5521(15)	7030(20)	168(12)
C(71)	12810(14)	5513(13)	6450(20)	155(11)
C(72)	13459(15)	5528(14)	6470(30)	185(18)
C(73)	12240(19)	5220(15)	5030(30)	184(16)
C(75)	12520(20)	6325(14)	6010(40)	230(20)
C(76)	12210(20)	6609(14)	5720(40)	230(20)
C(77)	8840(20)	7775(13)	510(20)	160(10)
C(78)	8592(19)	8141(13)	680(30)	172(16)
C(79)	8860(20)	7002(14)	140(20)	169(12)
C(200)	6918(13)	5727(9)	5708(17)	93(7)
C(304)	6980(30)	8163(17)	550(30)	219(19)
C(303)	6810(20)	8015(18)	-90(30)	208(13)
C(307)	1650(30)	6080(30)	3310(40)	390(30)
C(306)	1680(30)	6480(20)	3670(30)	360(20)
O(305)	5715(10)	5266(8)	7593(12)	125(7)
C(302)	8580(20)	7631(17)	-1050(30)	220(20)
C(301)	8150(20)	7594(14)	-630(20)	171(11)
C(308)	1350(20)	6910(30)	2500(30)	360(20)
C(311)	2390(30)	7660(20)	2310(40)	303(19)
C(313)	11910(20)	5911(14)	7410(20)	164(12)
C(314)	8695(18)	7239(14)	1910(20)	121(9)
C(315)	4316(17)	6143(13)	5800(20)	133(10)
C(316)	5529(17)	5070(14)	7060(20)	104(8)
C(317)	12319(19)	5645(14)	5110(20)	157(11)
C(318)	11650(30)	6355(12)	7320(30)	250(30)
C(319)	10240(20)	5760(20)	6910(40)	310(30)
C(4S)	2200(30)	7030(20)	1540(30)	298(18)
C(8S)	3460(30)	7620(20)	1780(40)	340(30)
C(10S)	2810(30)	7850(20)	2920(40)	320(30)
C(12S)	5280(20)	5310(20)	8690(30)	250(16)
C(14S)	5920(20)	4510(10)	8790(30)	269(16)
C(18S)	3430(20)	7270(20)	2210(30)	288(18)
C(19S)	2370(30)	7260(30)	4370(30)	450(40)
C(20S)	6620(30)	7000(20)	-850(30)	270(20)
C(29S)	6390(30)	5030(20)	9730(30)	264(16)
C(34S)	5950(30)	4880(30)	10060(30)	330(30)
C(35S)	4840(20)	5110(20)	8990(30)	310(30)
C(36S)	6430(40)	4205(15)	9010(50)	400(40)
C(37S)	6540(30)	7450(20)	-800(30)	243(15)

C(38S)	6278(18)	7360(20)	260(20)	224(14)
C(39S)	5639(16)	7510(20)	-50(30)	290(30)
C(40S)	1880(20)	7205(17)	3720(30)	380(20)
C(41S)	760(20)	6990(30)	2610(30)	370(30)
C(43S)	2410(40)	6610(20)	1410(40)	350(30)
C(44S)	7570(40)	4340(14)	9050(50)	470(40)
C(45S)	7560(30)	5614(15)	9470(30)	340(20)
C(46S)	8050(30)	5390(30)	8750(30)	360(20)
C(47S)	7780(30)	4767(14)	9270(30)	370(20)
C(48S)	8650(20)	5520(30)	9230(30)	390(30)
C(49S)	7810(40)	5940(30)	9140(40)	410(40)
C(50S)	8590(30)	6631(15)	-130(30)	199(18)
S(500)	10652(8)	7317(6)	5641(10)	232(8)
O(501)	10572(18)	7669(9)	5930(18)	286(18)
O(502)	11123(15)	7081(12)	6002(19)	318(19)
O(503)	10155(12)	7112(10)	5271(16)	225(14)
C(500)	10932(15)	7505(11)	4981(18)	288(14)
F(501)	11410(19)	7735(16)	5310(20)	440(30)
F(502)	11071(19)	7143(13)	4770(20)	368(19)
F(503)	10440(20)	7703(13)	4582(18)	380(20)
S(501)	6390(20)	6855(10)	7370(20)	590(30)
O(504)	6740(30)	6817(15)	6990(30)	600(40)
O(505)	6220(30)	6505(12)	7600(30)	640(40)
O(506)	6490(30)	7187(14)	7760(30)	580(40)
C(501)	5640(30)	7003(16)	6760(30)	650(30)
F(504)	5490(30)	6650(20)	6430(40)	720(40)
F(505)	5330(30)	7090(20)	7180(40)	730(40)
F(506)	5810(30)	7320(17)	6470(30)	630(40)
S(502)	9350(30)	5084(15)	7750(30)	750(40)
O(507)	8970(40)	5320(20)	7950(40)	700(40)
O(508)	9500(40)	4713(16)	8030(40)	720(40)
O(509)	9310(40)	5110(20)	7110(30)	710(50)
C(502)	10080(30)	5370(20)	8130(40)	770(40)
F(507)	10210(40)	5250(30)	8760(30)	790(50)
F(508)	10420(40)	5210(30)	7790(50)	770(50)
F(509)	9870(50)	5755(17)	7970(50)	820(50)
S(503)	4020(40)	7247(17)	-230(40)	1090(60)
O(510)	3960(60)	7000(20)	250(60)	1060(70)
O(511)	4530(50)	7210(30)	-380(70)	1100(70)
O(512)	3500(50)	7330(30)	-720(60)	1080(70)
C(503)	4160(40)	7752(18)	200(50)	1090(70)
F(510)	4750(50)	7710(20)	580(70)	1050(70)
F(511)	3740(60)	7750(20)	500(70)	1060(70)

**Table 8.** Bond lengths [Å] and angles [°] for **BT4**.

Pt(1)-O(1)	2.01(2)
Pt(1)-N(5)	2.16(2)
Pt(1)-P(1)	2.207(12)
Pt(1)-P(2)	2.264(9)
Pt(2)-N(6)	2.088(15)
Pt(2)-O(3)	2.11(3)
Pt(2)-P(4)	2.194(15)
Pt(2)-P(3)	2.302(12)
Pt(3)-N(7)	2.10(3)
Pt(3)-O(5)	2.15(3)
Pt(3)-P(6)	2.236(14)
Pt(3)-P(5)	2.266(16)
Pt(4)-O(305)	2.00(3)
Pt(4)-N(8)	2.100(17)
Pt(4)-P(8)	2.17(2)
Pt(4)-P(7)	2.256(14)
Zn(1)-N(1)	2.072(16)
Zn(1)-N(2)	2.077(13)
Zn(1)-N(4)	2.080(13)
Zn(1)-O(9W)	2.11(2)
Zn(1)-N(3)	2.113(15)
P(4)-C(37S)	1.68(5)
P(4)-C(38S)	1.76(5)
P(4)-C(303)	1.97(6)
P(4)-C(20S)	2.29(7)
P(5)-C(4S)	1.67(7)
P(5)-C(18S)	1.90(5)
P(5)-C(311)	1.92(7)
P(6)-C(308)	1.67(6)
P(6)-C(306)	1.82(2)
P(6)-C(40S)	1.83(2)
P(7)-C(29S)	1.72(5)
P(7)-C(14S)	1.82(2)
P(7)-C(12S)	1.97(6)
P(8)-C(46S)	1.72(6)
P(8)-C(47S)	1.81(2)
P(8)-C(45S)	1.82(2)
O(1)-C(41)	1.29(4)
O(2)-C(41)	1.29(4)

O(3)-C(314)	1.44(5)
O(4)-C(314)	1.19(4)
O(5)-C(57)	1.37(6)
O(6)-C(57)	1.21(6)
O(8)-C(316)	1.30(4)
N(5)-C(24)	1.31(3)
N(5)-C(23)	1.32(3)
C(29)-C(26)	1.39
C(29)-C(30)	1.39
C(29)-H(29)	0.95
C(26)-C(27)	1.39
C(26)-C(10)	1.50(3)
C(27)-C(28)	1.39
C(27)-H(27)	0.95
C(28)-N(6)	1.39
C(28)-H(28)	0.95
N(6)-C(30)	1.39
C(30)-H(500)	0.95
P(1)-C(65)	1.77(4)
P(1)-C(67)	1.840(19)
P(1)-C(313)	1.85(4)
N(8)-C(36)	1.39
N(8)-C(40)	1.39
C(36)-C(37)	1.39
C(36)-H(36)	0.95
C(37)-C(38)	1.39
C(37)-H(37)	0.95
C(38)-C(39)	1.39
C(38)-C(200)	1.45(3)
C(39)-C(40)	1.39
C(39)-H(39)	0.95
C(40)-H(40)	0.95
C(34)-C(35)	1.24(4)
C(34)-C(31)	1.49(5)
C(34)-H(34)	0.95
C(31)-C(32)	1.25(4)
C(31)-C(14)	1.46(4)
C(32)-C(33)	1.39(4)
C(32)-H(32)	0.95
C(33)-N(7)	1.38(5)
C(33)-H(33)	0.95
N(7)-C(35)	1.36(5)
C(35)-H(35)	0.95



P(2)-C(71)	1.74(4)
P(2)-C(317)	1.75(5)
P(2)-C(75)	1.99(5)
N(1)-C(1)	1.42
N(1)-C(4')	1.42
C(1)-C(200)	1.34(3)
C(1)-C(2)	1.42
C(2)-C(4)	1.42
C(2)-H(2)	0.95
C(4)-C(4')	1.42
C(4)-H(4)	0.95
C(4')-C(5)	1.38(3)
P(3)-C(301)	1.61(4)
P(3)-C(77)	1.80(5)
P(3)-C(79)	1.81(4)
C(13)-C(14)	1.28(3)
C(13)-C(3)	1.42
C(13)-N(3)	1.42
C(3)-C(11)	1.42
C(3)-H(3)	0.95
C(11)-C(3')	1.42
C(11)-H(11)	0.95
C(3')-C(10)	1.38(3)
C(3')-N(3)	1.42
C(5)-C(6)	1.41(3)
C(5)-C(21)	1.43(4)
N(2)-C(9)	1.42
N(2)-C(6)	1.42
C(6)-C(7)	1.42
C(7)-C(8)	1.42
C(7)-H(7)	0.95
C(8)-C(9)	1.42
C(8)-H(8)	0.95
C(9)-C(10)	1.38(3)
C(14)-C(16)	1.42(3)
N(4)-C(19)	1.42
N(4)-C(16)	1.42
C(16)-C(17)	1.42
C(17)-C(18)	1.42
C(17)-H(17)	0.95
C(18)-C(19)	1.42
C(18)-H(18)	0.95
C(19)-C(200)	1.42(3)

C(21)-C(25)	1.36(4)
C(21)-C(22)	1.39(4)
C(22)-C(23)	1.36(3)
C(22)-H(22)	0.95
C(23)-H(23)	0.95
C(24)-C(25)	1.39(3)
C(24)-H(24)	0.95
C(25)-H(25)	0.95
C(41)-C(42)	1.43(4)
C(42)-C(47)	1.39(5)
C(42)-C(43)	1.45(4)
C(43)-C(45)	1.41(3)
C(43)-H(43)	0.95
C(44)-C(45)	1.39
C(44)-C(52)	1.39
C(44)-C(46)	1.42(3)
C(45)-C(48)	1.39
C(48)-C(49)	1.39
C(48)-H(48)	0.95
C(49)-C(51)	1.39
C(49)-H(49)	0.95
C(51)-C(52)	1.39
C(51)-C(314)	1.46(4)
C(52)-H(52)	0.95
C(46)-C(47)	1.46(4)
C(46)-H(46)	0.95
C(47)-H(47)	0.95
C(55)-C(59)	1.36(6)
C(55)-C(60)	1.43(4)
C(55)-H(55)	0.95
C(57)-C(59)	1.63(7)
C(58)-C(59)	1.38(6)
C(58)-C(315)	1.46(5)
C(58)-H(58)	0.95
C(60)-C(61)	1.39
C(60)-C(56')	1.39
C(61)-C(62)	1.39
C(61)-H(61)	0.95
C(62)-C(63)	1.39
C(62)-H(62)	0.95
C(63)-C(56)	1.39
C(63)-C(316)	1.47(5)
C(56)-C(56')	1.39

C(56)-H(56)	0.95
C(56')-C(315)	1.44(4)
C(65)-C(66)	1.36(5)
C(65)-H(65A)	0.99
C(65)-H(65B)	0.99
C(66)-H(66A)	0.98
C(66)-H(66B)	0.98
C(66)-H(66C)	0.98
C(67)-C(319)	1.54(2)
C(67)-H(67A)	0.99
C(67)-H(67B)	0.99
C(71)-C(72)	1.54(4)
C(71)-H(71A)	0.99
C(71)-H(71B)	0.99
C(72)-H(72A)	0.98
C(72)-H(72B)	0.98
C(72)-H(72C)	0.98
C(73)-C(317)	1.44(5)
C(73)-H(73A)	0.98
C(73)-H(73B)	0.98
C(73)-H(73C)	0.98
C(75)-C(76)	1.26(6)
C(75)-H(75A)	0.99
C(75)-H(75B)	0.99
C(76)-H(76A)	0.9818
C(76)-H(76B)	0.9818
C(76)-H(76C)	0.9818
C(77)-C(78)	1.47(5)
C(77)-H(77A)	0.99
C(77)-H(77B)	0.99
C(78)-H(78A)	0.98
C(78)-H(78B)	0.98
C(78)-H(78C)	0.98
C(79)-C(50S)	1.44(6)
C(79)-H(79A)	0.99
C(79)-H(79B)	0.99
C(304)-C(303)	1.44(7)
C(304)-H(501)	0.98
C(304)-H(502)	0.98
C(304)-H(30C)	0.98
C(303)-H(503)	0.99
C(303)-H(504)	0.99
C(307)-C(306)	1.55(2)

C(307)-H(30D)	1.1182
C(307)-H(30E)	1.1157
C(307)-H(30F)	1.1154
C(306)-H(30G)	0.99
C(306)-H(30H)	0.99
O(305)-C(316)	1.30(4)
C(302)-C(301)	1.60(5)
C(302)-H(505)	0.9802
C(302)-H(506)	0.9802
C(302)-H(30I)	0.9802
C(301)-H(30J)	0.99
C(301)-H(30K)	0.99
C(308)-C(41S)	1.55(2)
C(308)-H(30L)	0.99
C(308)-H(30M)	0.99
C(311)-C(10S)	1.55(2)
C(311)-H(31A)	0.99
C(311)-H(31B)	0.99
C(313)-C(318)	1.61(6)
C(313)-H(317)	0.99
C(313)-H(318)	0.99
C(315)-H(400)	0.95
C(317)-H(315)	0.99
C(317)-H(316)	0.99
C(318)-H(310)	0.98
C(318)-H(311)	0.98
C(318)-H(312)	0.98
C(319)-H(313)	0.98
C(319)-H(31E)	0.98
C(319)-H(31F)	0.98
C(4S)-C(43S)	1.54(2)
C(4S)-H(4S1)	0.99
C(4S)-H(4S2)	0.99
C(8S)-C(18S)	1.55(2)
C(8S)-H(8S1)	1.0258
C(8S)-H(8S2)	1.026
C(8S)-H(8S3)	1.0253
C(10S)-H(10A)	0.9944
C(10S)-H(10B)	0.9947
C(10S)-H(10C)	0.9948
C(12S)-C(35S)	1.55(2)
C(12S)-H(12A)	0.99
C(12S)-H(12B)	0.99

C(14S)-C(36S)	1.55(2)
C(14S)-H(14A)	0.99
C(14S)-H(14B)	0.99
C(18S)-H(18A)	0.99
C(18S)-H(18B)	0.99
C(19S)-C(40S)	1.55(2)
C(19S)-H(19A)	0.9813
C(19S)-H(19B)	0.9813
C(19S)-H(19C)	0.9813
C(20S)-C(37S)	1.54(2)
C(20S)-H(20A)	0.98
C(20S)-H(20B)	0.98
C(20S)-H(20C)	0.98
C(29S)-C(34S)	1.54(2)
C(29S)-H(29A)	0.99
C(29S)-H(29B)	0.99
C(34S)-H(34A)	1.0196
C(34S)-H(34B)	1.0208
C(34S)-H(34C)	1.0179
C(35S)-H(35A)	0.9807
C(35S)-H(35B)	0.9806
C(35S)-H(35C)	0.9806
C(36S)-H(36A)	0.9989
C(36S)-H(36B)	0.9994
C(36S)-H(36C)	0.9989
C(37S)-H(37A)	0.99
C(37S)-H(37B)	0.99
C(38S)-C(39S)	1.55(2)
C(38S)-H(38A)	0.99
C(38S)-H(38B)	0.99
C(39S)-H(39A)	0.98
C(39S)-H(39B)	0.98
C(39S)-H(39C)	0.98
C(40S)-H(40A)	0.99
C(40S)-H(40B)	0.99
C(41S)-H(41A)	0.9992
C(41S)-H(41B)	0.9988
C(41S)-H(41C)	0.999
C(43S)-H(43A)	1.0837
C(43S)-H(43B)	1.0856
C(43S)-H(43C)	1.0826
C(44S)-C(47S)	1.55(2)
C(44S)-H(44A)	0.9814

C(44S)-H(44B)	0.9814
C(44S)-H(44C)	0.9815
C(45S)-C(49S)	1.54(2)
C(45S)-H(45A)	0.99
C(45S)-H(45B)	0.99
C(46S)-C(48S)	1.54(2)
C(46S)-H(46A)	0.99
C(46S)-H(46B)	0.99
C(47S)-H(47A)	0.99
C(47S)-H(47B)	0.99
C(48S)-H(48A)	0.98
C(48S)-H(48B)	0.98
C(48S)-H(48C)	0.98
C(49S)-H(49A)	1.0063
C(49S)-H(49B)	1.0073
C(49S)-H(49C)	1.0067
C(50S)-H(50A)	0.98
C(50S)-H(50B)	0.98
C(50S)-H(50C)	0.98
S(500)-O(503)	1.387(19)
S(500)-O(501)	1.392(19)
S(500)-O(502)	1.396(19)
S(500)-C(500)	1.92(5)
C(500)-F(501)	1.375(19)
C(500)-F(502)	1.39(2)
C(500)-F(503)	1.40(2)
S(501)-O(504)	1.391(19)
S(501)-O(506)	1.393(19)
S(501)-O(505)	1.40(2)
S(501)-C(501)	1.93(5)
C(501)-F(506)	1.38(2)
C(501)-F(504)	1.39(2)
C(501)-F(505)	1.39(2)
S(502)-O(508)	1.39(2)
S(502)-O(507)	1.39(2)
S(502)-O(509)	1.40(2)
S(502)-C(502)	1.93(5)
C(502)-F(507)	1.39(2)
C(502)-F(508)	1.39(2)
C(502)-F(509)	1.40(2)
S(503)-O(510)	1.39(2)
S(503)-O(512)	1.39(2)
S(503)-O(511)	1.39(2)

S(503)-C(503)	1.92(5)
C(503)-F(510)	1.39(2)
C(503)-F(511)	1.39(2)
C(503)-F(512)	1.39(2)
O(1)-Pt(1)-N(5)	82.2(9)
O(1)-Pt(1)-P(1)	173.5(6)
N(5)-Pt(1)-P(1)	91.9(7)
O(1)-Pt(1)-P(2)	88.2(6)
N(5)-Pt(1)-P(2)	170.1(7)
P(1)-Pt(1)-P(2)	97.6(4)
N(6)-Pt(2)-O(3)	81.6(8)
N(6)-Pt(2)-P(4)	93.2(7)
O(3)-Pt(2)-P(4)	174.8(7)
N(6)-Pt(2)-P(3)	167.2(7)
O(3)-Pt(2)-P(3)	85.6(7)
P(4)-Pt(2)-P(3)	99.6(5)
N(7)-Pt(3)-O(5)	80.3(11)
N(7)-Pt(3)-P(6)	170.6(11)
O(5)-Pt(3)-P(6)	90.6(8)
N(7)-Pt(3)-P(5)	92.9(10)
O(5)-Pt(3)-P(5)	167.0(12)
P(6)-Pt(3)-P(5)	95.6(6)
O(305)-Pt(4)-N(8)	81.2(8)
O(305)-Pt(4)-P(8)	172.1(9)
N(8)-Pt(4)-P(8)	93.0(7)
O(305)-Pt(4)-P(7)	86.7(7)
N(8)-Pt(4)-P(7)	167.8(8)
P(8)-Pt(4)-P(7)	99.2(6)
N(1)-Zn(1)-N(2)	89.7(8)
N(1)-Zn(1)-N(4)	89.1(8)
N(2)-Zn(1)-N(4)	161.6(8)
N(1)-Zn(1)-O(9W)	105.5(9)
N(2)-Zn(1)-O(9W)	95.4(9)
N(4)-Zn(1)-O(9W)	102.6(9)
N(1)-Zn(1)-N(3)	162.3(8)
N(2)-Zn(1)-N(3)	90.5(7)
N(4)-Zn(1)-N(3)	85.3(7)
O(9W)-Zn(1)-N(3)	92.1(9)
C(37S)-P(4)-C(38S)	102(3)
C(37S)-P(4)-C(303)	83(3)
C(38S)-P(4)-C(303)	97(3)
C(37S)-P(4)-Pt(2)	137(2)

C(38S)-P(4)-Pt(2)	113.8(15)
C(303)-P(4)-Pt(2)	113.7(19)
C(37S)-P(4)-C(20S)	42.3(16)
C(38S)-P(4)-C(20S)	100(3)
C(303)-P(4)-C(20S)	125(2)
Pt(2)-P(4)-C(20S)	106.1(19)
C(4S)-P(5)-C(18S)	111(3)
C(4S)-P(5)-C(311)	96(3)
C(18S)-P(5)-C(311)	98(3)
C(4S)-P(5)-Pt(3)	125(3)
C(18S)-P(5)-Pt(3)	108.2(16)
C(311)-P(5)-Pt(3)	116(2)
C(308)-P(6)-C(306)	111(3)
C(308)-P(6)-C(40S)	105(4)
C(306)-P(6)-C(40S)	86(4)
C(308)-P(6)-Pt(3)	119.2(18)
C(306)-P(6)-Pt(3)	118(2)
C(40S)-P(6)-Pt(3)	112(2)
C(29S)-P(7)-C(14S)	99(3)
C(29S)-P(7)-C(12S)	111(3)
C(14S)-P(7)-C(12S)	108(3)
C(29S)-P(7)-Pt(4)	124.3(19)
C(14S)-P(7)-Pt(4)	103(2)
C(12S)-P(7)-Pt(4)	110.2(16)
C(46S)-P(8)-C(47S)	93(5)
C(46S)-P(8)-C(45S)	86(4)
C(47S)-P(8)-C(45S)	109(3)
C(46S)-P(8)-Pt(4)	129(2)
C(47S)-P(8)-Pt(4)	121(2)
C(45S)-P(8)-Pt(4)	113(3)
C(41)-O(1)-Pt(1)	125(2)
C(314)-O(3)-Pt(2)	115(2)
C(57)-O(5)-Pt(3)	111(3)
C(24)-N(5)-C(23)	123(2)
C(24)-N(5)-Pt(1)	112.4(16)
C(23)-N(5)-Pt(1)	121.6(16)
C(26)-C(29)-C(30)	120
C(26)-C(29)-H(29)	120
C(30)-C(29)-H(29)	120
C(27)-C(26)-C(29)	120
C(27)-C(26)-C(10)	120(2)
C(29)-C(26)-C(10)	120(2)
C(26)-C(27)-C(28)	120



C(26)-C(27)-H(27)	120
C(28)-C(27)-H(27)	120
N(6)-C(28)-C(27)	120
N(6)-C(28)-H(28)	120
C(27)-C(28)-H(28)	120
C(30)-N(6)-C(28)	120
C(30)-N(6)-Pt(2)	116.7(13)
C(28)-N(6)-Pt(2)	120.9(14)
N(6)-C(30)-C(29)	120
N(6)-C(30)-H(500)	120
C(29)-C(30)-H(500)	120
C(65)-P(1)-C(67)	104(2)
C(65)-P(1)-C(313)	106(2)
C(67)-P(1)-C(313)	100(2)
C(65)-P(1)-Pt(1)	116.0(15)
C(67)-P(1)-Pt(1)	114.3(15)
C(313)-P(1)-Pt(1)	115.2(17)
C(36)-N(8)-C(40)	120
C(36)-N(8)-Pt(4)	123.2(15)
C(40)-N(8)-Pt(4)	115.9(15)
N(8)-C(36)-C(37)	120
N(8)-C(36)-H(36)	120
C(37)-C(36)-H(36)	120
C(36)-C(37)-C(38)	120
C(36)-C(37)-H(37)	120
C(38)-C(37)-H(37)	120
C(39)-C(38)-C(37)	120
C(39)-C(38)-C(200)	119(2)
C(37)-C(38)-C(200)	121(2)
C(38)-C(39)-C(40)	120
C(38)-C(39)-H(39)	120
C(40)-C(39)-H(39)	120
C(39)-C(40)-N(8)	120
C(39)-C(40)-H(40)	120
N(8)-C(40)-H(40)	120
C(35)-C(34)-C(31)	124(4)
C(35)-C(34)-H(34)	118.2
C(31)-C(34)-H(34)	118.2
C(32)-C(31)-C(14)	126(4)
C(32)-C(31)-C(34)	114(3)
C(14)-C(31)-C(34)	120(3)
C(31)-C(32)-C(33)	125(4)
C(31)-C(32)-H(32)	117.7

C(33)-C(32)-H(32)	117.6
N(7)-C(33)-C(32)	118(4)
N(7)-C(33)-H(33)	120.9
C(32)-C(33)-H(33)	120.9
C(35)-N(7)-C(33)	118(3)
C(35)-N(7)-Pt(3)	122(3)
C(33)-N(7)-Pt(3)	118(3)
C(34)-C(35)-N(7)	121(4)
C(34)-C(35)-H(35)	119.5
N(7)-C(35)-H(35)	119.5
C(71)-P(2)-C(317)	111(2)
C(71)-P(2)-C(75)	102(3)
C(317)-P(2)-C(75)	106(3)
C(71)-P(2)-Pt(1)	119.9(13)
C(317)-P(2)-Pt(1)	110.7(15)
C(75)-P(2)-Pt(1)	106.4(14)
C(1)-N(1)-C(4')	108
C(1)-N(1)-Zn(1)	128.7(11)
C(4')-N(1)-Zn(1)	123.3(11)
C(200)-C(1)-C(2)	129(2)
C(200)-C(1)-N(1)	123(2)
C(2)-C(1)-N(1)	108
C(1)-C(2)-C(4)	108
C(1)-C(2)-H(2)	126
C(4)-C(2)-H(2)	126
C(4')-C(4)-C(2)	108
C(4')-C(4)-H(4)	126
C(2)-C(4)-H(4)	126
C(5)-C(4')-C(4)	121.7(19)
C(5)-C(4')-N(1)	130.2(19)
C(4)-C(4')-N(1)	108
C(301)-P(3)-C(77)	100(2)
C(301)-P(3)-C(79)	110(2)
C(77)-P(3)-C(79)	98(3)
C(301)-P(3)-Pt(2)	129.0(18)
C(77)-P(3)-Pt(2)	108.0(15)
C(79)-P(3)-Pt(2)	107.6(13)
C(14)-C(13)-C(3)	129.4(19)
C(14)-C(13)-N(3)	122.5(19)
C(3)-C(13)-N(3)	108
C(13)-C(3)-C(11)	108
C(13)-C(3)-H(3)	126
C(11)-C(3)-H(3)	126

C(3)-C(11)-C(3')	108
C(3)-C(11)-H(11)	126
C(3')-C(11)-H(11)	126
C(10)-C(3')-N(3)	127.4(19)
C(10)-C(3')-C(11)	124.5(19)
N(3)-C(3')-C(11)	108
C(3')-N(3)-C(13)	108
C(3')-N(3)-Zn(1)	122.2(10)
C(13)-N(3)-Zn(1)	128.7(10)
C(4')-C(5)-C(6)	124(2)
C(4')-C(5)-C(21)	122(3)
C(6)-C(5)-C(21)	114(2)
C(9)-N(2)-C(6)	108
C(9)-N(2)-Zn(1)	124.6(11)
C(6)-N(2)-Zn(1)	126.4(11)
C(5)-C(6)-C(7)	127.0(17)
C(5)-C(6)-N(2)	124.9(17)
C(7)-C(6)-N(2)	108
C(6)-C(7)-C(8)	108
C(6)-C(7)-H(7)	126
C(8)-C(7)-H(7)	126
C(7)-C(8)-C(9)	108
C(7)-C(8)-H(8)	126
C(9)-C(8)-H(8)	126
C(10)-C(9)-N(2)	125.3(18)
C(10)-C(9)-C(8)	126.7(18)
N(2)-C(9)-C(8)	108
C(3')-C(10)-C(9)	128(3)
C(3')-C(10)-C(26)	116(2)
C(9)-C(10)-C(26)	116(2)
C(13)-C(14)-C(16)	131(2)
C(13)-C(14)-C(31)	118(3)
C(16)-C(14)-C(31)	111(2)
C(19)-N(4)-C(16)	108
C(19)-N(4)-Zn(1)	123.4(11)
C(16)-N(4)-Zn(1)	127.9(11)
C(17)-C(16)-N(4)	108
C(17)-C(16)-C(14)	129.9(16)
N(4)-C(16)-C(14)	122.1(16)
C(18)-C(17)-C(16)	108
C(18)-C(17)-H(17)	126
C(16)-C(17)-H(17)	126
C(19)-C(18)-C(17)	108

C(19)-C(18)-H(18)	126
C(17)-C(18)-H(18)	126
N(4)-C(19)-C(18)	108
N(4)-C(19)-C(200)	126.6(18)
C(18)-C(19)-C(200)	125.3(18)
C(25)-C(21)-C(22)	116(3)
C(25)-C(21)-C(5)	122(3)
C(22)-C(21)-C(5)	122(3)
C(23)-C(22)-C(21)	123(3)
C(23)-C(22)-H(22)	118.5
C(21)-C(22)-H(22)	118.5
N(5)-C(23)-C(22)	118(2)
N(5)-C(23)-H(23)	121.2
C(22)-C(23)-H(23)	121.2
N(5)-C(24)-C(25)	120(2)
N(5)-C(24)-H(24)	120.1
C(25)-C(24)-H(24)	120.1
C(21)-C(25)-C(24)	120(3)
C(21)-C(25)-H(25)	120
C(24)-C(25)-H(25)	119.9
O(1)-C(41)-O(2)	117(3)
O(1)-C(41)-C(42)	122(4)
O(2)-C(41)-C(42)	121(4)
C(47)-C(42)-C(41)	120(4)
C(47)-C(42)-C(43)	120(3)
C(41)-C(42)-C(43)	119(4)
C(45)-C(43)-C(42)	120(3)
C(45)-C(43)-H(43)	120.1
C(42)-C(43)-H(43)	120.1
C(45)-C(44)-C(52)	120
C(45)-C(44)-C(46)	121(2)
C(52)-C(44)-C(46)	118(2)
C(48)-C(45)-C(44)	120
C(48)-C(45)-C(43)	120(2)
C(44)-C(45)-C(43)	120(2)
C(49)-C(48)-C(45)	120
C(49)-C(48)-H(48)	120
C(45)-C(48)-H(48)	120
C(48)-C(49)-C(51)	120
C(48)-C(49)-H(49)	120
C(51)-C(49)-H(49)	120
C(49)-C(51)-C(52)	120
C(49)-C(51)-C(314)	112(3)

C(52)-C(51)-C(314)	128(3)
C(51)-C(52)-C(44)	120
C(51)-C(52)-H(52)	120
C(44)-C(52)-H(52)	120
C(44)-C(46)-C(47)	118(3)
C(44)-C(46)-H(46)	120.9
C(47)-C(46)-H(46)	120.8
C(42)-C(47)-C(46)	120(4)
C(42)-C(47)-H(47)	120.1
C(46)-C(47)-H(47)	120.2
C(59)-C(55)-C(60)	119(5)
C(59)-C(55)-H(55)	120.4
C(60)-C(55)-H(55)	120.4
O(6)-C(57)-O(5)	136(6)
O(6)-C(57)-C(59)	121(6)
O(5)-C(57)-C(59)	101(5)
C(59)-C(58)-C(315)	122(5)
C(59)-C(58)-H(58)	119
C(315)-C(58)-H(58)	119
C(55)-C(59)-C(58)	123(5)
C(55)-C(59)-C(57)	111(5)
C(58)-C(59)-C(57)	127(5)
C(61)-C(60)-C(56')	120
C(61)-C(60)-C(55)	122(3)
C(56')-C(60)-C(55)	118(3)
C(60)-C(61)-C(62)	120
C(60)-C(61)-H(61)	120
C(62)-C(61)-H(61)	120
C(61)-C(62)-C(63)	120
C(61)-C(62)-H(62)	120
C(63)-C(62)-H(62)	120
C(56)-C(63)-C(62)	120
C(56)-C(63)-C(316)	123(3)
C(62)-C(63)-C(316)	117(3)
C(63)-C(56)-C(56')	120
C(63)-C(56)-H(56)	120
C(56')-C(56)-H(56)	120
C(56)-C(56')-C(60)	120
C(56)-C(56')-C(315)	115(3)
C(60)-C(56')-C(315)	125(3)
C(66)-C(65)-P(1)	116(3)
C(66)-C(65)-H(65A)	108.2
P(1)-C(65)-H(65A)	108.2

C(66)-C(65)-H(65B)	108.1
P(1)-C(65)-H(65B)	108.1
H(65A)-C(65)-H(65B)	107.3
C(65)-C(66)-H(66A)	109.5
C(65)-C(66)-H(66B)	109.5
H(66A)-C(66)-H(66B)	109.5
C(65)-C(66)-H(66C)	109.4
H(66A)-C(66)-H(66C)	109.5
H(66B)-C(66)-H(66C)	109.5
C(319)-C(67)-P(1)	137(4)
C(319)-C(67)-H(67A)	103.1
P(1)-C(67)-H(67A)	102.9
C(319)-C(67)-H(67B)	103
P(1)-C(67)-H(67B)	103
H(67A)-C(67)-H(67B)	105.1
C(72)-C(71)-P(2)	120(3)
C(72)-C(71)-H(71A)	107.2
P(2)-C(71)-H(71A)	107.3
C(72)-C(71)-H(71B)	107.3
P(2)-C(71)-H(71B)	107.2
H(71A)-C(71)-H(71B)	106.9
C(71)-C(72)-H(72A)	109.4
C(71)-C(72)-H(72B)	109.6
H(72A)-C(72)-H(72B)	109.5
C(71)-C(72)-H(72C)	109.4
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
C(317)-C(73)-H(73A)	109.5
C(317)-C(73)-H(73B)	109.4
H(73A)-C(73)-H(73B)	109.5
C(317)-C(73)-H(73C)	109.4
H(73A)-C(73)-H(73C)	109.5
H(73B)-C(73)-H(73C)	109.5
C(76)-C(75)-P(2)	122(5)
C(76)-C(75)-H(75A)	106.6
P(2)-C(75)-H(75A)	106.8
C(76)-C(75)-H(75B)	106.8
P(2)-C(75)-H(75B)	106.7
H(75A)-C(75)-H(75B)	106.6
C(75)-C(76)-H(76A)	109.7
C(75)-C(76)-H(76B)	109.6
H(76A)-C(76)-H(76B)	109.2
C(75)-C(76)-H(76C)	109.8

H(76A)-C(76)-H(76C)	109.2
H(76B)-C(76)-H(76C)	109.3
C(78)-C(77)-P(3)	118(4)
C(78)-C(77)-H(77A)	107.7
P(3)-C(77)-H(77A)	107.9
C(78)-C(77)-H(77B)	107.9
P(3)-C(77)-H(77B)	107.9
H(77A)-C(77)-H(77B)	107.2
C(77)-C(78)-H(78A)	109.4
C(77)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
C(77)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5
C(50S)-C(79)-P(3)	114(4)
C(50S)-C(79)-H(79A)	108.7
P(3)-C(79)-H(79A)	108.7
C(50S)-C(79)-H(79B)	108.8
P(3)-C(79)-H(79B)	108.8
H(79A)-C(79)-H(79B)	107.6
C(1)-C(200)-C(19)	128(3)
C(1)-C(200)-C(38)	114(3)
C(19)-C(200)-C(38)	118(2)
C(303)-C(304)-H(501)	109.5
C(303)-C(304)-H(502)	109.5
H(501)-C(304)-H(502)	109.5
C(303)-C(304)-H(30C)	109.4
H(501)-C(304)-H(30C)	109.5
H(502)-C(304)-H(30C)	109.5
C(304)-C(303)-P(4)	106(3)
C(304)-C(303)-H(503)	110.6
P(4)-C(303)-H(503)	110.6
C(304)-C(303)-H(504)	110.5
P(4)-C(303)-H(504)	110.6
H(503)-C(303)-H(504)	108.7
C(306)-C(307)-H(30D)	123
C(306)-C(307)-H(30E)	122.6
H(30D)-C(307)-H(30E)	93.4
C(306)-C(307)-H(30F)	122.6
H(30D)-C(307)-H(30F)	93.5
H(30E)-C(307)-H(30F)	93.6
C(307)-C(306)-P(6)	101(5)
C(307)-C(306)-H(30G)	111.7

P(6)-C(306)-H(30G)	111.5
C(307)-C(306)-H(30H)	111.5
P(6)-C(306)-H(30H)	111.6
H(30G)-C(306)-H(30H)	109.4
C(316)-O(305)-Pt(4)	125(3)
C(301)-C(302)-H(505)	109.4
C(301)-C(302)-H(506)	109.4
H(505)-C(302)-H(506)	109.5
C(301)-C(302)-H(30I)	109.7
H(505)-C(302)-H(30I)	109.5
H(506)-C(302)-H(30I)	109.5
C(302)-C(301)-P(3)	126(4)
C(302)-C(301)-H(30J)	105.7
P(3)-C(301)-H(30J)	105.9
C(302)-C(301)-H(30K)	106
P(3)-C(301)-H(30K)	106
H(30J)-C(301)-H(30K)	106.2
C(41S)-C(308)-P(6)	113(4)
C(41S)-C(308)-H(30L)	109
P(6)-C(308)-H(30L)	108.8
C(41S)-C(308)-H(30M)	108.8
P(6)-C(308)-H(30M)	109
H(30L)-C(308)-H(30M)	107.7
C(10S)-C(311)-P(5)	108(4)
C(10S)-C(311)-H(31A)	110.2
P(5)-C(311)-H(31A)	110.2
C(10S)-C(311)-H(31B)	110
P(5)-C(311)-H(31B)	110.1
H(31A)-C(311)-H(31B)	108.5
C(318)-C(313)-P(1)	114(3)
C(318)-C(313)-H(317)	108.7
P(1)-C(313)-H(317)	108.7
C(318)-C(313)-H(318)	108.7
P(1)-C(313)-H(318)	108.8
H(317)-C(313)-H(318)	107.7
O(4)-C(314)-O(3)	121(4)
O(4)-C(314)-C(51)	131(5)
O(3)-C(314)-C(51)	107(4)
C(56')-C(315)-C(58)	113(4)
C(56')-C(315)-H(400)	123.6
C(58)-C(315)-H(400)	123.6
O(8)-C(316)-O(305)	112(4)
O(8)-C(316)-C(63)	123(4)



O(305)-C(316)-C(63)	125(4)
C(73)-C(317)-P(2)	106(4)
C(73)-C(317)-H(315)	110.5
P(2)-C(317)-H(315)	110.5
C(73)-C(317)-H(316)	110.5
P(2)-C(317)-H(316)	110.5
H(315)-C(317)-H(316)	108.7
C(313)-C(318)-H(310)	109.4
C(313)-C(318)-H(311)	109.6
H(310)-C(318)-H(311)	109.5
C(313)-C(318)-H(312)	109.4
H(310)-C(318)-H(312)	109.5
H(311)-C(318)-H(312)	109.5
C(67)-C(319)-H(313)	109.5
C(67)-C(319)-H(31E)	109.6
H(313)-C(319)-H(31E)	109.5
C(67)-C(319)-H(31F)	109.4
H(313)-C(319)-H(31F)	109.5
H(31E)-C(319)-H(31F)	109.5
C(43S)-C(4S)-P(5)	102(4)
C(43S)-C(4S)-H(4S1)	111.3
P(5)-C(4S)-H(4S1)	111.2
C(43S)-C(4S)-H(4S2)	111.5
P(5)-C(4S)-H(4S2)	111.4
H(4S1)-C(4S)-H(4S2)	109.2
C(18S)-C(8S)-H(8S1)	114.2
C(18S)-C(8S)-H(8S2)	113.7
H(8S1)-C(8S)-H(8S2)	104.7
C(18S)-C(8S)-H(8S3)	113.7
H(8S1)-C(8S)-H(8S3)	104.7
H(8S2)-C(8S)-H(8S3)	104.8
C(311)-C(10S)-H(10A)	110.7
C(311)-C(10S)-H(10B)	110.9
H(10A)-C(10S)-H(10B)	108.1
C(311)-C(10S)-H(10C)	111
H(10A)-C(10S)-H(10C)	108
H(10B)-C(10S)-H(10C)	108
C(35S)-C(12S)-P(7)	114(4)
C(35S)-C(12S)-H(12A)	108.3
P(7)-C(12S)-H(12A)	108.7
C(35S)-C(12S)-H(12B)	109.5
P(7)-C(12S)-H(12B)	108.7
H(12A)-C(12S)-H(12B)	107.7

C(36S)-C(14S)-P(7)	121(3)
C(36S)-C(14S)-H(14A)	107.2
P(7)-C(14S)-H(14A)	107
C(36S)-C(14S)-H(14B)	107
P(7)-C(14S)-H(14B)	107.1
H(14A)-C(14S)-H(14B)	106.8
C(8S)-C(18S)-P(5)	118(3)
C(8S)-C(18S)-H(18A)	107.6
P(5)-C(18S)-H(18A)	107.5
C(8S)-C(18S)-H(18B)	108
P(5)-C(18S)-H(18B)	108
H(18A)-C(18S)-H(18B)	107.1
C(40S)-C(19S)-H(19A)	109.6
C(40S)-C(19S)-H(19B)	109.6
H(19A)-C(19S)-H(19B)	109.3
C(40S)-C(19S)-H(19C)	109.6
H(19A)-C(19S)-H(19C)	109.4
H(19B)-C(19S)-H(19C)	109.3
C(37S)-C(20S)-P(4)	47(3)
C(37S)-C(20S)-H(20A)	109.5
P(4)-C(20S)-H(20A)	67.8
C(37S)-C(20S)-H(20B)	109.5
P(4)-C(20S)-H(20B)	145.3
H(20A)-C(20S)-H(20B)	109.5
C(37S)-C(20S)-H(20C)	109.4
P(4)-C(20S)-H(20C)	103.5
H(20A)-C(20S)-H(20C)	109.5
H(20B)-C(20S)-H(20C)	109.5
C(34S)-C(29S)-P(7)	111(4)
C(34S)-C(29S)-H(29A)	109.1
P(7)-C(29S)-H(29A)	109.6
C(34S)-C(29S)-H(29B)	109.5
P(7)-C(29S)-H(29B)	109.5
H(29A)-C(29S)-H(29B)	108.1
C(29S)-C(34S)-H(34A)	113.4
C(29S)-C(34S)-H(34B)	113.7
H(34A)-C(34S)-H(34B)	105.3
C(29S)-C(34S)-H(34C)	112.9
H(34A)-C(34S)-H(34C)	105.4
H(34B)-C(34S)-H(34C)	105.5
C(12S)-C(35S)-H(35A)	110.1
C(12S)-C(35S)-H(35B)	109.7
H(35A)-C(35S)-H(35B)	109.4

C(12S)-C(35S)-H(35C)	108.9
H(35A)-C(35S)-H(35C)	109.4
H(35B)-C(35S)-H(35C)	109.4
C(14S)-C(36S)-H(36A)	111.2
C(14S)-C(36S)-H(36B)	111.5
H(36A)-C(36S)-H(36B)	107.5
C(14S)-C(36S)-H(36C)	111.2
H(36A)-C(36S)-H(36C)	107.6
H(36B)-C(36S)-H(36C)	107.6
C(20S)-C(37S)-P(4)	90(4)
C(20S)-C(37S)-H(37A)	113.6
P(4)-C(37S)-H(37A)	113.6
C(20S)-C(37S)-H(37B)	113.5
P(4)-C(37S)-H(37B)	113.6
H(37A)-C(37S)-H(37B)	110.9
C(39S)-C(38S)-P(4)	126(4)
C(39S)-C(38S)-H(38A)	105.8
P(4)-C(38S)-H(38A)	105.9
C(39S)-C(38S)-H(38B)	105.8
P(4)-C(38S)-H(38B)	105.9
H(38A)-C(38S)-H(38B)	106.2
C(38S)-C(39S)-H(39A)	109.5
C(38S)-C(39S)-H(39B)	109.5
H(39A)-C(39S)-H(39B)	109.5
C(38S)-C(39S)-H(39C)	109.4
H(39A)-C(39S)-H(39C)	109.5
H(39B)-C(39S)-H(39C)	109.5
C(19S)-C(40S)-P(6)	122(3)
C(19S)-C(40S)-H(40A)	106.8
P(6)-C(40S)-H(40A)	106.8
C(19S)-C(40S)-H(40B)	106.9
P(6)-C(40S)-H(40B)	106.9
H(40A)-C(40S)-H(40B)	106.7
C(308)-C(41S)-H(41A)	111.4
C(308)-C(41S)-H(41B)	111.2
H(41A)-C(41S)-H(41B)	107.6
C(308)-C(41S)-H(41C)	111.3
H(41A)-C(41S)-H(41C)	107.5
H(41B)-C(41S)-H(41C)	107.6
C(4S)-C(43S)-H(43A)	119.6
C(4S)-C(43S)-H(43B)	119.8
H(43A)-C(43S)-H(43B)	97.6
C(4S)-C(43S)-H(43C)	119.4

H(43A)-C(43S)-H(43C)	97.8
H(43B)-C(43S)-H(43C)	97.6
C(47S)-C(44S)-H(44A)	109.5
C(47S)-C(44S)-H(44B)	109.6
H(44A)-C(44S)-H(44B)	109.3
C(47S)-C(44S)-H(44C)	109.7
H(44A)-C(44S)-H(44C)	109.3
H(44B)-C(44S)-H(44C)	109.3
C(49S)-C(45S)-P(8)	101(6)
C(49S)-C(45S)-H(45A)	111.6
P(8)-C(45S)-H(45A)	111.6
C(49S)-C(45S)-H(45B)	111.7
P(8)-C(45S)-H(45B)	111.8
H(45A)-C(45S)-H(45B)	109.5
C(48S)-C(46S)-P(8)	130(5)
C(48S)-C(46S)-H(46A)	104.9
P(8)-C(46S)-H(46A)	104.9
C(48S)-C(46S)-H(46B)	104.7
P(8)-C(46S)-H(46B)	104.7
H(46A)-C(46S)-H(46B)	105.8
C(44S)-C(47S)-P(8)	125(3)
C(44S)-C(47S)-H(47A)	106
P(8)-C(47S)-H(47A)	106.1
C(44S)-C(47S)-H(47B)	106.2
P(8)-C(47S)-H(47B)	106.1
H(47A)-C(47S)-H(47B)	106.3
C(46S)-C(48S)-H(48A)	109.5
C(46S)-C(48S)-H(48B)	109.5
H(48A)-C(48S)-H(48B)	109.5
C(46S)-C(48S)-H(48C)	109.3
H(48A)-C(48S)-H(48C)	109.5
H(48B)-C(48S)-H(48C)	109.5
C(45S)-C(49S)-H(49A)	111.9
C(45S)-C(49S)-H(49B)	112.3
H(49A)-C(49S)-H(49B)	106.7
C(45S)-C(49S)-H(49C)	112
H(49A)-C(49S)-H(49C)	106.8
H(49B)-C(49S)-H(49C)	106.8
C(79)-C(50S)-H(50A)	109.4
C(79)-C(50S)-H(50B)	109.5
H(50A)-C(50S)-H(50B)	109.5
C(79)-C(50S)-H(50C)	109.5
H(50A)-C(50S)-H(50C)	109.5

H(50B)-C(50S)-H(50C)	109.5
O(503)-S(500)-O(501)	118(2)
O(503)-S(500)-O(502)	116(2)
O(501)-S(500)-O(502)	115(2)
O(503)-S(500)-C(500)	98.9(18)
O(501)-S(500)-C(500)	102.6(19)
O(502)-S(500)-C(500)	102.2(19)
F(501)-C(500)-F(502)	115(2)
F(501)-C(500)-F(503)	117(2)
F(502)-C(500)-F(503)	117(2)
F(501)-C(500)-S(500)	102(2)
F(502)-C(500)-S(500)	99(2)
F(503)-C(500)-S(500)	102(2)
O(504)-S(501)-O(506)	117(2)
O(504)-S(501)-O(505)	117(2)
O(506)-S(501)-O(505)	117(2)
O(504)-S(501)-C(501)	101(2)
O(506)-S(501)-C(501)	99(2)
O(505)-S(501)-C(501)	98(2)
F(506)-C(501)-F(504)	119(2)
F(506)-C(501)-F(505)	117(2)
F(504)-C(501)-F(505)	116(2)
F(506)-C(501)-S(501)	100(2)
F(504)-C(501)-S(501)	100(2)
F(505)-C(501)-S(501)	99(2)
O(508)-S(502)-O(507)	118(2)
O(508)-S(502)-O(509)	116(2)
O(507)-S(502)-O(509)	117(2)
O(508)-S(502)-C(502)	100(2)
O(507)-S(502)-C(502)	99(2)
O(509)-S(502)-C(502)	99(2)
F(507)-C(502)-F(508)	118(2)
F(507)-C(502)-F(509)	117(2)
F(508)-C(502)-F(509)	117(2)
F(507)-C(502)-S(502)	100(2)
F(508)-C(502)-S(502)	100(2)
F(509)-C(502)-S(502)	99(2)
O(510)-S(503)-O(512)	117(2)
O(510)-S(503)-O(511)	117(2)
O(512)-S(503)-O(511)	116(2)
O(510)-S(503)-C(503)	101(2)
O(512)-S(503)-C(503)	100(2)
O(511)-S(503)-C(503)	100(2)

F(510)-C(503)-F(511)	117(2)
F(510)-C(503)-F(512)	116(2)
F(511)-C(503)-F(512)	117(2)
F(510)-C(503)-S(503)	101(2)
F(511)-C(503)-S(503)	101(2)
F(512)-C(503)-S(503)	100(2)

**Table 9.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **BT2**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
Pt(1)	5816(1)	3577(1)	4430(1)	28(1)
Pt(2)	6648(1)	10841(1)	7624(1)	31(1)
S(1)	5841(1)	9864(3)	4772(2)	56(1)
S(2)	6862(1)	5026(3)	1953(3)	72(2)
P(1)	5391(1)	2790(2)	4385(2)	34(1)
P(2)	6120(1)	2824(2)	4013(2)	34(1)
P(3)	6376(1)	11249(2)	8280(2)	44(1)
P(4)	6983(1)	11847(3)	7697(2)	51(1)
F(1)	5361(5)	9151(11)	4997(14)	198(12)
F(2)	5351(4)	10414(11)	5084(9)	143(8)
F(3)	5690(7)	9795(14)	5788(10)	208(13)
F(4)	7043(4)	4415(7)	2994(7)	124(7)
F(5)	6475(4)	4441(7)	2572(5)	94(4)
F(6)	6715(3)	5486(6)	2935(4)	79(4)
O(1)	5589(2)	4297(5)	4910(5)	37(2)
O(2)	5375(3)	5114(7)	4130(6)	62(4)
O(3)	6341(3)	9883(6)	7490(5)	40(2)
O(4)	6775(3)	9106(6)	8007(5)	49(3)
O(5)	6032(4)	10497(7)	5080(8)	106(7)
O(6)	5652(4)	9994(11)	4157(6)	110(7)
O(7)	6012(3)	9150(7)	4900(7)	77(4)
O(8)	6882(4)	4286(6)	1720(5)	76(5)
O(9)	6565(3)	5436(10)	1586(6)	82(5)
O(10)	7132(3)	5512(7)	2125(6)	65(4)
N(1)	7384(3)	6487(5)	4577(5)	24(2)
N(2)	7052(2)	7543(6)	5213(4)	21(2)
N(3)	6147(3)	4493(7)	4539(5)	30(3)
N(4)	6837(3)	10267(6)	6993(5)	26(2)
C(1)	7563(3)	6036(7)	4309(6)	27(3)
C(2)	7417(4)	5304(8)	4162(7)	35(3)
C(3)	7131(4)	5312(8)	4311(7)	36(3)

C(4)	7108(3)	6066(7)	4572(5)	23(3)
C(5)	6850(3)	6281(7)	4797(6)	28(3)
C(6)	6824(3)	6951(7)	5093(6)	23(3)
C(7)	6564(3)	7184(8)	5345(7)	34(3)
C(8)	6646(3)	7859(7)	5629(6)	31(3)
C(9)	6956(3)	8109(7)	5545(6)	22(3)
C(10)	7131(3)	8765(7)	5781(6)	26(3)
C(11)	6589(3)	5705(8)	4721(6)	30(3)
C(12)	6365(3)	5563(8)	4146(6)	28(3)
C(13)	6146(3)	4972(8)	4068(6)	28(3)
C(14)	6348(3)	4656(8)	5104(6)	33(3)
C(15)	6571(3)	5236(8)	5203(6)	30(3)
C(16)	7014(3)	9274(7)	6190(6)	24(3)
C(17)	6723(3)	9692(7)	6005(6)	26(3)
C(18)	6646(3)	10159(7)	6413(6)	31(3)
C(19)	7112(3)	9847(8)	7168(6)	32(3)
C(20)	7210(3)	9369(8)	6786(6)	28(3)
C(21)	5508(4)	4973(10)	4671(9)	49(4)
C(22)	5612(3)	5615(8)	5126(7)	34(3)
C(23)	5792(4)	5456(9)	5739(8)	47(4)
C(24)	5929(4)	6049(9)	6139(8)	49(4)
C(25)	5869(3)	6809(9)	5948(7)	35(3)
C(26)	5688(3)	6960(9)	5357(7)	40(4)
C(27)	5563(3)	6372(9)	4939(7)	40(4)
C(28)	6023(4)	7410(8)	6385(6)	32(3)
C(29)	6341(4)	7337(8)	6797(7)	37(3)
C(30)	6485(4)	7922(8)	7199(6)	35(3)
C(31)	6332(4)	8582(8)	7182(6)	33(3)
C(32)	6023(4)	8681(9)	6778(8)	45(4)
C(33)	5878(3)	8106(10)	6384(7)	43(4)
C(34)	6502(4)	9220(9)	7624(7)	40(4)
C(35)	5362(4)	1841(9)	4047(7)	40(4)
C(36)	5026(4)	1448(10)	3953(8)	50(4)
C(37)	5014(4)	3298(10)	3986(8)	51(4)
C(38)	4996(4)	3490(10)	3309(7)	51(4)
C(39)	5366(5)	2634(13)	5165(8)	73(7)
C(40)	5674(5)	2307(14)	5593(7)	82(8)
C(41)	6245(5)	1952(10)	4396(10)	66(6)
C(42)	6486(6)	2055(13)	5069(11)	84(7)
C(43)	5920(5)	2589(11)	3220(9)	60(5)
C(44)	5831(6)	3302(15)	2801(8)	82(7)
C(45)	6503(4)	3289(9)	4024(7)	41(4)
C(46)	6741(4)	2814(14)	3785(10)	74(6)

C(47)	6579(6)	10927(15)	9057(10)	85(7)
C(48)	6635(5)	10148(13)	9194(9)	73(6)
C(49)	5974(5)	10852(12)	8066(9)	63(5)
C(50)	5800(4)	11117(13)	7443(10)	72(6)
C(51)	6323(5)	12242(9)	8417(9)	55(4)
C(52)	6076(6)	12416(11)	8782(10)	75(6)
C(53)	7297(5)	11688(13)	7308(11)	73(6)
C(54)	7561(7)	12298(17)	7401(15)	116(9)
C(55)	6783(5)	12741(10)	7373(10)	70(6)
C(56)	6557(7)	12667(14)	6711(11)	93(8)
C(57)	7220(5)	12036(12)	8473(10)	78(6)
C(58)	7424(5)	11348(11)	8772(10)	69(5)
C(63)	5566(5)	9793(10)	5156(11)	100(9)
C(64)	6768(4)	4825(9)	2641(9)	94(9)
C(65)	5000	1060(14)	2500	65(8)
C(66)	4699(7)	589(13)	2383(10)	92(8)
O(67)	5000	1730(9)	2500	80(7)

**Table 10.** Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **BT2'**.

Pt(1)-O(1)	2.088(9)
Pt(1)-N(3)	2.100(11)
Pt(1)-P(2)	2.247(4)
Pt(1)-P(1)	2.249(4)
Pt(2)-O(3)	2.093(10)
Pt(2)-N(4)	2.101(11)
Pt(2)-P(4)	2.240(4)
Pt(2)-P(3)	2.263(4)
S(1)-O(6)	1.411(11)
S(1)-O(5)	1.429(11)
S(1)-O(7)	1.433(10)
S(1)-C(63)	1.66(3)
S(2)-O(10)	1.388(11)
S(2)-O(8)	1.415(10)
S(2)-O(9)	1.477(11)
S(2)-C(64)	1.77(2)
P(1)-C(37)	1.821(18)
P(1)-C(35)	1.823(15)
P(1)-C(39)	1.835(17)
P(2)-C(41)	1.762(17)
P(2)-C(43)	1.803(18)
P(2)-C(45)	1.812(16)
P(3)-C(49)	1.775(19)



P(3)-C(51)	1.795(16)
P(3)-C(47)	1.82(2)
P(4)-C(57)	1.79(2)
P(4)-C(55)	1.83(2)
P(4)-C(53)	1.83(2)
F(1)-C(63)	1.403(15)
F(2)-C(63)	1.399(15)
F(3)-C(63)	1.381(16)
F(4)-C(64)	1.406(14)
F(5)-C(64)	1.383(14)
F(6)-C(64)	1.388(13)
O(1)-C(21)	1.31(2)
O(2)-C(21)	1.22(2)
O(3)-C(34)	1.336(18)
O(4)-C(34)	1.246(19)
N(1)-C(1)	1.363(16)
N(1)-C(4)	1.381(15)
N(1)-H(1)	0.88
N(2)-C(9)	1.381(15)
N(2)-C(6)	1.392(16)
N(3)-C(14)	1.350(17)
N(3)-C(13)	1.362(17)
N(4)-C(19)	1.338(17)
N(4)-C(18)	1.345(17)
C(1)-C(2)	1.421(18)
C(1)-C(10)#1	1.421(17)
C(2)-C(3)	1.36(2)
C(2)-H(2)	0.95
C(3)-C(4)	1.464(18)
C(3)-H(3)	0.95
C(4)-C(5)	1.394(18)
C(5)-C(6)	1.376(18)
C(5)-C(11)	1.474(17)
C(6)-C(7)	1.444(17)
C(7)-C(8)	1.346(19)
C(7)-H(7)	0.95
C(8)-C(9)	1.454(18)
C(8)-H(8)	0.95
C(9)-C(10)	1.387(18)
C(10)-C(16)	1.479(17)
C(11)-C(15)	1.392(19)
C(11)-C(12)	1.394(19)
C(12)-C(13)	1.368(18)

C(12)-H(12)	0.95
C(13)-H(13)	0.95
C(14)-C(15)	1.361(18)
C(14)-H(14)	0.95
C(15)-H(15)	0.95
C(16)-C(20)	1.379(17)
C(16)-C(17)	1.389(17)
C(17)-C(18)	1.352(18)
C(17)-H(17)	0.95
C(18)-H(18)	0.95
C(19)-C(20)	1.362(18)
C(19)-H(19)	0.95
C(20)-H(20)	0.95
C(21)-C(22)	1.50(2)
C(22)-C(27)	1.39(2)
C(22)-C(23)	1.41(2)
C(23)-C(24)	1.39(2)
C(23)-H(23)	0.95
C(24)-C(25)	1.40(2)
C(24)-H(24)	0.95
C(25)-C(26)	1.36(2)
C(25)-C(28)	1.465(19)
C(26)-C(27)	1.40(2)
C(26)-H(26)	0.95
C(27)-H(27)	0.95
C(28)-C(33)	1.36(2)
C(28)-C(29)	1.41(2)
C(29)-C(30)	1.39(2)
C(29)-H(29)	0.95
C(30)-C(31)	1.32(2)
C(30)-H(30)	0.95
C(31)-C(32)	1.37(2)
C(31)-C(34)	1.53(2)
C(32)-C(33)	1.37(2)
C(32)-H(32)	0.95
C(33)-H(33)	0.95
C(35)-C(36)	1.541(19)
C(35)-H(35A)	0.99
C(35)-H(35B)	0.99
C(36)-H(36A)	0.98
C(36)-H(36B)	0.98
C(36)-H(36C)	0.98
C(37)-C(38)	1.56(2)

C(37)-H(37A)	0.99
C(37)-H(37B)	0.99
C(38)-H(38A)	0.98
C(38)-H(38B)	0.98
C(38)-H(38C)	0.98
C(39)-C(40)	1.50(3)
C(39)-H(39A)	0.99
C(39)-H(39B)	0.99
C(40)-H(40A)	0.98
C(40)-H(40B)	0.98
C(40)-H(40C)	0.98
C(41)-C(42)	1.58(3)
C(41)-H(41A)	0.99
C(41)-H(41B)	0.99
C(42)-H(42A)	0.98
C(42)-H(42B)	0.98
C(42)-H(42C)	0.98
C(43)-C(44)	1.55(3)
C(43)-H(43A)	0.99
C(43)-H(43B)	0.99
C(44)-H(44A)	0.98
C(44)-H(44B)	0.98
C(44)-H(44C)	0.98
C(45)-C(46)	1.53(2)
C(45)-H(45A)	0.99
C(45)-H(45B)	0.99
C(46)-H(46A)	0.98
C(46)-H(46B)	0.98
C(46)-H(46C)	0.98
C(47)-C(48)	1.41(3)
C(47)-H(47A)	0.99
C(47)-H(47B)	0.99
C(48)-H(48A)	0.98
C(48)-H(48B)	0.98
C(48)-H(48C)	0.98
C(49)-C(50)	1.47(3)
C(49)-H(49A)	0.99
C(49)-H(49B)	0.99
C(50)-H(50A)	0.98
C(50)-H(50B)	0.98
C(50)-H(50C)	0.98
C(51)-C(52)	1.55(3)
C(51)-H(51A)	0.99

C(51)-H(51B)	0.99
C(52)-H(52A)	0.98
C(52)-H(52B)	0.98
C(52)-H(52C)	0.98
C(53)-C(54)	1.52(3)
C(53)-H(53A)	0.99
C(53)-H(53B)	0.99
C(54)-H(54A)	0.98
C(54)-H(54B)	0.98
C(54)-H(54C)	0.98
C(55)-C(56)	1.53(3)
C(55)-H(55A)	0.99
C(55)-H(55B)	0.99
C(56)-H(56A)	0.98
C(56)-H(56B)	0.98
C(56)-H(56C)	0.98
C(57)-C(58)	1.52(3)
C(57)-H(57A)	0.99
C(57)-H(57B)	0.99
C(58)-H(58A)	0.98
C(58)-H(58B)	0.98
C(58)-H(58C)	0.98
C(65)-O(67)	1.17(3)
C(65)-C(66)#2	1.48(3)
C(65)-C(66)	1.48(3)
C(66)-H(66A)	0.98
C(66)-H(66B)	0.98
C(66)-H(66C)	0.98
O(1)-Pt(1)-N(3)	82.7(4)
O(1)-Pt(1)-P(2)	172.6(3)
N(3)-Pt(1)-P(2)	92.9(3)
O(1)-Pt(1)-P(1)	84.5(3)
N(3)-Pt(1)-P(1)	166.9(3)
P(2)-Pt(1)-P(1)	100.16(14)
O(3)-Pt(2)-N(4)	82.2(4)
O(3)-Pt(2)-P(4)	175.6(3)
N(4)-Pt(2)-P(4)	93.7(3)
O(3)-Pt(2)-P(3)	86.0(3)
N(4)-Pt(2)-P(3)	168.2(3)
P(4)-Pt(2)-P(3)	98.10(15)
O(6)-S(1)-O(5)	115.9(11)
O(6)-S(1)-O(7)	116.5(10)

O(5)-S(1)-O(7)	113.5(9)
O(6)-S(1)-C(63)	104.8(11)
O(5)-S(1)-C(63)	100.5(11)
O(7)-S(1)-C(63)	102.7(9)
O(10)-S(2)-O(8)	122.1(10)
O(10)-S(2)-O(9)	110.9(10)
O(8)-S(2)-O(9)	111.7(9)
O(10)-S(2)-C(64)	105.0(8)
O(8)-S(2)-C(64)	101.9(8)
O(9)-S(2)-C(64)	102.7(8)
C(37)-P(1)-C(35)	107.2(8)
C(37)-P(1)-C(39)	105.2(10)
C(35)-P(1)-C(39)	105.0(9)
C(37)-P(1)-Pt(1)	107.3(6)
C(35)-P(1)-Pt(1)	122.0(5)
C(39)-P(1)-Pt(1)	109.0(6)
C(41)-P(2)-C(43)	106.3(10)
C(41)-P(2)-C(45)	104.4(8)
C(43)-P(2)-C(45)	105.6(8)
C(41)-P(2)-Pt(1)	115.2(7)
C(43)-P(2)-Pt(1)	113.6(7)
C(45)-P(2)-Pt(1)	110.9(5)
C(49)-P(3)-C(51)	105.5(9)
C(49)-P(3)-C(47)	106.5(11)
C(51)-P(3)-C(47)	100.3(11)
C(49)-P(3)-Pt(2)	109.6(6)
C(51)-P(3)-Pt(2)	122.4(7)
C(47)-P(3)-Pt(2)	111.2(7)
C(57)-P(4)-C(55)	107.3(10)
C(57)-P(4)-C(53)	103.4(10)
C(55)-P(4)-C(53)	104.6(10)
C(57)-P(4)-Pt(2)	112.1(8)
C(55)-P(4)-Pt(2)	115.8(7)
C(53)-P(4)-Pt(2)	112.5(7)
C(21)-O(1)-Pt(1)	115.7(10)
C(34)-O(3)-Pt(2)	114.3(10)
C(1)-N(1)-C(4)	105.8(10)
C(1)-N(1)-H(1)	127.1
C(4)-N(1)-H(1)	127.1
C(9)-N(2)-C(6)	109.9(10)
C(14)-N(3)-C(13)	118.4(11)
C(14)-N(3)-Pt(1)	119.1(9)
C(13)-N(3)-Pt(1)	122.2(8)

C(19)-N(4)-C(18)	115.7(11)
C(19)-N(4)-Pt(2)	122.5(8)
C(18)-N(4)-Pt(2)	120.1(9)
N(1)-C(1)-C(2)	111.5(11)
N(1)-C(1)-C(10)#1	125.6(11)
C(2)-C(1)-C(10)#1	122.8(12)
C(3)-C(2)-C(1)	107.0(12)
C(3)-C(2)-H(2)	126.5
C(1)-C(2)-H(2)	126.5
C(2)-C(3)-C(4)	106.5(12)
C(2)-C(3)-H(3)	126.7
C(4)-C(3)-H(3)	126.7
N(1)-C(4)-C(5)	127.6(11)
N(1)-C(4)-C(3)	109.0(11)
C(5)-C(4)-C(3)	123.3(11)
C(6)-C(5)-C(4)	127.0(11)
C(6)-C(5)-C(11)	118.2(12)
C(4)-C(5)-C(11)	114.8(11)
C(5)-C(6)-N(2)	125.3(11)
C(5)-C(6)-C(7)	128.4(12)
N(2)-C(6)-C(7)	106.3(11)
C(8)-C(7)-C(6)	108.8(11)
C(8)-C(7)-H(7)	125.6
C(6)-C(7)-H(7)	125.6
C(7)-C(8)-C(9)	108.3(11)
C(7)-C(8)-H(8)	125.8
C(9)-C(8)-H(8)	125.8
N(2)-C(9)-C(10)	126.6(11)
N(2)-C(9)-C(8)	106.5(11)
C(10)-C(9)-C(8)	126.8(11)
C(9)-C(10)-C(1)#1	123.7(11)
C(9)-C(10)-C(16)	120.2(11)
C(1)#1-C(10)-C(16)	115.9(11)
C(15)-C(11)-C(12)	117.1(12)
C(15)-C(11)-C(5)	121.9(12)
C(12)-C(11)-C(5)	120.8(12)
C(13)-C(12)-C(11)	120.3(12)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
N(3)-C(13)-C(12)	121.5(12)
N(3)-C(13)-H(13)	119.3
C(12)-C(13)-H(13)	119.3
N(3)-C(14)-C(15)	121.8(13)

N(3)-C(14)-H(14)	119.1
C(15)-C(14)-H(14)	119.1
C(14)-C(15)-C(11)	120.7(13)
C(14)-C(15)-H(15)	119.7
C(11)-C(15)-H(15)	119.7
C(20)-C(16)-C(17)	117.3(12)
C(20)-C(16)-C(10)	118.4(11)
C(17)-C(16)-C(10)	124.2(11)
C(18)-C(17)-C(16)	119.1(12)
C(18)-C(17)-H(17)	120.4
C(16)-C(17)-H(17)	120.4
N(4)-C(18)-C(17)	124.4(13)
N(4)-C(18)-H(18)	117.8
C(17)-C(18)-H(18)	117.8
N(4)-C(19)-C(20)	123.7(12)
N(4)-C(19)-H(19)	118.1
C(20)-C(19)-H(19)	118.1
C(19)-C(20)-C(16)	119.6(12)
C(19)-C(20)-H(20)	120.2
C(16)-C(20)-H(20)	120.2
O(2)-C(21)-O(1)	126.2(15)
O(2)-C(21)-C(22)	119.9(17)
O(1)-C(21)-C(22)	113.8(15)
C(27)-C(22)-C(23)	118.6(14)
C(27)-C(22)-C(21)	121.1(15)
C(23)-C(22)-C(21)	119.9(14)
C(24)-C(23)-C(22)	120.1(15)
C(24)-C(23)-H(23)	119.9
C(22)-C(23)-H(23)	119.9
C(23)-C(24)-C(25)	120.3(17)
C(23)-C(24)-H(24)	119.9
C(25)-C(24)-H(24)	119.9
C(26)-C(25)-C(24)	119.3(15)
C(26)-C(25)-C(28)	122.6(14)
C(24)-C(25)-C(28)	118.0(14)
C(25)-C(26)-C(27)	121.3(15)
C(25)-C(26)-H(26)	119.4
C(27)-C(26)-H(26)	119.4
C(22)-C(27)-C(26)	120.3(14)
C(22)-C(27)-H(27)	119.9
C(26)-C(27)-H(27)	119.9
C(33)-C(28)-C(29)	115.3(13)
C(33)-C(28)-C(25)	122.2(14)

C(29)-C(28)-C(25)	122.4(12)
C(30)-C(29)-C(28)	121.2(13)
C(30)-C(29)-H(29)	119.4
C(28)-C(29)-H(29)	119.4
C(31)-C(30)-C(29)	120.8(15)
C(31)-C(30)-H(30)	119.6
C(29)-C(30)-H(30)	119.6
C(30)-C(31)-C(32)	119.6(14)
C(30)-C(31)-C(34)	119.3(14)
C(32)-C(31)-C(34)	121.2(13)
C(33)-C(32)-C(31)	120.2(14)
C(33)-C(32)-H(32)	119.9
C(31)-C(32)-H(32)	119.9
C(28)-C(33)-C(32)	122.8(14)
C(28)-C(33)-H(33)	118.6
C(32)-C(33)-H(33)	118.6
O(4)-C(34)-O(3)	127.3(14)
O(4)-C(34)-C(31)	120.1(13)
O(3)-C(34)-C(31)	112.1(14)
C(36)-C(35)-P(1)	114.2(11)
C(36)-C(35)-H(35A)	108.7
P(1)-C(35)-H(35A)	108.7
C(36)-C(35)-H(35B)	108.7
P(1)-C(35)-H(35B)	108.7
H(35A)-C(35)-H(35B)	107.6
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(38)-C(37)-P(1)	112.2(12)
C(38)-C(37)-H(37A)	109.2
P(1)-C(37)-H(37A)	109.2
C(38)-C(37)-H(37B)	109.2
P(1)-C(37)-H(37B)	109.2
H(37A)-C(37)-H(37B)	107.9
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5



C(40)-C(39)-P(1)	113.5(14)
C(40)-C(39)-H(39A)	108.9
P(1)-C(39)-H(39A)	108.9
C(40)-C(39)-H(39B)	108.9
P(1)-C(39)-H(39B)	108.9
H(39A)-C(39)-H(39B)	107.7
C(39)-C(40)-H(40A)	109.5
C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(39)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(42)-C(41)-P(2)	113.2(15)
C(42)-C(41)-H(41A)	108.9
P(2)-C(41)-H(41A)	108.9
C(42)-C(41)-H(41B)	108.9
P(2)-C(41)-H(41B)	108.9
H(41A)-C(41)-H(41B)	107.8
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(44)-C(43)-P(2)	113.0(13)
C(44)-C(43)-H(43A)	109
P(2)-C(43)-H(43A)	109
C(44)-C(43)-H(43B)	109
P(2)-C(43)-H(43B)	109
H(43A)-C(43)-H(43B)	107.8
C(43)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(46)-C(45)-P(2)	115.9(12)
C(46)-C(45)-H(45A)	108.3
P(2)-C(45)-H(45A)	108.3
C(46)-C(45)-H(45B)	108.3
P(2)-C(45)-H(45B)	108.3
H(45A)-C(45)-H(45B)	107.4
C(45)-C(46)-H(46A)	109.5

C(45)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(45)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(48)-C(47)-P(3)	121.2(19)
C(48)-C(47)-H(47A)	107
P(3)-C(47)-H(47A)	107
C(48)-C(47)-H(47B)	107
P(3)-C(47)-H(47B)	107
H(47A)-C(47)-H(47B)	106.8
C(47)-C(48)-H(48A)	109.5
C(47)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(47)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(50)-C(49)-P(3)	107.9(15)
C(50)-C(49)-H(49A)	110.1
P(3)-C(49)-H(49A)	110.1
C(50)-C(49)-H(49B)	110.1
P(3)-C(49)-H(49B)	110.1
H(49A)-C(49)-H(49B)	108.4
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(52)-C(51)-P(3)	115.1(14)
C(52)-C(51)-H(51A)	108.5
P(3)-C(51)-H(51A)	108.5
C(52)-C(51)-H(51B)	108.5
P(3)-C(51)-H(51B)	108.5
H(51A)-C(51)-H(51B)	107.5
C(51)-C(52)-H(52A)	109.5
C(51)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(51)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(54)-C(53)-P(4)	116.1(16)
C(54)-C(53)-H(53A)	108.3

P(4)-C(53)-H(53A)	108.3
C(54)-C(53)-H(53B)	108.3
P(4)-C(53)-H(53B)	108.3
H(53A)-C(53)-H(53B)	107.4
C(53)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(56)-C(55)-P(4)	113.8(15)
C(56)-C(55)-H(55A)	108.8
P(4)-C(55)-H(55A)	108.8
C(56)-C(55)-H(55B)	108.8
P(4)-C(55)-H(55B)	108.8
H(55A)-C(55)-H(55B)	107.7
C(55)-C(56)-H(56A)	109.5
C(55)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5
C(55)-C(56)-H(56C)	109.5
H(56A)-C(56)-H(56C)	109.5
H(56B)-C(56)-H(56C)	109.5
C(58)-C(57)-P(4)	112.0(12)
C(58)-C(57)-H(57A)	109.2
P(4)-C(57)-H(57A)	109.2
C(58)-C(57)-H(57B)	109.2
P(4)-C(57)-H(57B)	109.2
H(57A)-C(57)-H(57B)	107.9
C(57)-C(58)-H(58A)	109.5
C(57)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(57)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
F(3)-C(63)-F(2)	98.8(19)
F(3)-C(63)-F(1)	107(3)
F(2)-C(63)-F(1)	105.1(19)
F(3)-C(63)-S(1)	116.3(17)
F(2)-C(63)-S(1)	114.6(16)
F(1)-C(63)-S(1)	113.8(16)
F(5)-C(64)-F(6)	101.1(13)
F(5)-C(64)-F(4)	112.6(16)
F(6)-C(64)-F(4)	112.1(15)

F(5)-C(64)-S(2)	115.5(12)
F(6)-C(64)-S(2)	112.0(12)
F(4)-C(64)-S(2)	103.9(12)
O(67)-C(65)-C(66)#2	124.0(14)
O(67)-C(65)-C(66)	124.0(14)
C(66)#2-C(65)-C(66)	112(3)
C(65)-C(66)-H(66A)	109.5
C(65)-C(66)-H(66B)	109.5
H(66A)-C(66)-H(66B)	109.5
C(65)-C(66)-H(66C)	109.5
H(66A)-C(66)-H(66C)	109.5
H(66B)-C(66)-H(66C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1  $-x+3/2, -y+3/2, -z+1$  #2  $-x+1, y, -z+1/2$

**Table 11.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **BT3'**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
Pt(1)	4111(1)	3450(1)	5479(1)	128(1)
Pt(2)	3825(1)	4802(1)	1183(1)	108(1)
P(1)	3645(5)	4940(5)	319(8)	152(5)
P(2)	4263(5)	5280(4)	1279(8)	140(5)
P(3)	4548(4)	3879(4)	5824(7)	125(5)
P(4)	4116(10)	3020(9)	6198(13)	311(18)
O(1)	4167(10)	3740(9)	4713(16)	140(10)
O(51)	3881(10)	4670(8)	1981(13)	141(9)
C(17)	1964(8)	1988(8)	1729(11)	94(10)
C(8)	1732(8)	1645(9)	1756(13)	117(11)
C(9)	1765(8)	1490(7)	2304(15)	111(11)
C(10)	2017(8)	1737(9)	2615(10)	97(9)
N(3)	2140(7)	2044(7)	2259(12)	98(9)
C(11)	2113(11)	1678(11)	3180(20)	88(9)
C(12)	2350(7)	1931(7)	3466(12)	95(9)
C(13)	2435(8)	1882(7)	4042(12)	99(9)
C(14)	2696(8)	2183(8)	4204(10)	104(10)
C(15)	2771(7)	2419(6)	3728(13)	91(9)
N(4)	2558(7)	2263(7)	3272(10)	89(8)
C(16)	2979(11)	2748(11)	3670(20)	87(9)
C(18)	3867(7)	2913(9)	4577(15)	128(11)
C(19)	3619(9)	2784(8)	4156(12)	108(10)
C(20)	3220(8)	2851(8)	4195(12)	101(10)

C(21)	3069(7)	3047(9)	4654(15)	127(11)
C(22)	3317(10)	3177(9)	5075(12)	140(12)
N(2)	3716(10)	3110(9)	5036(12)	141(11)
C(23)	3610(40)	3460(30)	6730(50)	420(40)
C(24)	4643(15)	3925(17)	6530(20)	149(12)
C(25)	4925(18)	4214(18)	6700(30)	180(20)
C(26)	4443(12)	4363(13)	5550(20)	121(11)
C(27)	4059(16)	4499(17)	5910(30)	170(19)
C(40)	4263(15)	5484(17)	1890(30)	183(14)
C(41)	3900(20)	5700(20)	2140(30)	240(30)
C(43)	3262(19)	4591(18)	40(30)	181(15)
C(45)	4090(20)	4880(20)	-230(30)	200(20)
C(46)	4956(19)	5310(20)	1920(40)	290(30)
C(50)	4065(14)	4382(13)	2158(13)	143(12)
C(56)	3938(11)	4047(11)	3889(10)	143(11)
C(57)	4203(9)	3866(8)	3534(16)	135(11)
C(58)	4221(8)	3972(9)	2975(15)	134(11)
C(59)	3974(10)	4260(10)	2770(11)	125(10)
C(60)	3709(8)	4441(7)	3124(16)	124(11)
C(61)	3691(9)	4335(9)	3684(15)	126(10)
C(62)	3900(15)	3955(16)	4520(14)	154(13)
O(63)	3567(15)	4032(15)	4770(20)	213(17)
O(65)	4248(15)	4151(12)	1837(19)	211(17)
C(67)	3097(7)	4368(6)	1536(12)	89(9)
C(68)	2900(6)	4032(7)	1695(12)	92(10)
C(69)	3049(7)	3668(6)	1556(12)	90(10)
C(70)	3396(8)	3640(5)	1257(12)	100(11)
C(71)	3593(6)	3977(7)	1099(11)	102(11)
N(1)	3444(7)	4341(6)	1238(11)	103(8)
C(74)	4639(11)	2850(20)	6330(30)	350(20)
C(73)	4250(20)	4540(20)	-70(30)	230(30)
C(108)	5218(19)	3473(19)	5190(30)	220(30)
C(109)	5034(14)	3785(17)	5550(30)	159(13)
C(110)	3030(20)	4800(30)	-490(30)	230(30)
C(112)	3430(20)	5397(17)	120(30)	180(14)
C(113)	3100(20)	5470(20)	590(30)	240(30)
C(114)	4370(20)	5666(17)	650(20)	240(30)
C(115)	4759(16)	5018(18)	1520(30)	193(15)
C(116)	4720(20)	5910(18)	860(30)	240(30)
C(117)	3810(20)	3080(30)	6940(30)	420(40)
C(118)	3727(17)	2629(17)	6070(40)	340(30)
C(119)	3860(30)	2220(16)	6260(50)	410(40)
C(120)	4680(30)	2700(40)	6940(30)	440(40)

S(1S)	4404(11)	1684(9)	7280(20)	390(20)
O(1S)	4598(16)	1360(14)	7460(30)	450(30)
O(2S)	4021(16)	1610(20)	7170(30)	450(30)
O(3S)	4600(20)	1894(18)	6900(30)	440(30)
C(1S)	4375(14)	1943(13)	7830(20)	420(30)
F(1S)	4688(18)	2050(20)	8040(30)	470(30)
F(2S)	4180(20)	2250(15)	7780(30)	450(30)
F(3S)	4210(20)	1783(19)	8240(20)	470(30)
S(2S)	5941(11)	5422(12)	2096(16)	359(19)
O(4S)	6030(15)	5130(14)	1730(20)	290(20)
O(5S)	5640(20)	5340(20)	2440(30)	410(30)
O(6S)	6260(19)	5560(20)	2370(30)	430(30)
C(2S)	5798(13)	5783(14)	1734(19)	370(20)
F(4S)	5518(18)	5730(18)	1410(30)	400(20)
F(5S)	5680(20)	6075(14)	2000(30)	410(20)
F(6S)	6040(19)	5947(16)	1420(30)	380(20)

**Table 12.** Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **BT3'**.

Pt(1)-N(2)	2.08(2)
Pt(1)-O(1)	2.10(4)
Pt(1)-P(3)	2.255(13)
Pt(1)-P(4)	2.27(2)
Pt(2)-O(51)	1.97(3)
Pt(2)-N(1)	2.057(19)
Pt(2)-P(1)	2.210(19)
Pt(2)-P(2)	2.236(13)
P(1)-C(112)	1.80(6)
P(1)-C(43)	1.89(6)
P(1)-C(45)	2.02(7)
P(2)-C(40)	1.61(6)
P(2)-C(115)	2.00(6)
P(2)-C(114)	2.04(2)
P(3)-C(24)	1.72(6)
P(3)-C(109)	1.82(5)
P(3)-C(26)	1.81(5)
P(4)-C(74)	1.91(2)
P(4)-C(118)	1.91(2)
P(4)-C(117)	2.07(2)
O(1)-C(62)	1.26(2)
O(51)-C(50)	1.25(2)
C(17)-C(16)#1	1.33(4)
C(17)-C(8)	1.42

C(17)-N(3)	1.42
C(8)-C(9)	1.42
C(8)-H(8)	0.95
C(9)-C(10)	1.42
C(9)-H(9)	0.95
C(10)-N(3)	1.42
C(10)-C(11)	1.42(5)
C(11)-C(12)	1.36(4)
C(11)-C(69)#1	1.45(4)
C(12)-C(13)	1.42
C(12)-N(4)	1.42
C(13)-C(14)	1.42
C(13)-H(13)	0.95
C(14)-C(15)	1.42
C(14)-H(14)	0.95
C(15)-C(16)	1.34(4)
C(15)-N(4)	1.42
N(4)-H(4)	0.88
C(16)-C(20)	1.55(5)
C(18)-C(19)	1.39
C(18)-N(2)	1.39
C(18)-H(18)	0.95
C(19)-C(20)	1.39
C(19)-H(19)	0.95
C(20)-C(21)	1.39
C(21)-C(22)	1.39
C(21)-H(21)	0.95
C(22)-N(2)	1.39
C(22)-H(22)	0.95
C(23)-C(117)	1.54(2)
C(23)-H(23A)	0.9972
C(23)-H(23B)	0.9995
C(23)-H(23C)	0.9981
C(24)-C(25)	1.45(6)
C(24)-H(24A)	0.99
C(24)-H(24B)	0.99
C(25)-H(25A)	0.98
C(25)-H(25B)	0.98
C(25)-H(25C)	0.98
C(26)-C(27)	1.63(7)
C(26)-H(26A)	0.99
C(26)-H(26B)	0.99
C(27)-H(27A)	1.0126

C(27)-H(27B)	1.014
C(27)-H(27C)	1.0134
C(40)-C(41)	1.56(2)
C(40)-H(40A)	0.99
C(40)-H(40B)	0.99
C(41)-H(41A)	0.9939
C(41)-H(41B)	0.9946
C(41)-H(41C)	0.994
C(43)-C(110)	1.67(9)
C(43)-H(43A)	0.99
C(43)-H(43B)	0.99
C(45)-C(73)	1.34(8)
C(45)-H(45A)	0.99
C(45)-H(45B)	0.99
C(46)-C(115)	1.55(2)
C(46)-H(46A)	0.9838
C(46)-H(46B)	0.9838
C(46)-H(46C)	0.9839
C(50)-O(65)	1.27(2)
C(50)-C(59)	1.56(2)
C(56)-C(57)	1.39
C(56)-C(61)	1.39
C(56)-C(62)	1.55(2)
C(57)-C(58)	1.39
C(57)-H(57)	0.95
C(58)-C(59)	1.39
C(58)-H(58)	0.95
C(59)-C(60)	1.39
C(60)-C(61)	1.39
C(60)-H(60)	0.95
C(61)-H(61)	0.95
C(62)-O(63)	1.32(6)
C(67)-C(68)	1.39
C(67)-N(1)	1.39
C(67)-H(67)	0.95
C(68)-C(69)	1.39
C(68)-H(68)	0.95
C(69)-C(70)	1.39
C(70)-C(71)	1.39
C(70)-H(70)	0.95
C(71)-N(1)	1.39
C(71)-H(71)	0.95
C(74)-C(120)	1.55(2)



C(74)-H(74A)	0.99
C(74)-H(74B)	0.99
C(73)-H(73A)	0.95
C(73)-H(73B)	0.95
C(108)-C(109)	1.52(2)
C(108)-H(10A)	0.9872
C(108)-H(10B)	0.9868
C(108)-H(10C)	0.9866
C(109)-H(10D)	0.99
C(109)-H(10E)	0.99
C(110)-H(11A)	1.0093
C(110)-H(11B)	1.0096
C(110)-H(11C)	1.0102
C(112)-C(113)	1.61(9)
C(112)-H(11D)	0.99
C(112)-H(11E)	0.99
C(113)-H(11F)	1.0391
C(113)-H(11G)	1.0376
C(113)-H(11H)	1.036
C(114)-C(116)	1.55(2)
C(114)-H(11I)	0.99
C(114)-H(11J)	0.99
C(115)-H(11K)	0.99
C(115)-H(11L)	0.99
C(116)-H(11M)	0.9903
C(116)-H(11N)	0.9903
C(116)-H(11O)	0.99
C(117)-H(11P)	0.99
C(117)-H(11Q)	0.99
C(118)-C(119)	1.55(2)
C(118)-H(11R)	0.99
C(118)-H(11S)	0.99
C(119)-H(11T)	0.9946
C(119)-H(11U)	0.9952
C(119)-H(11V)	0.9948
C(120)-H(12A)	1.113
C(120)-H(12B)	1.1285
C(120)-H(12C)	1.1366
S(1S)-O(3S)	1.34(4)
S(1S)-O(2S)	1.36(3)
S(1S)-O(1S)	1.37(3)
S(1S)-C(1S)	1.59(2)
C(1S)-F(1S)	1.24(3)

C(1S)-F(2S)	1.25(3)
C(1S)-F(3S)	1.25(3)
S(2S)-O(4S)	1.36(3)
S(2S)-O(5S)	1.36(3)
S(2S)-O(6S)	1.37(4)
S(2S)-C(2S)	1.59(3)
C(2S)-F(4S)	1.25(3)
C(2S)-F(6S)	1.25(3)
C(2S)-F(5S)	1.26(3)
N(2)-Pt(1)-O(1)	83.1(11)
N(2)-Pt(1)-P(3)	170.2(9)
O(1)-Pt(1)-P(3)	87.1(9)
N(2)-Pt(1)-P(4)	91.5(10)
O(1)-Pt(1)-P(4)	166.6(16)
P(3)-Pt(1)-P(4)	98.2(7)
O(51)-Pt(2)-N(1)	79.8(11)
O(51)-Pt(2)-P(1)	169.2(11)
N(1)-Pt(2)-P(1)	92.7(9)
O(51)-Pt(2)-P(2)	90.1(10)
N(1)-Pt(2)-P(2)	169.9(9)
P(1)-Pt(2)-P(2)	97.4(6)
C(112)-P(1)-C(43)	100(3)
C(112)-P(1)-C(45)	102(3)
C(43)-P(1)-C(45)	103(3)
C(112)-P(1)-Pt(2)	124(3)
C(43)-P(1)-Pt(2)	113(2)
C(45)-P(1)-Pt(2)	112(2)
C(40)-P(2)-C(115)	87(3)
C(40)-P(2)-C(114)	113(3)
C(115)-P(2)-C(114)	111(3)
C(40)-P(2)-Pt(2)	114(2)
C(115)-P(2)-Pt(2)	105.6(17)
C(114)-P(2)-Pt(2)	121.1(16)
C(24)-P(3)-C(109)	101(3)
C(24)-P(3)-C(26)	107(3)
C(109)-P(3)-C(26)	103(3)
C(24)-P(3)-Pt(1)	123.0(19)
C(109)-P(3)-Pt(1)	111.2(19)
C(26)-P(3)-Pt(1)	109.6(14)
C(74)-P(4)-C(118)	118.1(18)
C(74)-P(4)-C(117)	111.0(15)
C(118)-P(4)-C(117)	82(4)

C(74)-P(4)-Pt(1)	109(2)
C(118)-P(4)-Pt(1)	109(2)
C(117)-P(4)-Pt(1)	126(3)
C(62)-O(1)-Pt(1)	122(3)
C(50)-O(51)-Pt(2)	124(2)
C(16)#1-C(17)-C(8)	133(3)
C(16)#1-C(17)-N(3)	119(3)
C(8)-C(17)-N(3)	108
C(17)-C(8)-C(9)	108
C(17)-C(8)-H(8)	126
C(9)-C(8)-H(8)	126
C(10)-C(9)-C(8)	108
C(10)-C(9)-H(9)	126
C(8)-C(9)-H(9)	126
N(3)-C(10)-C(9)	108
N(3)-C(10)-C(11)	128(3)
C(9)-C(10)-C(11)	124(3)
C(10)-N(3)-C(17)	108
C(12)-C(11)-C(10)	121(3)
C(12)-C(11)-C(69)#1	123(9)
C(10)-C(11)-C(69)#1	116(8)
C(11)-C(12)-C(13)	122(3)
C(11)-C(12)-N(4)	130(3)
C(13)-C(12)-N(4)	108
C(14)-C(13)-C(12)	108
C(14)-C(13)-H(13)	126
C(12)-C(13)-H(13)	126
C(13)-C(14)-C(15)	108
C(13)-C(14)-H(14)	126
C(15)-C(14)-H(14)	126
C(16)-C(15)-N(4)	121(3)
C(16)-C(15)-C(14)	131(3)
N(4)-C(15)-C(14)	108
C(15)-N(4)-C(12)	108
C(15)-N(4)-H(4)	126
C(12)-N(4)-H(4)	126
C(17)#1-C(16)-C(15)	137(4)
C(17)#1-C(16)-C(20)	110(3)
C(15)-C(16)-C(20)	113(3)
C(19)-C(18)-N(2)	120
C(19)-C(18)-H(18)	120
N(2)-C(18)-H(18)	120
C(20)-C(19)-C(18)	120

C(20)-C(19)-H(19)	120
C(18)-C(19)-H(19)	120
C(21)-C(20)-C(19)	120
C(21)-C(20)-C(16)	124(3)
C(19)-C(20)-C(16)	116(3)
C(22)-C(21)-C(20)	120
C(22)-C(21)-H(21)	120
C(20)-C(21)-H(21)	120
C(21)-C(22)-N(2)	120
C(21)-C(22)-H(22)	120
N(2)-C(22)-H(22)	120
C(22)-N(2)-C(18)	120
C(22)-N(2)-Pt(1)	121(2)
C(18)-N(2)-Pt(1)	116(2)
C(117)-C(23)-H(23A)	110.6
C(117)-C(23)-H(23B)	111.9
H(23A)-C(23)-H(23B)	107.8
C(117)-C(23)-H(23C)	111.2
H(23A)-C(23)-H(23C)	107.6
H(23B)-C(23)-H(23C)	107.5
C(25)-C(24)-P(3)	118(4)
C(25)-C(24)-H(24A)	107.8
P(3)-C(24)-H(24A)	107.8
C(25)-C(24)-H(24B)	107.6
P(3)-C(24)-H(24B)	107.7
H(24A)-C(24)-H(24B)	107.1
C(24)-C(25)-H(25A)	109.6
C(24)-C(25)-H(25B)	109.4
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.4
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(27)-C(26)-P(3)	104(4)
C(27)-C(26)-H(26A)	110.9
P(3)-C(26)-H(26A)	111.1
C(27)-C(26)-H(26B)	111
P(3)-C(26)-H(26B)	111.1
H(26A)-C(26)-H(26B)	109.1
C(26)-C(27)-H(27A)	112.3
C(26)-C(27)-H(27B)	112.7
H(27A)-C(27)-H(27B)	106.4
C(26)-C(27)-H(27C)	112.5
H(27A)-C(27)-H(27C)	106.3

H(27B)-C(27)-H(27C)	106.2
C(41)-C(40)-P(2)	123(4)
C(41)-C(40)-H(40A)	106.4
P(2)-C(40)-H(40A)	106.4
C(41)-C(40)-H(40B)	106.6
P(2)-C(40)-H(40B)	106.7
H(40A)-C(40)-H(40B)	106.6
C(40)-C(41)-H(41A)	110.6
C(40)-C(41)-H(41B)	111.1
H(41A)-C(41)-H(41B)	108
C(40)-C(41)-H(41C)	110.7
H(41A)-C(41)-H(41C)	108.1
H(41B)-C(41)-H(41C)	108.1
C(110)-C(43)-P(1)	109(4)
C(110)-C(43)-H(43A)	110
P(1)-C(43)-H(43A)	109.9
C(110)-C(43)-H(43B)	109.9
P(1)-C(43)-H(43B)	109.7
H(43A)-C(43)-H(43B)	108.3
C(73)-C(45)-P(1)	102(5)
C(73)-C(45)-H(45A)	111.3
P(1)-C(45)-H(45A)	111.4
C(73)-C(45)-H(45B)	111.4
P(1)-C(45)-H(45B)	111.4
H(45A)-C(45)-H(45B)	109.3
C(115)-C(46)-H(46A)	109.6
C(115)-C(46)-H(46B)	109.9
H(46A)-C(46)-H(46B)	109.1
C(115)-C(46)-H(46C)	110
H(46A)-C(46)-H(46C)	109.1
H(46B)-C(46)-H(46C)	109.1
O(51)-C(50)-O(65)	123(3)
O(51)-C(50)-C(59)	116(3)
O(65)-C(50)-C(59)	120(4)
C(57)-C(56)-C(61)	120
C(57)-C(56)-C(62)	124(3)
C(61)-C(56)-C(62)	116(3)
C(58)-C(57)-C(56)	120
C(58)-C(57)-H(57)	120
C(56)-C(57)-H(57)	120
C(59)-C(58)-C(57)	120
C(59)-C(58)-H(58)	120
C(57)-C(58)-H(58)	120

C(58)-C(59)-C(60)	120
C(58)-C(59)-C(50)	114(3)
C(60)-C(59)-C(50)	126(3)
C(61)-C(60)-C(59)	120
C(61)-C(60)-H(60)	120
C(59)-C(60)-H(60)	120
C(60)-C(61)-C(56)	120
C(60)-C(61)-H(61)	120
C(56)-C(61)-H(61)	120
O(1)-C(62)-O(63)	125(4)
O(1)-C(62)-C(56)	115(4)
O(63)-C(62)-C(56)	118(4)
C(68)-C(67)-N(1)	120
C(68)-C(67)-H(67)	120
N(1)-C(67)-H(67)	120
C(67)-C(68)-C(69)	120
C(67)-C(68)-H(68)	120
C(69)-C(68)-H(68)	120
C(70)-C(69)-C(68)	120
C(70)-C(69)-C(11)#1	120(2)
C(68)-C(69)-C(11)#1	119(2)
C(69)-C(70)-C(71)	120
C(69)-C(70)-H(70)	120
C(71)-C(70)-H(70)	120
N(1)-C(71)-C(70)	120
N(1)-C(71)-H(71)	120
C(70)-C(71)-H(71)	120
C(71)-N(1)-C(67)	120
C(71)-N(1)-Pt(2)	116.1(13)
C(67)-N(1)-Pt(2)	121.7(14)
C(120)-C(74)-P(4)	110(3)
C(120)-C(74)-H(74A)	108.8
P(4)-C(74)-H(74A)	109.7
C(120)-C(74)-H(74B)	110.4
P(4)-C(74)-H(74B)	109.9
H(74A)-C(74)-H(74B)	108.3
C(45)-C(73)-H(73A)	120
C(45)-C(73)-H(73B)	120
H(73A)-C(73)-H(73B)	120
C(109)-C(108)-H(10A)	110.7
C(109)-C(108)-H(10B)	110
H(10A)-C(108)-H(10B)	108.8
C(109)-C(108)-H(10C)	109.8

H(10A)-C(108)-H(10C)	108.7
H(10B)-C(108)-H(10C)	108.8
C(108)-C(109)-P(3)	135(4)
C(108)-C(109)-H(10D)	103.6
P(3)-C(109)-H(10D)	103.4
C(108)-C(109)-H(10E)	102.8
P(3)-C(109)-H(10E)	103.4
H(10D)-C(109)-H(10E)	105.2
C(43)-C(110)-H(11A)	112
C(43)-C(110)-H(11B)	112.1
H(11A)-C(110)-H(11B)	106.7
C(43)-C(110)-H(11C)	112.3
H(11A)-C(110)-H(11C)	106.8
H(11B)-C(110)-H(11C)	106.7
C(113)-C(112)-P(1)	103(4)
C(113)-C(112)-H(11D)	111.3
P(1)-C(112)-H(11D)	111.2
C(113)-C(112)-H(11E)	110.8
P(1)-C(112)-H(11E)	111.1
H(11D)-C(112)-H(11E)	109.1
C(112)-C(113)-H(11F)	115.1
C(112)-C(113)-H(11G)	114.8
H(11F)-C(113)-H(11G)	103.7
C(112)-C(113)-H(11H)	114.4
H(11F)-C(113)-H(11H)	103.6
H(11G)-C(113)-H(11H)	103.8
C(116)-C(114)-P(2)	104(2)
C(116)-C(114)-H(11I)	111
P(2)-C(114)-H(11I)	110.9
C(116)-C(114)-H(11J)	110.9
P(2)-C(114)-H(11J)	110.8
H(11I)-C(114)-H(11J)	108.9
C(46)-C(115)-P(2)	105(4)
C(46)-C(115)-H(11K)	110.7
P(2)-C(115)-H(11K)	110.7
C(46)-C(115)-H(11L)	111
P(2)-C(115)-H(11L)	111
H(11K)-C(115)-H(11L)	108.9
C(114)-C(116)-H(11M)	110.6
C(114)-C(116)-H(11N)	110.5
H(11M)-C(116)-H(11N)	108.5
C(114)-C(116)-H(11O)	110.3
H(11M)-C(116)-H(11O)	108.4

H(11N)-C(116)-H(11O)	108.5
C(23)-C(117)-P(4)	92(6)
C(23)-C(117)-H(11P)	113.4
P(4)-C(117)-H(11P)	113.3
C(23)-C(117)-H(11Q)	112.9
P(4)-C(117)-H(11Q)	113.3
H(11P)-C(117)-H(11Q)	110.7
C(119)-C(118)-P(4)	112(3)
C(119)-C(118)-H(11R)	109
P(4)-C(118)-H(11R)	109.1
C(119)-C(118)-H(11S)	109.4
P(4)-C(118)-H(11S)	109.2
H(11R)-C(118)-H(11S)	107.9
C(118)-C(119)-H(11T)	110.7
C(118)-C(119)-H(11U)	111.1
H(11T)-C(119)-H(11U)	107.9
C(118)-C(119)-H(11V)	110.9
H(11T)-C(119)-H(11V)	108
H(11U)-C(119)-H(11V)	108
C(74)-C(120)-H(12A)	122.2
C(74)-C(120)-H(12B)	123.9
H(12A)-C(120)-H(12B)	92.5
C(74)-C(120)-H(12C)	124.8
H(12A)-C(120)-H(12C)	92.8
H(12B)-C(120)-H(12C)	91.5
O(3S)-S(1S)-O(2S)	116(3)
O(3S)-S(1S)-O(1S)	114(3)
O(2S)-S(1S)-O(1S)	113(3)
O(3S)-S(1S)-C(1S)	107(3)
O(2S)-S(1S)-C(1S)	102(3)
O(1S)-S(1S)-C(1S)	103(3)
F(1S)-C(1S)-F(2S)	104(4)
F(1S)-C(1S)-F(3S)	103(4)
F(2S)-C(1S)-F(3S)	102(4)
F(1S)-C(1S)-S(1S)	117(3)
F(2S)-C(1S)-S(1S)	115(3)
F(3S)-C(1S)-S(1S)	115(3)
O(4S)-S(2S)-O(5S)	115(3)
O(4S)-S(2S)-O(6S)	113(3)
O(5S)-S(2S)-O(6S)	113(3)
O(4S)-S(2S)-C(2S)	107(3)
O(5S)-S(2S)-C(2S)	105(3)
O(6S)-S(2S)-C(2S)	103(3)



F(4S)-C(2S)-F(6S)	101(4)
F(4S)-C(2S)-F(5S)	101(4)
F(6S)-C(2S)-F(5S)	100(4)
F(4S)-C(2S)-S(2S)	118(3)
F(6S)-C(2S)-S(2S)	118(3)
F(5S)-C(2S)-S(2S)	116(3)

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Symmetry transformations used to generate equivalent atoms:

#1  $-x+1/2, -y+1/2, -z+1/2$

## References

- S1. S. Muratsugu, A. Yamaguchi, G. I. Yokota, T. Maeno and M. Tada, *Chem. Commun.* 2018, **54**, 4842–4845.
- S2. P. J. Stang, D. H. Cao, S. Saito and A. M. Arif, *J. Am. Chem. Soc.* 1995, **117**, 6273–6283.
- S3. Y. Shi, I. Sánchez-Molina, C. Cao, T. R. Cook and P. J. Stang, *Proc. Natl. Acad. Sci.*, 2014, **111**, 9390–9395.
- S4. (a) Thordarson, P. *Chem. Soc. Rev.* 2011, **40**, 1305-1323. (b) [www.supramolecular.org](http://www.supramolecular.org)