

[(1,2,5,6- η)-Cycloocta-1,5-diene]bis(4-methylphenyl)platinum(II)

Zhi-Wei Wang, Ran Liu, Hong-Yu Liu and Chong-Qing Wan*

Department of Chemistry, Capital Normal University, Beijing 100048, People's Republic of China
Correspondence e-mail: wanchqing@yahoo.com.cn

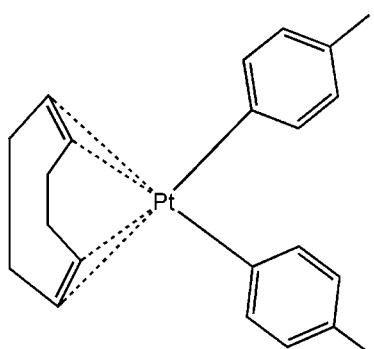
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Key indicators: single-crystal X-ray study; $T = 293\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$; R factor = 0.022; wR factor = 0.061; data-to-parameter ratio = 15.0.

In the mononuclear title complex, $[\text{Pt}(\text{C}_7\text{H}_7)_2(\text{C}_8\text{H}_{12})]$, the Pt^{II} ion exhibits a square-planar coordination geometry defined by two methylphenyl ligands and the mid-points of the two π -coordinated double bonds of cycloocta-1,5-diene. The two methylphenyl groups have a *cis* relationship with a $\text{C}-\text{Pt}-\text{C}$ bond angle of $88.54(18)^\circ$ and a dihedral angle between the mean planes of the benzene rings of $83.87(1)^\circ$. Each complex molecule links to four symmetry-related ones through intermolecular $\text{C}-\text{H}\cdots\pi$ interactions, forming a layer almost parallel to the bc plane.

Related literature

For general background to Pt^{II} complexes with cycloocta-1,5-diene, see: Goel *et al.* (1982); Syed *et al.* (1984). For the structures of analogous Pt^{II} complexes, see: Deacon *et al.* (1993); Debaerdemaeker *et al.* (1987, 1991); Roviello *et al.* (2006). For $\text{C}-\text{H}\cdots\pi$ interactions, see: Umezawa *et al.* (1998). For the preparation, see: Chaudhury & Puddephatt (1975).



Experimental

Crystal data

$[\text{Pt}(\text{C}_7\text{H}_7)_2(\text{C}_8\text{H}_{12})]$

$M_r = 485.52$

Monoclinic, $C2/c$
 $a = 25.029(13)\text{ \AA}$
 $b = 8.172(4)\text{ \AA}$
 $c = 19.674(10)\text{ \AA}$
 $\beta = 118.417(8)^\circ$
 $V = 3539(3)\text{ \AA}^3$

$Z = 8$
Mo $K\alpha$ radiation
 $\mu = 7.93\text{ mm}^{-1}$
 $T = 293\text{ K}$
 $0.36 \times 0.30 \times 0.20\text{ mm}$

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
 $T_{\min} = 0.584$, $T_{\max} = 1.000$

8906 measured reflections
3113 independent reflections
2884 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.061$
 $S = 1.11$
3113 reflections

208 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 2.74\text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.99\text{ e \AA}^{-3}$

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

Cg1 and *Cg2* are the centroids of the C9–C14 and C2–C7 rings, respectively.

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|--|-------------|---------------------|----------------------------|-------------------------------|
| C1—H1B \cdots <i>Cg1</i> ⁱ | 0.96 | 2.93 | 3.615 (4) | 129 |
| C20—H20B \cdots <i>Cg1</i> ⁱⁱ | 0.96 | 2.85 | 3.749 (5) | 155 |
| C21—H21A \cdots <i>Cg2</i> ⁱⁱ | 0.97 | 2.83 | 3.411 (4) | 119 |
| C8—H8C \cdots <i>Cg2</i> ⁱⁱⁱ | 0.96 | 2.85 | 3.509 (2) | 126 |

Symmetry codes: (i) $x, -y + 2, z + \frac{1}{2}$; (ii) $x, y - 1, z$; (iii) $x, -y + 2, z - \frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *APEX2* and *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2077).

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supporting information

Acta Cryst. (2011). E67, m37 [https://doi.org/10.1107/S1600536810049664]

[(1,2,5,6- η)-Cycloocta-1,5-diene]bis(4-methylphenyl)platinum(II)

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S1. Comment

The Pt^{II} complexes with cycloocta-1,5-diene (COD) are versatile precursors in inorganic synthesis (Goel *et al.*, 1982; Syed *et al.*, 1984). Herein, we report the structure of the bis-aryl complex [(COD)Pt(C₇H₇)₂]. In the crystal structure of the title complex, the center Pt^{II} adopts a square-planar coordination geometry with two methylphenyl groups depositing in a *cis* relationship, and the cycloocta-1,5-diene bonding to the ion with a 1,2,5,6- η^4 -coordination mode (Fig. 1). The Pt1—C5 and Pt1—C12 bond lengths equal 2.028 (4) Å, while the distances from the Pt^{II} to the doubly-bonded C atoms lie within the range of 2.256 (4)–2.279 (4) Å, all of which are comparable to that of similar complexes. The two methylphenyl groups site in a *cis* relationship with a C5—Pt1—C12 bond angle of 88.54 (18) $^\circ$ and a dihedral angle between the two benzene rings of 83.87 (1) $^\circ$. Each of such mononuclear complex moiety links four symmetry-related ones through two types of intermolecular C—H··· π interactions [C—H(methylene)··· π and C—H(methyl)··· π] to form a layer almost parallel to the *bc* plane, as shown in Fig. 2. The C···centroid distances vary from 3.411 (4) to 3.749 (5) Å, and C—H···centroid bond angles lie within the range of 119–155 $^\circ$ (Umezawa *et al.* 1998).

S2. Experimental

The title complex was obtained following a reaction procedure from literature (Chaudhury *et al.*, 1975). Reaction of aryl Grignard reagents (C₆H₄-4-CH₃)MgBr (0.195 g, 1 mmol) with (COD)PtCl₂ (0.086 g, 0.8 mmol) in ether formed the title compound as a white powder, crystals of which were obtained after four days by recrystallization from CH₂Cl₂/n-hexane, yield: 0.233 g (60%).

S3. Refinement

The hydrogen atoms were placed in idealized positions and allowed to ride on the relevant carbon atoms, with C—H = 0.93 and 0.97 Å for aryl and methylene H atoms, respectively, and with $U_{iso}(\text{H}) = 1.2U_{eq}(\text{C})$.

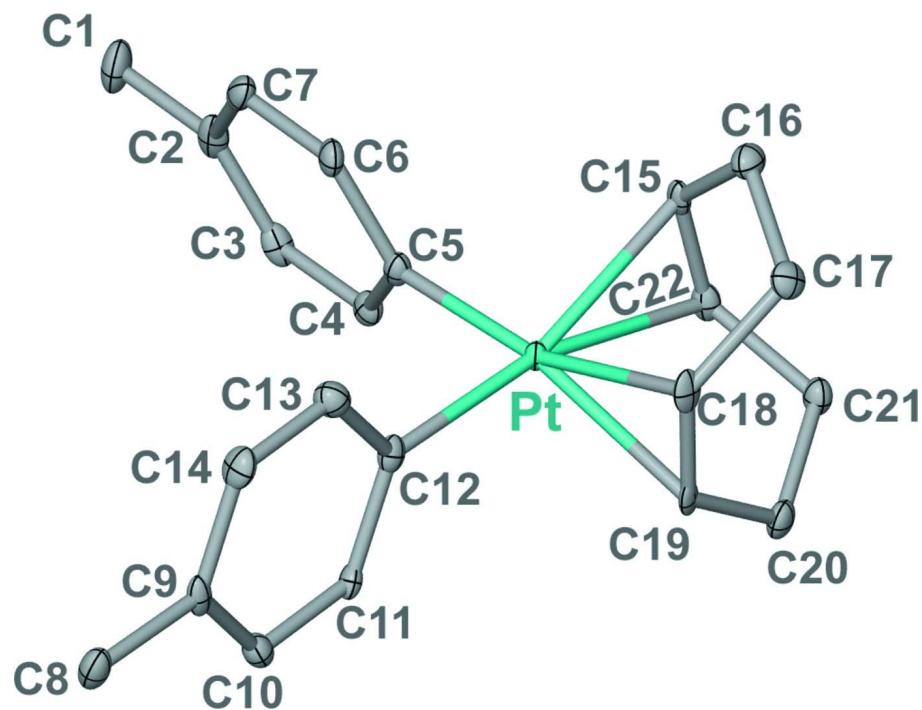
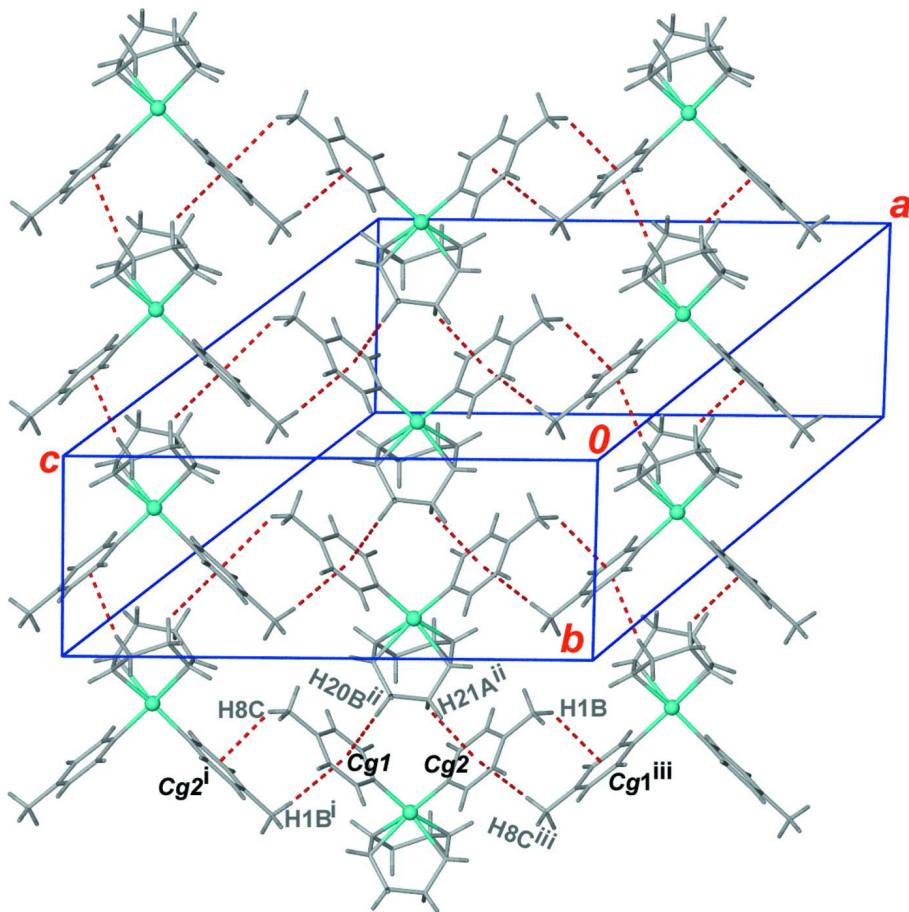


Figure 1

The atom-numbering scheme of the title complex. Displacement ellipsoids are drawn at the 30% probability level and H atoms are omitted for clarity.

**Figure 2**

The C—H(methyl)··· π and C—H(methylene)··· π interactions between the mononuclear units, forming a layer in the bc plane. The $Cg1$ and $Cg2$ are the centroids of the $C9—C10—C11—C12—C13—C14$ and $C2—C3—C4—C5—C6—C7$ rings, respectively. Symmetry codes: (i) $x, -y + 2, z - 1/2$; (ii) $x, y + 1, z$; (iii) $x, -y + 2, z + 1/2$.

$[(1,2,5,6-\eta)\text{-Cycloocta-1,5-diene}] \text{bis}(4\text{-methylphenyl})\text{platinum(II)}$

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Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

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$b = 8.172 (4)$ Å

$c = 19.674 (10)$ Å

$\beta = 118.417 (8)^\circ$

$V = 3539 (3)$ Å 3

$Z = 8$

$F(000) = 1888$

$D_x = 1.823$ Mg m $^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

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$T = 293$ K

Block, colourless

$0.36 \times 0.30 \times 0.20$ mm

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Bruker APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2007)

$T_{\min} = 0.584$, $T_{\max} = 1.000$

8906 measured reflections

3113 independent reflections

2884 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$
 $\theta_{\text{max}} = 25.0^\circ, \theta_{\text{min}} = 2.2^\circ$

$h = -29 \rightarrow 17$
 $k = -9 \rightarrow 9$
 $l = -20 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.061$
 $S = 1.11$
3113 reflections
208 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0308P)^2 + 23.1984P]$ $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.004$
 $\Delta\rho_{\text{max}} = 2.74 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.99 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|---------------|--------------|----------------------------------|
| Pt1 | 0.625760 (7) | 0.723387 (19) | 0.445111 (9) | 0.00847 (8) |
| C5 | 0.6352 (2) | 0.8997 (5) | 0.5226 (2) | 0.0123 (9) |
| C12 | 0.6322 (2) | 0.9000 (5) | 0.3769 (2) | 0.0119 (9) |
| C15 | 0.5845 (2) | 0.5524 (5) | 0.4975 (2) | 0.0118 (9) |
| H15A | 0.5749 | 0.6041 | 0.5353 | 0.014* |
| C19 | 0.6452 (2) | 0.5268 (5) | 0.3793 (2) | 0.0110 (9) |
| H19A | 0.6613 | 0.5682 | 0.3458 | 0.013* |
| C18 | 0.5828 (2) | 0.5402 (5) | 0.3479 (2) | 0.0137 (9) |
| H18A | 0.5628 | 0.5894 | 0.2962 | 0.016* |
| C9 | 0.6352 (2) | 1.1307 (5) | 0.2696 (2) | 0.0126 (9) |
| C11 | 0.6864 (2) | 0.9413 (5) | 0.3760 (2) | 0.0106 (9) |
| H11A | 0.7225 | 0.8924 | 0.4116 | 0.013* |
| C8 | 0.6356 (2) | 1.2543 (6) | 0.2132 (3) | 0.0172 (10) |
| H8A | 0.6763 | 1.2668 | 0.2210 | 0.026* |
| H8B | 0.6212 | 1.3575 | 0.2213 | 0.026* |
| H8C | 0.6096 | 1.2174 | 0.1614 | 0.026* |
| C21 | 0.6671 (2) | 0.3611 (5) | 0.5002 (2) | 0.0139 (9) |
| H21A | 0.6357 | 0.2780 | 0.4800 | 0.017* |
| H21B | 0.7020 | 0.3150 | 0.5446 | 0.017* |
| C20 | 0.6854 (2) | 0.4039 (5) | 0.4380 (3) | 0.0148 (9) |
| H20A | 0.7266 | 0.4459 | 0.4633 | 0.018* |
| H20B | 0.6854 | 0.3042 | 0.4112 | 0.018* |

| | | | | |
|------|------------|------------|------------|-------------|
| C6 | 0.5846 (2) | 0.9915 (5) | 0.5136 (3) | 0.0136 (9) |
| H6A | 0.5472 | 0.9738 | 0.4703 | 0.016* |
| C7 | 0.5889 (2) | 1.1085 (5) | 0.5680 (3) | 0.0162 (10) |
| H7A | 0.5545 | 1.1665 | 0.5601 | 0.019* |
| C1 | 0.6475 (3) | 1.2679 (6) | 0.6911 (3) | 0.0246 (12) |
| H1A | 0.6883 | 1.2740 | 0.7328 | 0.037* |
| H1B | 0.6205 | 1.2389 | 0.7112 | 0.037* |
| H1C | 0.6358 | 1.3723 | 0.6659 | 0.037* |
| C13 | 0.5800 (2) | 0.9798 (6) | 0.3221 (3) | 0.0153 (9) |
| H13A | 0.5431 | 0.9575 | 0.3207 | 0.018* |
| C17 | 0.5429 (2) | 0.4230 (6) | 0.3636 (2) | 0.0144 (9) |
| H17A | 0.5622 | 0.3163 | 0.3757 | 0.017* |
| H17B | 0.5044 | 0.4120 | 0.3168 | 0.017* |
| C14 | 0.5813 (2) | 1.0902 (5) | 0.2700 (3) | 0.0154 (9) |
| H14A | 0.5452 | 1.1389 | 0.2342 | 0.019* |
| C22 | 0.6441 (2) | 0.5074 (5) | 0.5265 (2) | 0.0133 (9) |
| H22A | 0.6694 | 0.5349 | 0.5812 | 0.016* |
| C4 | 0.6897 (2) | 0.9310 (5) | 0.5893 (2) | 0.0136 (9) |
| H4A | 0.7241 | 0.8714 | 0.5984 | 0.016* |
| C10 | 0.6876 (2) | 1.0531 (5) | 0.3235 (2) | 0.0134 (9) |
| H10A | 0.7244 | 1.0763 | 0.3246 | 0.016* |
| C2 | 0.6439 (2) | 1.1394 (6) | 0.6337 (3) | 0.0181 (10) |
| C16 | 0.5305 (2) | 0.4754 (6) | 0.4297 (3) | 0.0152 (9) |
| H16A | 0.4972 | 0.5528 | 0.4098 | 0.018* |
| H16B | 0.5179 | 0.3801 | 0.4478 | 0.018* |
| C3 | 0.6939 (2) | 1.0492 (6) | 0.6427 (2) | 0.0158 (9) |
| H3A | 0.7314 | 1.0683 | 0.6857 | 0.019* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|-------------|--------------|
| Pt1 | 0.01211 (11) | 0.00610 (11) | 0.00793 (11) | -0.00017 (6) | 0.00537 (8) | -0.00012 (6) |
| C5 | 0.019 (2) | 0.009 (2) | 0.012 (2) | -0.0001 (18) | 0.0095 (19) | 0.0006 (17) |
| C12 | 0.015 (2) | 0.009 (2) | 0.009 (2) | 0.0004 (17) | 0.0042 (18) | -0.0013 (17) |
| C15 | 0.021 (2) | 0.007 (2) | 0.011 (2) | -0.0015 (18) | 0.0101 (19) | 0.0012 (16) |
| C19 | 0.021 (2) | 0.004 (2) | 0.011 (2) | -0.0019 (17) | 0.0103 (19) | -0.0031 (16) |
| C18 | 0.022 (3) | 0.009 (2) | 0.009 (2) | -0.0033 (18) | 0.0059 (19) | -0.0051 (16) |
| C9 | 0.023 (2) | 0.007 (2) | 0.0093 (19) | -0.0021 (18) | 0.0085 (19) | -0.0019 (16) |
| C11 | 0.013 (2) | 0.006 (2) | 0.010 (2) | 0.0017 (17) | 0.0036 (18) | 0.0008 (16) |
| C8 | 0.028 (3) | 0.011 (2) | 0.016 (2) | 0.0040 (19) | 0.014 (2) | 0.0011 (18) |
| C21 | 0.018 (2) | 0.010 (2) | 0.013 (2) | 0.0005 (18) | 0.0080 (19) | 0.0011 (17) |
| C20 | 0.021 (2) | 0.009 (2) | 0.016 (2) | 0.0010 (18) | 0.010 (2) | -0.0024 (17) |
| C6 | 0.018 (2) | 0.007 (2) | 0.016 (2) | 0.0005 (17) | 0.0080 (19) | 0.0019 (17) |
| C7 | 0.024 (3) | 0.009 (2) | 0.022 (2) | 0.0046 (19) | 0.016 (2) | 0.0041 (18) |
| C1 | 0.041 (3) | 0.011 (2) | 0.023 (3) | 0.002 (2) | 0.017 (3) | -0.0013 (19) |
| C13 | 0.016 (2) | 0.016 (2) | 0.015 (2) | -0.0010 (18) | 0.0082 (19) | 0.0001 (18) |
| C17 | 0.014 (2) | 0.014 (2) | 0.013 (2) | -0.0039 (18) | 0.0046 (18) | -0.0045 (17) |
| C14 | 0.018 (2) | 0.013 (2) | 0.012 (2) | 0.0049 (18) | 0.0049 (19) | 0.0042 (18) |

| | | | | | | |
|-----|-----------|-----------|-----------|--------------|-------------|--------------|
| C22 | 0.020 (2) | 0.011 (2) | 0.010 (2) | -0.0017 (18) | 0.0079 (19) | 0.0001 (17) |
| C4 | 0.017 (2) | 0.011 (2) | 0.014 (2) | 0.0019 (18) | 0.0085 (19) | 0.0035 (17) |
| C10 | 0.016 (2) | 0.012 (2) | 0.014 (2) | -0.0029 (18) | 0.0085 (19) | -0.0013 (17) |
| C2 | 0.035 (3) | 0.011 (2) | 0.014 (2) | 0.000 (2) | 0.017 (2) | 0.0016 (18) |
| C16 | 0.014 (2) | 0.014 (2) | 0.018 (2) | -0.0009 (18) | 0.0069 (19) | -0.0024 (18) |
| C3 | 0.021 (2) | 0.014 (2) | 0.009 (2) | -0.0057 (19) | 0.0044 (19) | -0.0007 (18) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|-------------|-------------|---------------|-----------|
| Pt1—C5 | 2.028 (4) | C21—C20 | 1.538 (6) |
| Pt1—C12 | 2.028 (4) | C21—H21A | 0.9700 |
| Pt1—C15 | 2.256 (4) | C21—H21B | 0.9700 |
| Pt1—C19 | 2.257 (4) | C20—H20A | 0.9700 |
| Pt1—C18 | 2.258 (4) | C20—H20B | 0.9700 |
| Pt1—C22 | 2.279 (4) | C6—C7 | 1.399 (6) |
| C5—C4 | 1.394 (6) | C6—H6A | 0.9300 |
| C5—C6 | 1.409 (6) | C7—C2 | 1.392 (7) |
| C12—C13 | 1.399 (6) | C7—H7A | 0.9300 |
| C12—C11 | 1.405 (6) | C1—C2 | 1.514 (7) |
| C15—C22 | 1.369 (7) | C1—H1A | 0.9600 |
| C15—C16 | 1.511 (6) | C1—H1B | 0.9600 |
| C15—H15A | 0.9800 | C1—H1C | 0.9600 |
| C19—C18 | 1.383 (6) | C13—C14 | 1.376 (6) |
| C19—C20 | 1.500 (6) | C13—H13A | 0.9300 |
| C19—H19A | 0.9800 | C17—C16 | 1.535 (6) |
| C18—C17 | 1.517 (6) | C17—H17A | 0.9700 |
| C18—H18A | 0.9800 | C17—H17B | 0.9700 |
| C9—C10 | 1.387 (6) | C14—H14A | 0.9300 |
| C9—C14 | 1.393 (7) | C22—H22A | 0.9800 |
| C9—C8 | 1.504 (6) | C4—C3 | 1.393 (6) |
| C11—C10 | 1.390 (6) | C4—H4A | 0.9300 |
| C11—H11A | 0.9300 | C10—H10A | 0.9300 |
| C8—H8A | 0.9600 | C2—C3 | 1.389 (7) |
| C8—H8B | 0.9600 | C16—H16A | 0.9700 |
| C8—H8C | 0.9600 | C16—H16B | 0.9700 |
| C21—C22 | 1.521 (6) | C3—H3A | 0.9300 |
| | | | |
| C5—Pt1—C12 | 88.54 (18) | H21A—C21—H21B | 107.7 |
| C5—Pt1—C15 | 90.66 (17) | C19—C20—C21 | 114.9 (4) |
| C12—Pt1—C15 | 160.11 (17) | C19—C20—H20A | 108.5 |
| C5—Pt1—C19 | 163.18 (18) | C21—C20—H20A | 108.5 |
| C12—Pt1—C19 | 91.14 (17) | C19—C20—H20B | 108.5 |
| C15—Pt1—C19 | 95.26 (16) | C21—C20—H20B | 108.5 |
| C5—Pt1—C18 | 161.08 (18) | H20A—C20—H20B | 107.5 |
| C12—Pt1—C18 | 93.84 (17) | C7—C6—C5 | 122.0 (4) |
| C15—Pt1—C18 | 80.76 (16) | C7—C6—H6A | 119.0 |
| C19—Pt1—C18 | 35.68 (16) | C5—C6—H6A | 119.0 |
| C5—Pt1—C22 | 96.28 (17) | C2—C7—C6 | 121.1 (4) |

| | | | |
|---------------|-------------|-----------------|------------|
| C12—Pt1—C22 | 164.40 (17) | C2—C7—H7A | 119.4 |
| C15—Pt1—C22 | 35.13 (16) | C6—C7—H7A | 119.4 |
| C19—Pt1—C22 | 79.97 (16) | C2—C1—H1A | 109.5 |
| C18—Pt1—C22 | 86.41 (16) | C2—C1—H1B | 109.5 |
| C4—C5—C6 | 116.0 (4) | H1A—C1—H1B | 109.5 |
| C4—C5—Pt1 | 123.3 (3) | C2—C1—H1C | 109.5 |
| C6—C5—Pt1 | 120.6 (3) | H1A—C1—H1C | 109.5 |
| C13—C12—C11 | 115.5 (4) | H1B—C1—H1C | 109.5 |
| C13—C12—Pt1 | 120.2 (3) | C14—C13—C12 | 122.4 (4) |
| C11—C12—Pt1 | 124.1 (3) | C14—C13—H13A | 118.8 |
| C22—C15—C16 | 126.5 (4) | C12—C13—H13A | 118.8 |
| C22—C15—Pt1 | 73.4 (3) | C18—C17—C16 | 114.5 (4) |
| C16—C15—Pt1 | 105.5 (3) | C18—C17—H17A | 108.6 |
| C22—C15—H15A | 114.2 | C16—C17—H17A | 108.6 |
| C16—C15—H15A | 114.2 | C18—C17—H17B | 108.6 |
| Pt1—C15—H15A | 114.2 | C16—C17—H17B | 108.6 |
| C18—C19—C20 | 126.7 (4) | H17A—C17—H17B | 107.6 |
| C18—C19—Pt1 | 72.2 (2) | C13—C14—C9 | 121.7 (4) |
| C20—C19—Pt1 | 106.5 (3) | C13—C14—H14A | 119.2 |
| C18—C19—H19A | 114.2 | C9—C14—H14A | 119.2 |
| C20—C19—H19A | 114.2 | C15—C22—C21 | 125.7 (4) |
| Pt1—C19—H19A | 114.2 | C15—C22—Pt1 | 71.5 (3) |
| C19—C18—C17 | 124.9 (4) | C21—C22—Pt1 | 110.6 (3) |
| C19—C18—Pt1 | 72.1 (2) | C15—C22—H22A | 113.7 |
| C17—C18—Pt1 | 109.8 (3) | C21—C22—H22A | 113.7 |
| C19—C18—H18A | 114.1 | Pt1—C22—H22A | 113.7 |
| C17—C18—H18A | 114.1 | C3—C4—C5 | 121.8 (4) |
| Pt1—C18—H18A | 114.1 | C3—C4—H4A | 119.1 |
| C10—C9—C14 | 117.0 (4) | C5—C4—H4A | 119.1 |
| C10—C9—C8 | 122.3 (4) | C9—C10—C11 | 121.4 (4) |
| C14—C9—C8 | 120.7 (4) | C9—C10—H10A | 119.3 |
| C10—C11—C12 | 122.0 (4) | C11—C10—H10A | 119.3 |
| C10—C11—H11A | 119.0 | C3—C2—C7 | 117.1 (4) |
| C12—C11—H11A | 119.0 | C3—C2—C1 | 122.9 (5) |
| C9—C8—H8A | 109.5 | C7—C2—C1 | 120.0 (5) |
| C9—C8—H8B | 109.5 | C15—C16—C17 | 114.0 (4) |
| H8A—C8—H8B | 109.5 | C15—C16—H16A | 108.7 |
| C9—C8—H8C | 109.5 | C17—C16—H16A | 108.7 |
| H8A—C8—H8C | 109.5 | C15—C16—H16B | 108.7 |
| H8B—C8—H8C | 109.5 | C17—C16—H16B | 108.7 |
| C22—C21—C20 | 113.4 (4) | H16A—C16—H16B | 107.6 |
| C22—C21—H21A | 108.9 | C2—C3—C4 | 122.1 (4) |
| C20—C21—H21A | 108.9 | C2—C3—H3A | 119.0 |
| C22—C21—H21B | 108.9 | C4—C3—H3A | 119.0 |
| C20—C21—H21B | 108.9 | | |
| C12—Pt1—C5—C4 | -100.7 (4) | C12—Pt1—C18—C17 | -151.9 (3) |
| C15—Pt1—C5—C4 | 99.1 (4) | C15—Pt1—C18—C17 | 8.8 (3) |

| | | | |
|-----------------|------------|-----------------|------------|
| C19—Pt1—C5—C4 | -11.6 (8) | C19—Pt1—C18—C17 | 121.5 (4) |
| C18—Pt1—C5—C4 | 161.7 (4) | C22—Pt1—C18—C17 | 43.7 (3) |
| C22—Pt1—C5—C4 | 64.4 (4) | C13—C12—C11—C10 | -0.6 (6) |
| C12—Pt1—C5—C6 | 83.4 (4) | Pt1—C12—C11—C10 | 174.2 (3) |
| C15—Pt1—C5—C6 | -76.7 (4) | C18—C19—C20—C21 | -37.3 (6) |
| C19—Pt1—C5—C6 | 172.5 (4) | Pt1—C19—C20—C21 | 42.5 (4) |
| C18—Pt1—C5—C6 | -14.2 (7) | C22—C21—C20—C19 | -38.0 (5) |
| C22—Pt1—C5—C6 | -111.5 (4) | C4—C5—C6—C7 | 0.7 (6) |
| C5—Pt1—C12—C13 | -89.5 (4) | Pt1—C5—C6—C7 | 176.9 (3) |
| C15—Pt1—C12—C13 | -1.6 (7) | C5—C6—C7—C2 | 0.1 (7) |
| C19—Pt1—C12—C13 | 107.3 (4) | C11—C12—C13—C14 | 0.7 (6) |
| C18—Pt1—C12—C13 | 71.7 (4) | Pt1—C12—C13—C14 | -174.3 (3) |
| C22—Pt1—C12—C13 | 162.1 (5) | C19—C18—C17—C16 | 93.6 (5) |
| C5—Pt1—C12—C11 | 95.9 (4) | Pt1—C18—C17—C16 | 12.0 (5) |
| C15—Pt1—C12—C11 | -176.2 (4) | C12—C13—C14—C9 | -0.9 (7) |
| C19—Pt1—C12—C11 | -67.3 (4) | C10—C9—C14—C13 | 0.8 (6) |
| C18—Pt1—C12—C11 | -102.9 (4) | C8—C9—C14—C13 | -178.7 (4) |
| C22—Pt1—C12—C11 | -12.5 (8) | C16—C15—C22—C21 | -5.3 (7) |
| C5—Pt1—C15—C22 | -100.0 (3) | Pt1—C15—C22—C21 | -102.5 (4) |
| C12—Pt1—C15—C22 | 172.5 (4) | C16—C15—C22—Pt1 | 97.2 (4) |
| C19—Pt1—C15—C22 | 64.2 (3) | C20—C21—C22—C15 | 94.0 (5) |
| C18—Pt1—C15—C22 | 96.9 (3) | C20—C21—C22—Pt1 | 12.4 (5) |
| C5—Pt1—C15—C16 | 135.8 (3) | C5—Pt1—C22—C15 | 82.2 (3) |
| C12—Pt1—C15—C16 | 48.3 (6) | C12—Pt1—C22—C15 | -170.5 (5) |
| C19—Pt1—C15—C16 | -60.0 (3) | C19—Pt1—C22—C15 | -114.4 (3) |
| C18—Pt1—C15—C16 | -27.3 (3) | C18—Pt1—C22—C15 | -79.0 (3) |
| C22—Pt1—C15—C16 | -124.2 (4) | C5—Pt1—C22—C21 | -155.7 (3) |
| C5—Pt1—C19—C18 | 176.3 (5) | C12—Pt1—C22—C21 | -48.4 (7) |
| C12—Pt1—C19—C18 | -95.0 (3) | C15—Pt1—C22—C21 | 122.1 (4) |
| C15—Pt1—C19—C18 | 66.1 (3) | C19—Pt1—C22—C21 | 7.7 (3) |
| C22—Pt1—C19—C18 | 97.9 (3) | C18—Pt1—C22—C21 | 43.1 (3) |
| C5—Pt1—C19—C20 | 52.3 (7) | C6—C5—C4—C3 | -1.6 (6) |
| C12—Pt1—C19—C20 | 141.0 (3) | Pt1—C5—C4—C3 | -177.6 (3) |
| C15—Pt1—C19—C20 | -57.9 (3) | C14—C9—C10—C11 | -0.7 (6) |
| C18—Pt1—C19—C20 | -124.0 (4) | C8—C9—C10—C11 | 178.9 (4) |
| C22—Pt1—C19—C20 | -26.1 (3) | C12—C11—C10—C9 | 0.6 (7) |
| C20—C19—C18—C17 | -4.5 (7) | C6—C7—C2—C3 | -0.1 (6) |
| Pt1—C19—C18—C17 | -102.1 (4) | C6—C7—C2—C1 | 179.4 (4) |
| C20—C19—C18—Pt1 | 97.6 (4) | C22—C15—C16—C17 | -37.5 (6) |
| C5—Pt1—C18—C19 | -176.7 (4) | Pt1—C15—C16—C17 | 43.0 (4) |
| C12—Pt1—C18—C19 | 86.6 (3) | C18—C17—C16—C15 | -38.4 (5) |
| C15—Pt1—C18—C19 | -112.7 (3) | C7—C2—C3—C4 | -0.8 (7) |
| C22—Pt1—C18—C19 | -77.8 (3) | C1—C2—C3—C4 | 179.7 (4) |
| C5—Pt1—C18—C17 | -55.2 (6) | C5—C4—C3—C2 | 1.7 (7) |

Hydrogen-bond geometry (Å, °)

Cg1 and Cg2 are the centroids of the C9–C14 and C2–C7 rings, respectively.

| <i>D</i> —H··· <i>A</i> | <i>D</i> —H | H··· <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> —H··· <i>A</i> |
|---------------------------------------|-------------|---------------|-----------------------|-------------------------|
| C1—H1 <i>B</i> ···Cg1 ⁱ | 0.96 | 2.93 | 3.615 (4) | 129 |
| C20—H20 <i>B</i> ···Cg1 ⁱⁱ | 0.96 | 2.85 | 3.749 (5) | 155 |
| C21—H21 <i>A</i> ···Cg2 ⁱⁱ | 0.97 | 2.83 | 3.411 (4) | 119 |
| C8—H8 <i>C</i> ···Cg2 ⁱⁱⁱ | 0.96 | 2.85 | 3.509 (2) | 126 |

Symmetry codes: (i) $x, -y+2, z+1/2$; (ii) $x, y-1, z$; (iii) $x, -y+2, z-1/2$.