

(Acetylacetonato- κ^2O,O')[1-(4-bromophenyl- κC^2)-3-methylimidazol-2-ylidene- κC^2]platinum(II)

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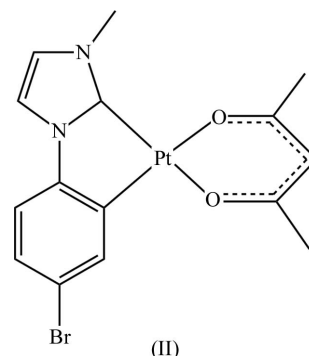
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The title platinum(II) complex, $[\text{Pt}(\text{C}_{10}\text{H}_8\text{BrN}_2)(\text{C}_5\text{H}_7\text{O}_2)]$, has a bidentate cyclometallated phenylimidazolylidene ligand and an acetylacetonate spectator ligand, which form a distorted square-planar coordination environment around the Pt^{II} centre. In the solid state, the molecules are oriented in a parallel fashion by intermolecular hydrogen bonding and π - π and $\text{C}-\text{H}\cdots\pi$ interactions, while close $\text{Pt}\cdots\text{Pt}$ contacts are not observed. The structure is only the second example for this new class of compounds.

Comment

Organic light-emitting diodes (OLEDs) currently attract attention as one of the promising technologies for a new generation of flat-panel displays or innovative lighting concepts. The photophysical properties of late transition metal complexes, especially of phosphorescent iridium and platinum compounds, have been intensively investigated and their exceptional luminescence properties allow for their use as emitters in light-emitting diodes (Chi & Chou, 2010; Kalinowski *et al.*, 2011; Rausch *et al.*, 2010; Williams, 2007; Williams *et al.*, 2008; Xiang *et al.*, 2008; Yersin, 2008). We recently reported a new class of platinum(II) compounds with cyclometallated N-heterocyclic carbene (NHC) ligands which are strongly emissive in the green-blue region of the spectrum (Unger *et al.*, 2010). Their properties differ from the previously known $\text{C}^{\wedge}\text{N}$ cyclometallating ligands derived from, for example, 2-phenylpyridine (ppy) (Chassot *et al.*, 1984) or from phenylazoles like phenylpyrazole or 2-phenylimidazole. The new class of $\text{Pt}(\text{C}^{\wedge}\text{C}^*)$ compounds opens up a new field of photophysically interesting compounds (BASF, 2006, 2007; Petretto *et al.*, 2010; Unger *et al.*, 2010). Only one solid-state structure of this new class of compounds is known, *viz.* (acetylacetonato- κ^2O,O')[1-(dibenzofuranyl- κC^2)-3-methylimidazol-2-ylidene- κC^2]platinum(II), (I) (Unger *et al.*, 2010). We report here and discuss a second solid-state structure, the title complex, (II). The synthesis of these platinum(II)-acetyl-

acetonate complexes starts with the reaction of the corresponding imidazolium salt with Ag_2O and $\text{Pt}(\text{COD})\text{Cl}_2$ (COD is cyclooctadiene), followed by addition of acetylacetonate and base. Details of the synthesis and the corresponding spectroscopic data have been published elsewhere (Unger *et al.*, 2010).



Single-crystal X-ray diffraction reveals that complex (II) crystallizes in the monoclinic space group $P2_1/c$. The asymmetric unit contains one complex molecule and is devoid of solvent molecules. Complex (II) (Fig. 1) consists of two bidentate ligands coordinating to a Pt^{II} cation. The phenylimidazolium-based NHC ligand is cyclometallated to the metal *via* carbene atom C1 and phenyl atom C6. The remaining two coordination sites are occupied by atoms O1 and O2 of the acetylacetonate anion. The planarity of the whole molecule is demonstrated by the torsion angles $\text{C12}-\text{O2}-\text{Pt1}-\text{C1} = 178.6(3)^\circ$, $\text{O1}-\text{Pt1}-\text{C6}-\text{C7} = -1.7(4)^\circ$ and $\text{C6}\cdots\text{C1}\cdots\text{O2}\cdots\text{O1} = -2.81(15)^\circ$. The dihedral angle between the benzene and imidazole rings ($\text{C6}-\text{C5}-\text{N1}-\text{C1}$) is also very close to planarity [$0.7(5)^\circ$]. The metal centre

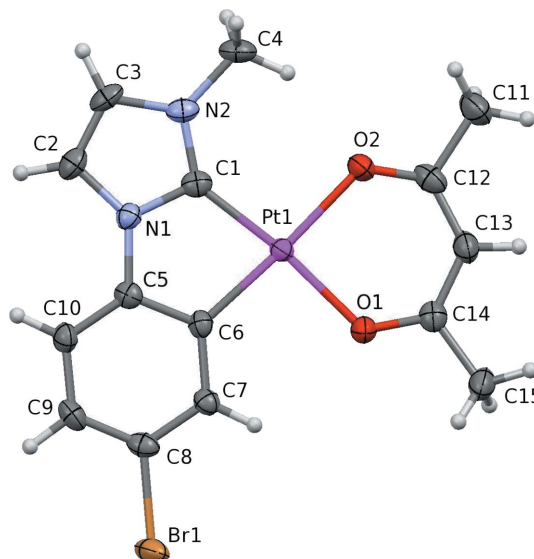


Figure 1
The solid-state structure of (II), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

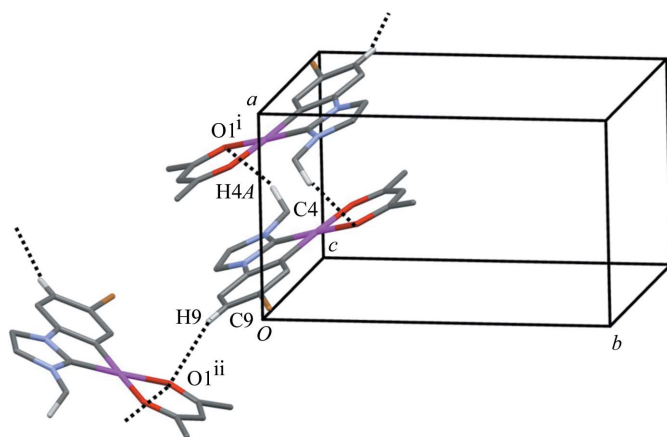


Figure 2
A packing diagram for (II), showing the intermolecular hydrogen bonds (dashed lines). [Symmetry codes: (i) $-x + 1, -y, -z + 1$; (ii) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$]

shows a quasi-square-planar coordination environment, since although the sum of all the central angles is 360° , deviations from orthogonality can be found. The small C1–Pt1–C6 angle of $79.96(16)^\circ$ leads to larger O2–Pt1–C1 and O1–Pt1–C6 angles between the two ligands, while the O1–Pt1–O2 angle is preserved, similar to the corresponding angles in (I) (Unger *et al.*, 2010). A comparison of bond lengths and angles in (I) and (II) is given in Table 1. The central bond lengths of both complexes are similar, with the exception of the Pt1–C6 bond length for the extended π -system (the dibenzofuranyl group), which is slightly shorter in (I) than in (II). The Pt1–C1 distance of (II) is in the range of platinum–carbene bonds known from other platinum NHC complexes (Meyer *et al.*, 2011; Sun *et al.*, 2011; O *et al.*, 2010).

In the crystal packing of (II) (Fig. 2), several interactions can be found between neighbouring molecules. Due to their planarity, the complexes are arranged in parallel stacks. Two molecules of each stack form dimers, which are characterized by small intermolecular distances of about 3.4 \AA . The complexes in the dimeric unit show an antiparallel arrangement because of the steric repulsion of the methyl groups. NHC groups are located next to acetylacetonate anions and show weak C4–H4A \cdots O1ⁱ hydrogen bonds [symmetry code: (i) $-x + 1, -y, -z + 1$], as well as π – π attractions. Due to the fact that the molecules are shifted in-plane with regard to the Pt^{II} centres, metallophilic Pt \cdots Pt contacts are not observed. The Pt \cdots Pt distance is $3.7105(7) \text{ \AA}$ and therefore exceeds the criterion of twice the van der Waals radius of 3.6 \AA (Bondi, 1964). Between the stacks, the complex dimers are linked by hydrogen bonds and C–H \cdots π interactions, with a distance of about 3.5 \AA between them. A weak C9–H9 \cdots O1ⁱⁱ hydrogen bond [symmetry code: (ii) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$] is observed connecting a benzene ring with an acetylacetonate ligand of a neighbouring stack. Additionally, the benzene ring participates in a C–H \cdots π interaction with the NHC fragment. A C–H \cdots π attractive interaction is found for C3–H3 \cdots C9(x, $-y - \frac{1}{2}, z + \frac{1}{2}$), with a H \cdots C distance of 2.74 \AA and an angle of 158° .

Experimental

The title compound was synthesized according to a previously reported literature procedure (Unger *et al.*, 2010). Colourless single crystals of (II) suitable for X-ray diffraction were grown within one week by slow evaporation from a solution of (II) in dichloromethane.

Crystal data

[Pt(C ₁₀ H ₈ BrN ₂)(C ₅ H ₇ O ₂)]	$V = 1507.8(4) \text{ \AA}^3$
$M_r = 530.29$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 7.5000(6) \text{ \AA}$	$\mu = 11.96 \text{ mm}^{-1}$
$b = 12.144(2) \text{ \AA}$	$T = 198 \text{ K}$
$c = 16.844(3) \text{ \AA}$	$0.76 \times 0.15 \times 0.13 \text{ mm}$
$\beta = 100.625(8)^\circ$	

Data collection

Nonius KappaCCD area-detector diffractometer	18494 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	2697 independent reflections
$T_{\min} = 0.039, T_{\max} = 0.301$	2263 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.019$	193 parameters
$wR(F^2) = 0.035$	H-atom parameters constrained
$S = 1.12$	$\Delta\rho_{\text{max}} = 0.55 \text{ e \AA}^{-3}$
2697 reflections	$\Delta\rho_{\text{min}} = -0.80 \text{ e \AA}^{-3}$

All H atoms were constrained to an ideal geometry using the standard riding model implemented in *SHELXL97* (Sheldrick, 2008). The H atoms were fixed, with C–H = 0.98 (methyl) or 0.95 \AA (aromatic) and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ (methyl) or $1.2U_{\text{eq}}(\text{C})$ (aromatic).

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: direct methods using *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

Table 1

Comparison of central bond lengths (\AA) and angles ($^\circ$) of (I) and (II).

	(I) ^a	(II) ^b
Pt1–C1	1.937 (8)	1.939 (4)
Pt1–C6	1.960 (6)	1.984 (4)
Pt1–O1	2.055 (6)	2.058 (3)
Pt1–O2	2.089 (6)	2.073 (3)
C1–Pt1–C6	80.5 (3)	79.96 (16)
O1–Pt1–O2	90.0 (2)	90.04 (10)
O1–Pt1–C6	91.4 (3)	93.40 (13)
O2–Pt1–C1	98.0 (3)	96.63 (14)

References: (a) Unger *et al.* (2010); (b) this work.

Table 2

Short-contact geometry ($\text{\AA}, ^\circ$) of (II).

$D\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
C4–H4A \cdots O1 ⁱ	0.98	2.71	3.394 (5)	127
C9–H9 \cdots O1 ⁱⁱ	0.95	2.64	3.540 (5)	158

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

Supplementary data for this paper are available from the IUCr electronic archives (Reference: EG3094). Services for accessing these data are described at the back of the journal.

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supplementary materials

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Crystal data

[Pt(C₁₀H₈BrN₂)(C₅H₇O₂)]

$M_r = 530.29$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.5000$ (6) Å

$b = 12.144$ (2) Å

$c = 16.844$ (3) Å

$\beta = 100.625$ (8)°

$V = 1507.8$ (4) Å³

$Z = 4$

$F(000) = 992$

$D_x = 2.336$ Mg m⁻³

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

Cell parameters from 960 reflections

$\theta = 4.1$ – 26.7 °

$\mu = 11.96$ mm⁻¹

$T = 198$ K

Fragment, colourless

$0.76 \times 0.15 \times 0.13$ mm

Data collection

Nonius KappaCCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 9 pixels mm⁻¹

φ scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 2003)

$T_{\min} = 0.039$, $T_{\max} = 0.301$

18494 measured reflections

2697 independent reflections

2263 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\max} = 25.4$ °, $\theta_{\min} = 3.2$ °

$h = -9 \rightarrow 7$

$k = -14 \rightarrow 14$

$l = -19 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.019$

$wR(F^2) = 0.035$

$S = 1.12$

2697 reflections

193 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

$w = 1/[\sigma^2(F_o^2) + (0.0101P)^2 + 2.5298P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.55$ e Å⁻³

$\Delta\rho_{\min} = -0.80$ e Å⁻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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Pt1	0.28982 (2)	0.077675 (12)	0.459620 (9)	0.01988 (5)
Br1	0.02024 (7)	-0.00071 (4)	0.11275 (2)	0.03870 (12)
O1	0.3538 (4)	0.2076 (2)	0.39165 (15)	0.0253 (6)
O2	0.3928 (4)	0.1634 (2)	0.56449 (15)	0.0283 (6)
N1	0.1295 (4)	-0.1326 (3)	0.46299 (19)	0.0231 (7)
N2	0.2333 (4)	-0.0939 (3)	0.58727 (19)	0.0264 (8)
C1	0.2201 (5)	-0.0536 (3)	0.5118 (2)	0.0243 (9)
C2	0.0851 (6)	-0.2210 (3)	0.5074 (3)	0.0300 (10)
C3	0.1511 (6)	-0.1967 (3)	0.5846 (3)	0.0308 (10)
C4	0.3239 (6)	-0.0412 (4)	0.6614 (2)	0.0334 (11)
C5	0.0999 (5)	-0.1098 (3)	0.3795 (2)	0.0218 (9)
C6	0.1742 (5)	-0.0079 (3)	0.3635 (2)	0.0217 (9)
C7	0.1506 (5)	0.0229 (3)	0.2822 (2)	0.0235 (9)
C8	0.0575 (5)	-0.0461 (3)	0.2236 (2)	0.0261 (9)
C9	-0.0138 (5)	-0.1462 (3)	0.2407 (2)	0.0273 (10)
C10	0.0084 (5)	-0.1792 (3)	0.3211 (2)	0.0263 (9)
C11	0.5281 (7)	0.3013 (4)	0.6514 (3)	0.0451 (12)
C12	0.4633 (6)	0.2579 (4)	0.5674 (2)	0.0323 (10)
C13	0.4846 (6)	0.3225 (4)	0.5017 (3)	0.0329 (10)
C14	0.4336 (5)	0.2957 (3)	0.4204 (2)	0.0262 (9)
C15	0.4736 (6)	0.3762 (4)	0.3583 (3)	0.0362 (11)
H2	0.0209	-0.2856	0.4872	0.036*
H3	0.1432	-0.2420	0.6298	0.037*
H4A	0.4290	-0.0854	0.6860	0.050*
H4B	0.2392	-0.0352	0.6991	0.050*
H4C	0.3643	0.0325	0.6491	0.050*
H7	0.1983	0.0907	0.2674	0.028*
H9	-0.0764	-0.1915	0.1986	0.033*
H10	-0.0383	-0.2477	0.3353	0.032*
H11A	0.4253	0.3322	0.6723	0.068*
H11B	0.6192	0.3588	0.6500	0.068*
H11C	0.5821	0.2411	0.6866	0.068*
H13	0.5398	0.3925	0.5135	0.039*
H15A	0.4958	0.3361	0.3106	0.054*
H15B	0.5815	0.4194	0.3810	0.054*
H15C	0.3699	0.4257	0.3428	0.054*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.02087 (9)	0.02025 (8)	0.01800 (8)	0.00008 (7)	0.00222 (5)	-0.00083 (7)
Br1	0.0582 (3)	0.0340 (3)	0.0208 (2)	0.0048 (2)	-0.00066 (19)	-0.00153 (19)
O1	0.0286 (16)	0.0241 (15)	0.0224 (14)	-0.0034 (13)	0.0028 (11)	0.0003 (12)
O2	0.0343 (17)	0.0264 (16)	0.0230 (15)	-0.0028 (14)	0.0019 (12)	-0.0038 (12)
N1	0.0246 (19)	0.0197 (17)	0.0253 (18)	0.0001 (15)	0.0053 (14)	0.0016 (15)
N2	0.0263 (19)	0.031 (2)	0.0218 (18)	0.0050 (16)	0.0056 (14)	0.0052 (15)
C1	0.019 (2)	0.030 (2)	0.024 (2)	0.0067 (17)	0.0045 (16)	0.0027 (17)
C2	0.033 (3)	0.022 (2)	0.037 (3)	0.0010 (19)	0.0115 (19)	0.0071 (19)
C3	0.036 (3)	0.026 (2)	0.033 (2)	0.005 (2)	0.0127 (19)	0.0140 (19)
C4	0.038 (3)	0.043 (3)	0.018 (2)	0.007 (2)	0.0026 (18)	0.0044 (19)
C5	0.021 (2)	0.022 (2)	0.023 (2)	0.0053 (16)	0.0048 (16)	-0.0014 (16)
C6	0.020 (2)	0.019 (2)	0.025 (2)	0.0017 (17)	0.0032 (16)	-0.0020 (17)
C7	0.022 (2)	0.025 (2)	0.023 (2)	0.0018 (18)	0.0021 (17)	-0.0015 (17)
C8	0.026 (2)	0.032 (2)	0.019 (2)	0.0087 (18)	0.0005 (17)	-0.0010 (17)
C9	0.027 (2)	0.026 (2)	0.027 (2)	-0.0012 (19)	0.0004 (18)	-0.0069 (19)
C10	0.028 (2)	0.021 (2)	0.031 (2)	-0.0024 (18)	0.0062 (18)	-0.0031 (18)
C11	0.058 (3)	0.042 (3)	0.032 (3)	-0.007 (3)	-0.001 (2)	-0.010 (2)
C12	0.033 (3)	0.035 (3)	0.027 (2)	0.009 (2)	-0.0003 (18)	-0.009 (2)
C13	0.037 (3)	0.025 (2)	0.034 (2)	-0.008 (2)	0.0001 (19)	-0.0027 (19)
C14	0.020 (2)	0.024 (2)	0.033 (2)	0.0020 (18)	0.0027 (17)	0.0006 (18)
C15	0.038 (3)	0.029 (2)	0.039 (3)	-0.009 (2)	0.001 (2)	0.006 (2)

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

Pt1—O1	2.058 (3)	C6—C5	1.404 (5)
Pt1—O2	2.073 (3)	C6—C7	1.398 (5)
Pt1—C1	1.939 (4)	C7—H7	0.9500
Pt1—C6	1.984 (4)	C8—C7	1.381 (5)
Br1—C8	1.918 (4)	C8—C9	1.380 (6)
O1—C14	1.276 (5)	C9—H9	0.9500
O2—C12	1.261 (5)	C10—C9	1.393 (5)
N1—C1	1.361 (5)	C10—H10	0.9500
N1—C2	1.384 (5)	C11—H11A	0.9800
N1—C5	1.410 (5)	C11—H11B	0.9800
N2—C1	1.348 (5)	C11—H11C	0.9800
N2—C3	1.390 (5)	C12—C11	1.504 (6)
N2—C4	1.455 (5)	C12—C13	1.390 (6)
C2—C3	1.335 (6)	C13—H13	0.9500
C2—H2	0.9500	C14—C13	1.391 (6)
C3—H3	0.9500	C14—C15	1.502 (6)
C4—H4A	0.9800	C15—H15A	0.9800
C4—H4B	0.9800	C15—H15B	0.9800
C4—H4C	0.9800	C15—H15C	0.9800
C5—C10	1.378 (5)		
O1—Pt1—O2	90.04 (10)	C6—C5—N1	111.7 (3)
C1—Pt1—O1	173.32 (13)	C6—C7—H7	120.2

C1—Pt1—O2	96.63 (14)	C7—C6—C5	116.1 (3)
C1—Pt1—C6	79.96 (16)	C7—C8—Br1	119.1 (3)
C6—Pt1—O1	93.40 (13)	C8—C7—C6	119.6 (4)
C6—Pt1—O2	175.27 (13)	C8—C7—H7	120.2
N1—C1—Pt1	116.8 (3)	C8—C9—C10	118.3 (4)
N2—C1—Pt1	138.3 (3)	C8—C9—H9	120.8
C5—C6—Pt1	115.7 (3)	C9—C8—Br1	117.6 (3)
C7—C6—Pt1	128.1 (3)	C9—C8—C7	123.3 (4)
C12—O2—Pt1	125.3 (3)	C9—C10—H10	120.9
C14—O1—Pt1	125.0 (2)	C10—C5—C6	124.4 (4)
O1—C14—C13	126.4 (4)	C10—C5—N1	124.0 (4)
O1—C14—C15	115.0 (4)	C10—C9—H9	120.8
O2—C12—C11	114.6 (4)	C12—C11—H11A	109.5
O2—C12—C13	126.3 (4)	C12—C11—H11B	109.5
N1—C2—H2	127.1	C12—C11—H11C	109.5
N2—C1—N1	104.8 (3)	C12—C13—C14	126.9 (4)
N2—C3—H3	125.9	C12—C13—H13	116.5
N2—C4—H4A	109.5	C13—C12—C11	119.1 (4)
N2—C4—H4B	109.5	C13—C14—C15	118.6 (4)
N2—C4—H4C	109.5	C14—C13—H13	116.5
C1—N1—C2	111.3 (3)	C14—C15—H15A	109.5
C1—N1—C5	115.7 (3)	C14—C15—H15B	109.5
C1—N2—C3	109.9 (3)	C14—C15—H15C	109.5
C1—N2—C4	126.2 (3)	H4A—C4—H4B	109.5
C2—N1—C5	133.0 (3)	H4A—C4—H4C	109.5
C2—C3—N2	108.2 (4)	H4B—C4—H4C	109.5
C2—C3—H3	125.9	H11A—C11—H11B	109.5
C3—N2—C4	123.9 (3)	H11A—C11—H11C	109.5
C3—C2—N1	105.8 (4)	H11B—C11—H11C	109.5
C3—C2—H2	127.1	H15A—C15—H15B	109.5
C5—C10—C9	118.2 (4)	H15A—C15—H15C	109.5
C5—C10—H10	120.9	H15B—C15—H15C	109.5
Pt1—O1—C14—C13	-3.0 (6)	O1—C14—C13—C12	1.9 (7)
Pt1—O1—C14—C15	177.1 (3)	O2—C12—C13—C14	-0.4 (7)
Pt1—O2—C12—C11	-179.8 (3)	N1—C2—C3—N2	0.6 (4)
Pt1—O2—C12—C13	0.4 (6)	N1—C5—C10—C9	179.1 (4)
Pt1—C6—C5—N1	-2.2 (4)	C1—N1—C2—C3	-0.7 (5)
Pt1—C6—C5—C10	177.6 (3)	C1—N2—C3—C2	-0.3 (5)
Pt1—C6—C7—C8	-176.6 (3)	C1—N1—C5—C6	0.7 (5)
O1—Pt1—O2—C12	-1.1 (3)	C1—N1—C5—C10	-179.0 (4)
O1—Pt1—C6—C5	-178.6 (3)	C2—N1—C1—N2	0.5 (4)
O1—Pt1—C6—C7	-1.7 (4)	C2—N1—C5—C10	1.2 (7)
O2—Pt1—O1—C14	2.3 (3)	C2—N1—C5—C6	-179.1 (4)
O2—Pt1—C1—N1	174.9 (3)	C3—N2—C1—N1	-0.1 (4)
O2—Pt1—C1—N2	-4.4 (4)	C4—N2—C1—N1	178.2 (3)
C1—Pt1—O2—C12	178.6 (3)	C4—N2—C3—C2	-178.7 (4)
C1—Pt1—C6—C5	2.2 (3)	C5—N1—C1—N2	-179.4 (3)
C1—Pt1—C6—C7	179.0 (4)	C5—N1—C2—C3	179.1 (4)

C6—Pt1—O1—C14	179.1 (3)	C5—C6—C7—C8	0.3 (5)
C6—Pt1—C1—N1	-1.7 (3)	C5—C10—C9—C8	0.3 (6)
C6—Pt1—C1—N2	178.9 (4)	C6—C5—C10—C9	-0.6 (6)
C2—N1—C1—Pt1	-179.1 (3)	C7—C6—C5—C10	0.3 (6)
C3—N2—C1—Pt1	179.3 (3)	C7—C6—C5—N1	-179.4 (3)
C4—N2—C1—Pt1	-2.3 (7)	C7—C8—C9—C10	0.3 (6)
C5—N1—C1—Pt1	1.1 (4)	C9—C8—C7—C6	-0.6 (6)
Br1—C8—C7—C6	178.2 (3)	C11—C12—C13—C14	179.8 (4)
Br1—C8—C9—C10	-178.5 (3)	C15—C14—C13—C12	-178.2 (4)

Hydrogen-bond geometry (Å, °)

<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>
C4—H4 <i>A</i> ...O1 ⁱ	0.98	2.71	3.394 (5)	127
C9—H9...O1 ⁱⁱ	0.95	2.64	3.540 (5)	158

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

Comparison of central bond lengths (Å) and angles (°) of [Pt(C₁₆H₁₁N₂O)(C₃H₇O₂)], (I), and [Pt(C₁₀H₈BrN₂)(C₃H₇O₂)], (II)

Bond lengths/angles	(I) ^a	(II) ^b
Pt1—C1	1.937 (8)	1.939 (4)
Pt1—C6	1.960 (6)	1.984 (4)
Pt1—O1	2.055 (6)	2.058 (3)
Pt1—O2	2.089 (6)	2.073 (3)
C1—Pt1—C6	80.5 (3)	79.96 (16)
O1—Pt1—O2	90.0 (2)	90.04 (10)
O1—Pt1—C6	91.4 (3)	93.40 (13)
O2—Pt1—C1	98.0 (3)	96.63 (14)

References: (a) Unger *et al.* (2010); (b) this work.