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Crystal structures of organoplatinum complexes containing alkyleugenoxyacetate and *p*-chloroaniline

Hai Le Thi Hong,[a] Diep Dao Thi Bich,[a] Ngan Nguyen Bich[a] and Luc Van Meervelt[b]*

[a]Chemistry Department, Hanoi National University of Education, 136 - Xuan Thuy - Cau Giay, Hanoi, Vietnam, and [b]KU Leuven - University of Leuven, Department of Chemistry, Celestijnenlaan 200F - bus 2404, B-3001 Heverlee, Belgium. *Correspondence e-mail: luc.vanmeervelt@kuleuven.be

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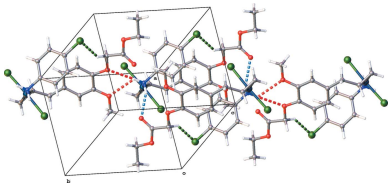
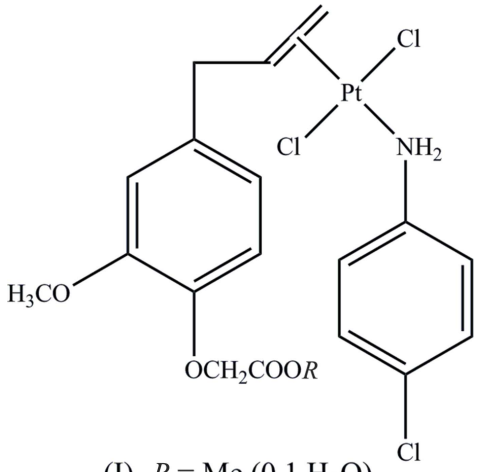
In the title complexes, *trans*-dichlorido(4-chloroaniline-κN){3-methoxy-4-methoxycarbonylmethoxy-1-[(2,3-η)-prop-2-en-1-yl]benzene}platinum(II) 0.1-hydrate, $[PtCl_2(C_6H_6ClN)(C_{13}H_{16}O_4)]\cdot 0.1H_2O$, (I), and *trans*-dichlorido(4-chloroaniline-κN){4-ethoxycarbonylmethoxy-3-methoxy-1-[(2,3-η)-prop-2-en-1-yl]benzene}platinum(II), $[PtCl_2(C_6H_6ClN)(C_{14}H_{18}O_4)]$, (II), the Pt^{II} metal atom displays a slightly distorted square-planar coordination geometry defined by the aniline N atom, two chloride anions (*trans*-positioned) and one ethylenic double bond. The least-squares planes through the two aromatic ring systems make an angle of 47.3 (3)° for (I) and 38.6 (2)° for (II). Both structures show disorder for the $PtCl_2$ fragment, in the case of (I) even further extended towards the CH_2—CH═CH_2 ligand. An intramolecular C—H···Cl hydrogen bond occurs in (I). In the crystal packing of (I), which is dominated by N—H···O and C—H···Cl interactions, a partially occupied water molecule is observed on a twofold rotation axis with a refined site occupancy of 0.10 (1). A C—H···π interaction is also present. In (II), inversion dimers form chains along the *b*-axis direction by N—H···O hydrogen bonds.

1. Chemical context

Complexes of platinum(II) such as cisplatin, carboplatin and oxaliplatin have been known to exhibit inhibitory activities on several human cancer cells and are widely used in pharmacy (Zhang *et al.*, 2006). However, many side effects and drug-resistant phenomena have been reported for the use of these complexes (Von Hoff *et al.*, 1979; Coates *et al.*, 1983; Griffin *et al.*, 1996). Therefore, it is necessary to design new complexes with high activities but low toxicity (Chabner & Roberts, 2005; Johnstone *et al.*, 2014). For this purpose, we have recently synthesized several Pt^{II} complexes containing natural aryl-olefines as ligand, *i.e.* derivatives of eugenol (4-allyl-2-methoxylphenol) such as methyleugenol and alkyleugenoxyacetate, with high toxicity towards human cancerous cells (IC_{50} values < 5 µg/mL; Da *et al.*, 2012; Da, Chi *et al.*, 2015; Da, Hai *et al.*, 2015). Interestingly, these complexes represent special arrangements in which the Pt^{II} atoms are coordinated by arylolefines through the C═C bond of the allyl group. Complexes of Pt^{II} containing methyl- or ethyleugenoxyl-acetate and *p*-chloroaniline were synthesized and their crystal and molecular structures characterized and reported here.





(I) R = Me (0.1 H_2O)
(II) R = Et

2. Structural commentary

The complexes crystallize in different space groups, $C2/c$ for the methyleugenoxyacetate derivative (I) and $P\overline{1}$ for the ethyleugenoxyacetate derivative (II). The central Pt^{II} metal atom displays a distorted square-planar coordination with the Pt^{II} atom coordinated by two Cl atoms, the NH_2-group of *p*-chloroaniline and the C=C double bond of the eugenol ligand. In both complexes, the Cl atoms are *trans* with respect to each other (Fig. 1). The eugenol ligand only interacts *via* the C=C double bond and not by a C atom of the phenyl ring. Both structures show some disorder of the Pt^{II} atom and its environment. In (I) the $PtCl_2CH_2$=$CH-CH_2$ fragment is disordered over two positions [population parameters 0.679 (8) and 0.321 (8)], while in (II) only the $PtCl_2$ fragment is disordered over two positions [population parameters 0.872 (6) and 0.128 (6)]. The angles between the best planes through the two aromatic rings are 47.3 (3) and 38.6 (2)° for (I) and (II), respectively. An intramolecular C—H···Cl interaction is observed for (II) with a H26*A*···Cl9 distance of 2.73 Å. In (I) the shortest intramolecular H···Cl contact distance is 3.13 Å for H29*A*···Cl9.

Table 1
Hydrogen-bond geometry (Å, °) for (I).

*Cg*1 is the centroid of the C20–C25 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*AA*···O26^{i}	0.91	2.45	3.027 (5)	122
N2—H2*AA*···O28^{i}	0.91	2.35	3.212 (6)	158
N2—H2*AB*···O31^{ii}	0.91	2.41	3.302 (3)	167
C16—H16*A*···Cl12	0.99	2.79	3.487 (10)	128
C16—H16*B*···Cl9^{iii}	0.99	2.76	3.472 (8)	129
C21—H21···Cl11^{iv}	0.95	2.82	3.726 (8)	159
C29—H29*B*···Cl12^{v}	0.99	2.80	3.651 (7)	145
C27—H27*B*···*Cg*1^{iv}	0.98	2.72	3.523 (6)	139

Symmetry codes: (i) $x+\frac{1}{2}, y-\frac{1}{2}, z$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x-\frac{1}{2}, y-\frac{1}{2}, z$; (iv) $-x+1, y, -z+\frac{3}{2}$; (v) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+2$.

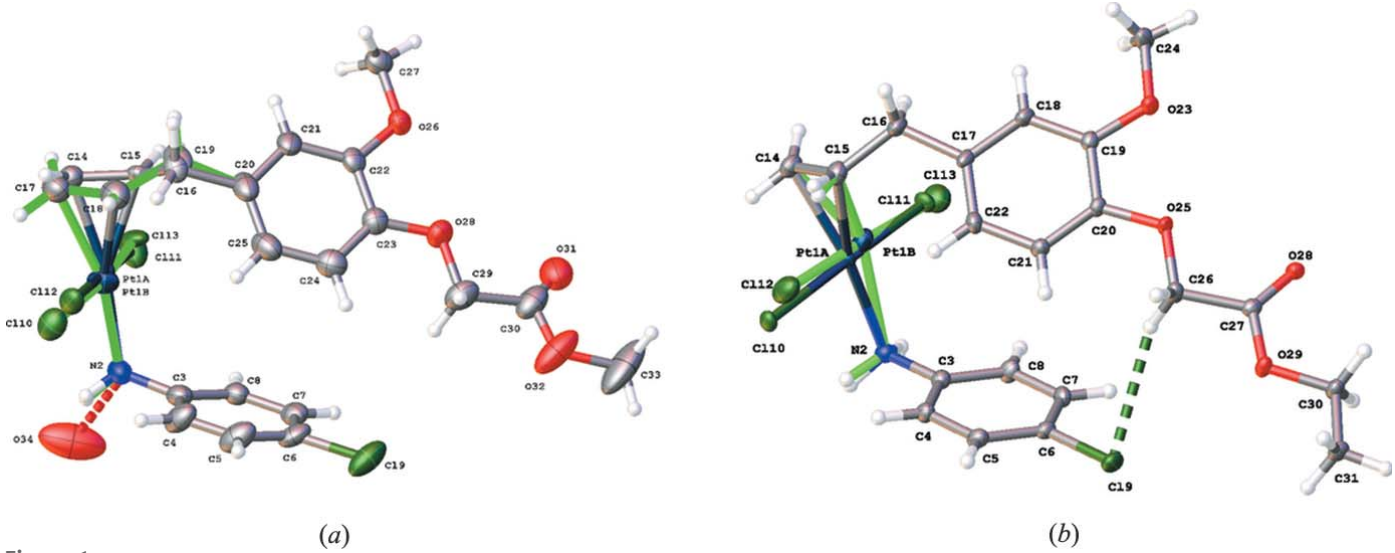
Table 2
Hydrogen-bond geometry (Å, °) for (II).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*AA*···O23^{i}	0.91	2.49	3.025 (5)	118
N2—H2*AA*···O25^{i}	0.91	2.47	3.377 (5)	174
N2—H2*AB*···O28^{ii}	0.91	2.22	3.085 (5)	158
C26—H26*A*···Cl9	0.99	2.73	3.581 (4)	144

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

3. Supramolecular features

The crystal packing of (I) is built up by N—H···O and C—H···Cl interactions (Table 1, Fig. 2). A water molecule O34 was identified at a special position [on a twofold rotation axis,



(*a*) (*b*)

Figure 1
Views of the asymmetric units in (*a*) (I) and (*b*) (II), showing the atom-labelling schemes. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular C—H···Cl interaction is shown as a green dotted line.

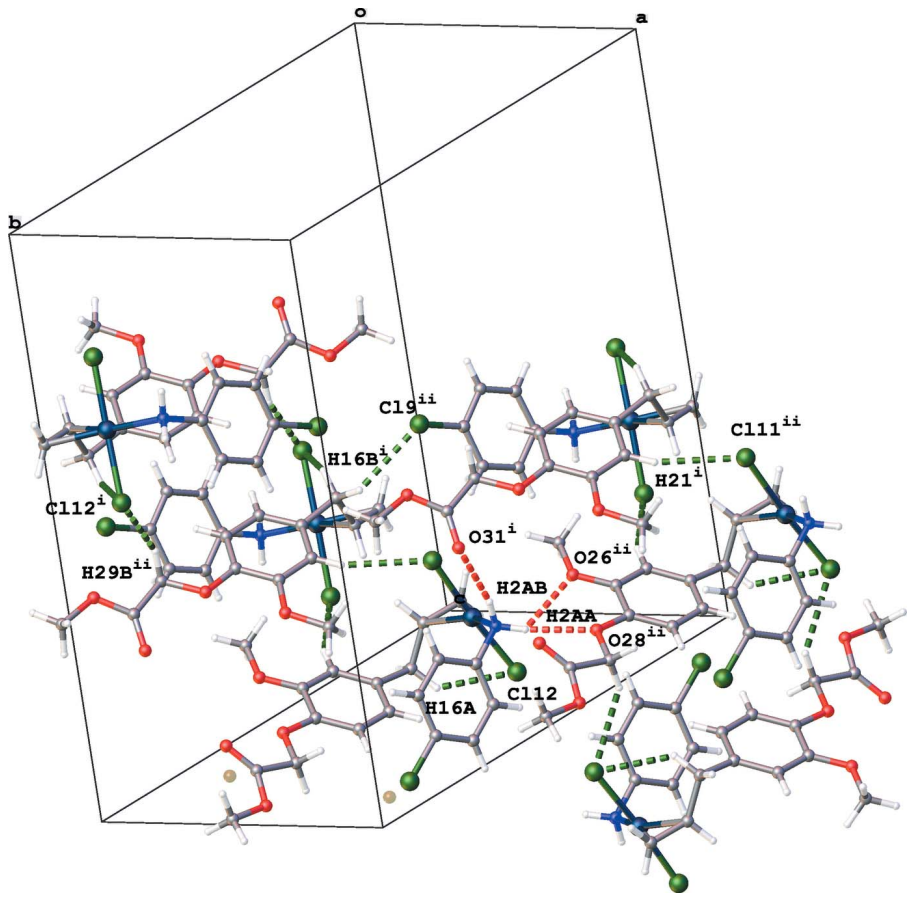


Figure 2
Partial packing diagram of (I), showing the N—H···O (red dotted lines) and C—H···Cl interactions (green dotted lines). [Symmetry codes: (i) $x+\frac{1}{2}, y-\frac{1}{2}, z$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x-\frac{1}{2}, y-\frac{1}{2}, z$; (iv) $x, -y+1, z-\frac{1}{2}$.]

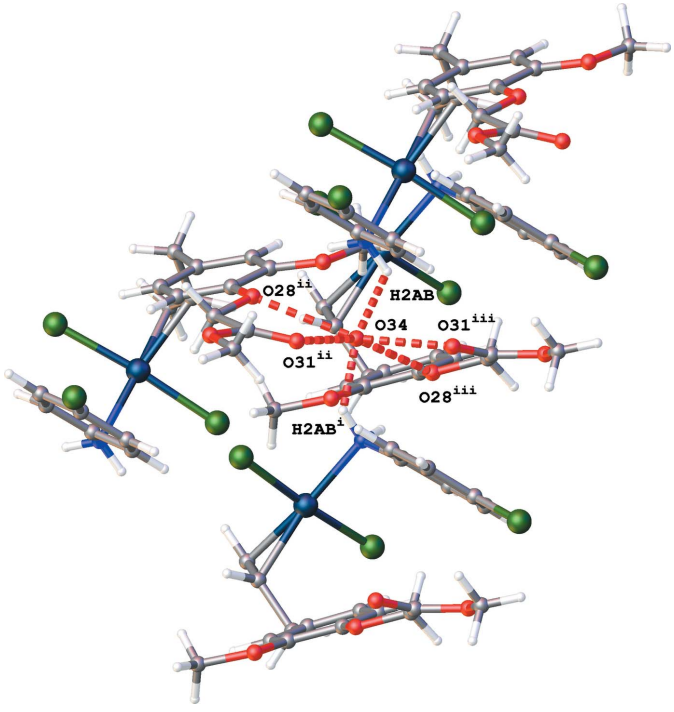


Figure 3
Partial packing diagram of (I), showing the interactions of water molecule O34 with N2, O28 and O31 (red dotted lines). [Symmetry codes: (i) $-x+2, y, -z+\frac{3}{2}$; (ii) $x+\frac{1}{2}, y-\frac{1}{2}, z$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.]

occupancy factor 0.10 (1)] where it interacts with atoms N2, O28 and O31 linking four molecules together (Fig. 3).

The crystal packing of (II) is dominated by hydrogen-bonding interactions (Table 2). Inversion dimers created by

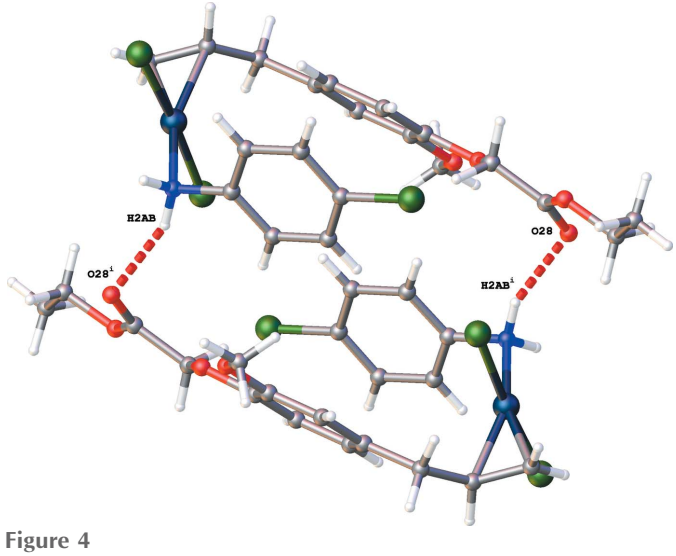


Figure 4
Formation of an inversion dimer by N—H···O hydrogen bonds drawn as red dashed lines in packing of (II). [Symmetry code: (i) $-x+1, -y, -z+1$.]

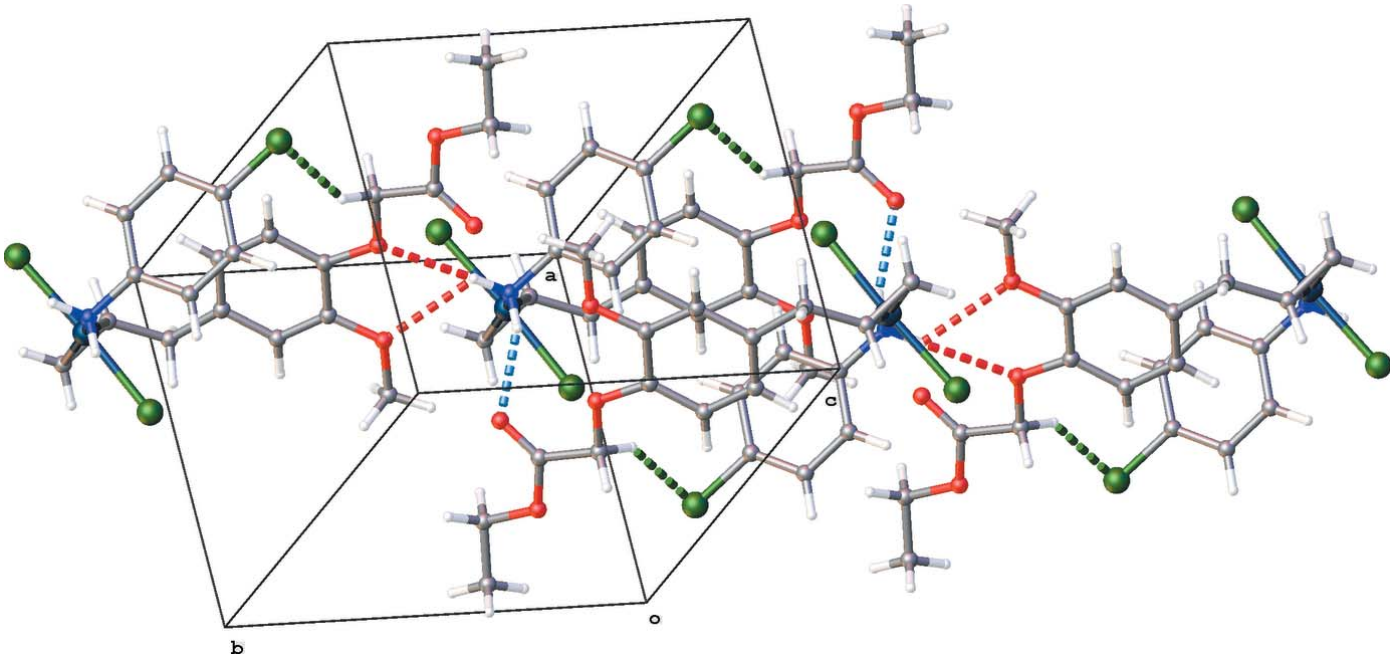


Figure 5
Chains of molecules in the *b*-direction in the packing of (II) by N—H···O hydrogen bonds (red dashed lines). Other N—H···O and C—H···Cl interactions shown as blue and green dashed lines, respectively.

N2—H2*AB*···O28^{i} hydrogen bonds are further linked into chains in the *b*-axis direction by N2—H2*AA*···(O23^{ii},O25^{ii}) hydrogen bonds [Figs. 4 and 5; symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x, y+1, z$].

No π–π interactions are observed in the packing of either structure. For (I) a C—H···π interaction is present [C27—H27*B*···*Cg*1^{iii}, H27*B*···*Cg*1^{iii} = 2.72 Å; *Cg*1 is the centroid of the C20-C25 ring; symmetry code: (iii) $-x+1, y, -z+\frac{3}{2}$].

4. Database survey

The Pt—N distances in (I) and (II) vary from 2.033 (6) to 2.273 (8) Å and deviate for the minor parts (Pt1*B*) due to the disorder from the average Pt—N distance of 2.09 (5) Å for Pt—NH_2—phenyl fragments present in the Cambridge Structural Database (CSD, Version 5.37; Groom *et al.*, 2016). The Pt1*A*—Cl distances are between 2.288 (4) and 2.305 (2) Å and agree well with the average Pt—Cl distance of 2.32 (3) Å for *trans* complexes present in the CSD. One Pt1*B*—Cl distance [2.151 (2) Å] deviates significantly from this average.

A search in the CSD for Pt complexes with Pt coordinated by Cl, NH_2 and C═C shows 11 hits. As fourth ligand we notice an additional Cl atom (eight hits, five *trans* and three *cis* coordinations) or C atom (two hits) or O atom (one hit). In the complex [PtCl(methyleugenol)(o-toluidine)] (CSD refcode GOYJEL; Da, Chi *et al.*, 2015), the central Pt atom coordinated by only one Cl atom, the NH_2 group of *o*-toluidine, the C═C double bond of the eugenol ligand and also a C atom of the eugenol ligand. In (I) and (II) this last interaction is not present and is replaced by an additional Cl atom.

5. Synthesis and crystallization

Synthesis of K[Pt(Alkeug)Cl$_3$]:

The mononuclear complexes K[Pt(Alkeug)Cl_3] (Alkeug are methyleugenoxylacetate or Meteug, and ethyleugenoxylacetate or Eteug) were synthesized following the protocol of Da and coworkers (Da *et al.*, 2012; Da, Chi *et al.*, 2015; Da, Hai *et al.*, 2015).

Synthesis of trans-[PtCl$_2$(Alkeug)(C$_6$H$_6$NCl)]:

A solution of 127.0 mg (1.0 mmol) p-chloroaniline in 10 mL acetone/ethanol (1:1 *v*/*v*) was added to a mixture of 1.0 mmol [K[Pt(Alkeug)Cl_3] and 10 mL acetone/ethanol (1:1 *v*/*v*). After two h stirring, a white precipitate of KCl was separated out. The remaining solution was stirred for two h at room temperature to obtain a yellow precipitate, which was collected by filtration, washed with ethanol and diethyl ether and dried in vacuum. The obtained crystals are soluble in chloroform and acetone, slightly soluble in ethanol and insoluble in water. The yield was 70–80%. Single crystals suitable for X-ray investigation were obtained by slow evaporation from a chloroform/ethanol (1:2 *v*/*v*) solution at room temperature.

Data for [PtCl$_2$(Meteug)(C$_6$H$_6$NCl)] (I):

IR (Impack-410 Nicolet spectrometer, KBr, cm^{-1}): 3243, 3164 (ν_{NH}); 3060, 2958, 2836 (ν_{CH}); 1746 ($\nu_{C=O}$); 1592, 1517 (aromatic, $\nu_{C=C}$, $\nu_{C=N}$); 545 (ν_{Pt-N}).

^{1}H NMR (δ p.p.m; 500 MHz, $CDCl_3$): 3.07 (*br*, 1H, $-CH_{2a}$); 3.40 (*dd*, ^2J = 15.0 Hz, ^3J = 8.0 Hz, $-CH_{2b}$); 5.54 (*br*, 1H, allyl); 4.54 (*br*, 1H, *cis*-alkene); 4.65 (*d*, *J* = 13.0 Hz, 1H, *trans*-alkene); 6.85 (*ov*, 1H, Ar); 6.83 (*ov*, 1H, Ar); 6.71 (*d*, *J* = 8.0 Hz, 1H, Ar); 3.82 (*ov*, 3H, $-OCH_3$); 4.69 (*s*, 2H, $-CH_2-$); 7.32 (*ov*, 4H, Ar), 6.10 (*br*, NH_2).

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$[PtCl_2(C_6H_6ClN)(C_{13}H_{16}O_4)]\cdot 0.1H_2O$	$[PtCl_2(C_6H_6ClN)(C_{14}H_{18}O_4)]$
M_r	631.61	643.84
Crystal system, space group	Monoclinic, $C2/c$	Triclinic, $P\overline{1}$
Temperature (K)	100	100
a, b, c (Å)	13.8322 (6), 15.0753 (4), 21.0367 (9)	9.9093 (3), 10.0102 (3), 11.1414 (4)
α, β, γ (°)	90, 106.683 (5), 90	97.302 (3), 99.706 (3), 92.572 (2)
V (Å^3)	4202.0 (3)	1078.01 (6)
Z	8	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	7.09	6.91
Crystal size (mm)	0.20 × 0.10 × 0.10	0.30 × 0.30 × 0.15
Data collection		
Diffractometer	Agilent SuperNova diffractometer (single source at offset, Eos detector)	Agilent SuperNova diffractometer (single source at offset, Eos detector)
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2012)	Multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min}, T_{max}	0.715, 1.000	0.547, 1.000
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	44052, 4295, 4033	22329, 4378, 4177
R_{int}	0.032	0.044
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.625
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.064, 1.22	0.026, 0.057, 1.20
No. of reflections	4295	4378
No. of parameters	315	292
No. of restraints	291	264
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.28, −0.92	0.97, −0.96

Computer programs: *CrysAlis PRO* (Agilent, 2012), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *olex2.solve* (Bourhis *et al.*, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

Data for [PtCl$_2$(Eteug)(C$_6$H$_6$NCl)] (II):

IR (KBr, cm^{-1}): 3239, 3160 (ν_{NH}); 3060, 2921, 2823 (ν_{CH}); 1746 ($\nu_{C=O}$); 1595, 1516 (aromatic, $\nu_{C=C}$, $\nu_{C=N}$); 550 ($\nu_{Pt\text{-}N}$).

^{1}H NMR (δ p.p.m; 500 MHz, $CDCl_3$): 3.08 (*br*, 1H, –CH_{2a}); 3.39 (*dd*, ^2J = 15.5 Hz, ^3J = 7.5 Hz, 1H, –CH_{2b}); 5.53 (*br*, 1H, allyl); 4.63 (*d*, J = 9.5 Hz, 1H, *cis*-alkene); 4.52 (*br*, 1H, *trans*-alkene); 6.78 (*ov*, 1H, Ar); 6.82 (*d*, J = 8.0 Hz, 1H, Ar); 6.70 (*d*, J = 8.0 Hz, 1H, Ar); 3.82 (*s*, 3H, –OCH_3); 4.28 (*q*, J = 7.0 Hz, 2H, –CH_2); 1.30 (*t*, J = 7.0 Hz, 3H, –CH_3); 4.67 (*s*, 2H, –CH_2–); 7.30 (*ov*, 4H, Ar), 6.20 (*br*, NH_2).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Both structures show disorder which was modelled as good as possible, but still some larger peaks are present in the difference maps.

In (I) the $PtCl_2CH_2{=}CH{-}CH_2$ fragment is disordered over two positions [population parameters 0.679 (8) and 0.321 (8)] and refined with constraints for the bond lengths present in this fragment. Refinement of the population parameter of oxygen atom O34 (at special position) converged to 0.10 (1). Water H atoms were not located.

In (II) only the $PtCl_2$ fragment is disordered over two positions [population parameters 0.872 (6) and 0.128 (6)].

All H atoms were placed in idealized positions and refined in riding mode, with U_{iso}(H) values assigned as 1.2U_{eq} of the parent atoms (1.5 times for methyl groups), with C—H distances of 0.95 (aromatic and $=CH_2$), 0.98 (CH_3), 0.99 (CH_2) and 1.00 Å (CH), and N—H distances of 0.91 Å (NH_2). Enhanced rigid bond restraints were used for the anisotropic temperature factors of the non-H atoms. In the final cycles of refinement, 7 and 15 outliers were omitted for (I) and (II), respectively.

Acknowledgements

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supporting information

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Crystal structures of organoplatinum complexes containing alkyl-eugenoxyacetate and *p*-chloroaniline

Hai Le Thi Hong, Diep Dao Thi Bich, Ngan Nguyen Bich and Luc Van Meervelt

Computing details

For both compounds, data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012). Program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008) for (I); olex2.solve (Bourhis *et al.*, 2015) for (II). For both compounds, program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

(I) *trans*-Dichlorido(4-chloroaniline-κN){3-methoxy-4-methoxycarbonylmethoxy-1-[(2,3-η)-prop-2-en-1-yl]benzene}platinum(II) 0.1-hydrate

Crystal data

$[PtCl_2(C_6H_6ClN)(C_{13}H_{16}O_4)]\cdot 0.1H_2O$
$M_r = 631.61$
Monoclinic, $C2/c$
$a = 13.8322$ (6) Å
$b = 15.0753$ (4) Å
$c = 21.0367$ (9) Å
$\beta = 106.683$ (5)°
$V = 4202.0$ (3) Å^3
$Z = 8$
$F(000) = 2440.0$
$D_x = 1.997$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 22209 reflections
$\theta = 3.3$–$28.6°$
$\mu = 7.09$ mm^{-1}
$T = 100$ K
Block, yellow
0.2 × 0.1 × 0.1 mm

Data collection

Agilent SuperNova diffractometer (single source at offset, Eos detector)
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 15.9631 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2012)
$T_{min} = 0.715$, $T_{max} = 1.000$
44052 measured reflections
4295 independent reflections
4033 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.9°$
$h = -17\rightarrow17$
$k = -18\rightarrow18$
$l = -26\rightarrow26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.064$
$S = 1.22$
4295 reflections
315 parameters
291 restraints
Primary atom site location: heavy-atom method

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + 46.5817P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.28$ e Å^{-3}
$\Delta\rho_{min} = -0.92$ e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Pt1A	0.75061 (14)	0.49179 (7)	0.82720 (10)	0.0213 (2)	0.679 (8)
Pt1B	0.7676 (3)	0.4904 (2)	0.8417 (2)	0.0349 (6)	0.321 (8)
N2	0.8940 (3)	0.5396 (3)	0.8235 (2)	0.0369 (10)	
H2AA	0.9427	0.4996	0.8432	0.044*	0.679 (8)
H2AB	0.8938	0.5459	0.7805	0.044*	0.679 (8)
H2BC	0.9465	0.5015	0.8389	0.044*	0.321 (8)
H2BD	0.8835	0.5469	0.7791	0.044*	0.321 (8)
C3	0.9164 (4)	0.6242 (3)	0.8573 (3)	0.0328 (11)	
C4	0.9600 (5)	0.6278 (4)	0.9245 (3)	0.0457 (14)	
H4	0.9792	0.5743	0.9487	0.055*	
C5	0.9763 (5)	0.7077 (4)	0.9572 (3)	0.0491 (15)	
H5	1.0047	0.7096	1.0040	0.059*	
C6	0.9509 (4)	0.7856 (4)	0.9213 (3)	0.0390 (12)	
C7	0.9087 (4)	0.7838 (4)	0.8539 (3)	0.0327 (11)	
H7	0.8915	0.8374	0.8295	0.039*	
C8	0.8913 (4)	0.7023 (3)	0.8218 (3)	0.0303 (11)	
H8	0.8621	0.7002	0.7751	0.036*	
Cl9	0.97029 (14)	0.88741 (11)	0.96197 (8)	0.0557 (4)	
Cl10	0.8612 (7)	0.4286 (5)	0.9395 (3)	0.0395 (16)	0.321 (8)
Cl11	0.6918 (4)	0.5297 (5)	0.7175 (2)	0.0425 (11)	0.679 (8)
Cl12	0.8205 (3)	0.4484 (2)	0.93519 (14)	0.0337 (6)	0.679 (8)
Cl13	0.6770 (6)	0.5272 (9)	0.7318 (4)	0.036 (2)	0.321 (8)
C14	0.6190 (7)	0.4194 (5)	0.8275 (4)	0.0265 (19)	0.679 (8)
H14A	0.6296	0.3818	0.8652	0.032*	0.679 (8)
H14B	0.6241	0.3962	0.7867	0.032*	0.679 (8)
C15	0.5959 (5)	0.5080 (4)	0.8322 (3)	0.0213 (15)	0.679 (8)
H15	0.5489	0.5324	0.7905	0.026*	0.679 (8)
C16	0.5856 (7)	0.5525 (4)	0.8945 (4)	0.0271 (18)	0.679 (8)
H16A	0.6411	0.5339	0.9335	0.032*	0.679 (8)
H16B	0.5205	0.5363	0.9022	0.032*	0.679 (8)
C17	0.6445 (18)	0.4012 (12)	0.8481 (11)	0.041 (5)	0.321 (8)
H17A	0.5949	0.3889	0.8073	0.050*	0.321 (8)
H17B	0.6967	0.3596	0.8662	0.050*	0.321 (8)
C18	0.6407 (13)	0.4798 (11)	0.8811 (10)	0.046 (4)	0.321 (8)

H18	0.6633	0.4711	0.9302	0.055*	0.321 (8)
C19	0.5657 (13)	0.5548 (7)	0.8620 (10)	0.042 (4)	0.321 (8)
H19A	0.5071	0.5376	0.8774	0.051*	0.321 (8)
H19B	0.5416	0.5552	0.8129	0.051*	0.321 (8)
C20	0.5902 (4)	0.6522 (4)	0.8837 (3)	0.0424 (13)	
C21	0.5064 (4)	0.7011 (3)	0.8465 (3)	0.0339 (11)	
H21	0.4456	0.6712	0.8242	0.041*	
C22	0.5118 (4)	0.7926 (3)	0.8422 (2)	0.0282 (10)	
C23	0.6008 (4)	0.8361 (3)	0.8764 (3)	0.0313 (11)	
C24	0.6828 (4)	0.7872 (4)	0.9122 (3)	0.0395 (12)	
H24	0.7435	0.8167	0.9352	0.047*	
C25	0.6774 (4)	0.6956 (4)	0.9150 (3)	0.0440 (13)	
H25	0.7349	0.6627	0.9389	0.053*	
O26	0.4355 (3)	0.8454 (2)	0.80566 (18)	0.0324 (8)	
C27	0.3460 (4)	0.8027 (4)	0.7673 (3)	0.0343 (12)	
H27A	0.3117	0.7750	0.7970	0.051*	
H27B	0.3635	0.7571	0.7393	0.051*	
H27C	0.3012	0.8465	0.7393	0.051*	
O28	0.5993 (3)	0.9267 (2)	0.86886 (19)	0.0372 (9)	
C29	0.6894 (5)	0.9716 (4)	0.9030 (3)	0.0446 (14)	
H29A	0.7479	0.9457	0.8914	0.054*	
H29B	0.7014	0.9667	0.9515	0.054*	
C30	0.6754 (5)	1.0688 (4)	0.8813 (3)	0.0480 (14)	
O31	0.6176 (4)	1.0965 (3)	0.8301 (3)	0.0582 (12)	
O32	0.7487 (5)	1.1132 (3)	0.9246 (2)	0.0740 (16)	
C33	0.7493 (9)	1.2074 (5)	0.9135 (5)	0.102 (3)	
H33A	0.7428	1.2188	0.8666	0.154*	
H33B	0.8128	1.2327	0.9410	0.154*	
H33C	0.6926	1.2349	0.9253	0.154*	
O34	1.0000	0.5000	0.7500	0.10 (2)	0.10 (1)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1A	0.0216 (4)	0.0167 (3)	0.0252 (5)	−0.00062 (18)	0.0064 (4)	−0.0012 (2)
Pt1B	0.0269 (10)	0.0479 (9)	0.0288 (12)	−0.0027 (5)	0.0061 (9)	−0.0021 (6)
N2	0.028 (2)	0.029 (2)	0.054 (3)	0.0035 (17)	0.0125 (19)	0.0060 (19)
C3	0.022 (2)	0.033 (2)	0.043 (3)	−0.0006 (19)	0.008 (2)	0.006 (2)
C4	0.045 (3)	0.039 (3)	0.046 (3)	−0.014 (2)	0.001 (2)	0.013 (2)
C5	0.052 (4)	0.052 (3)	0.039 (3)	−0.020 (3)	0.005 (3)	0.009 (2)
C6	0.034 (3)	0.041 (3)	0.042 (3)	−0.018 (2)	0.011 (2)	0.001 (2)
C7	0.027 (3)	0.033 (2)	0.040 (3)	−0.003 (2)	0.012 (2)	0.008 (2)
C8	0.022 (2)	0.032 (2)	0.036 (3)	0.0006 (19)	0.008 (2)	0.0055 (19)
Cl9	0.0722 (11)	0.0515 (9)	0.0477 (9)	−0.0338 (8)	0.0242 (8)	−0.0125 (7)
Cl10	0.049 (4)	0.037 (3)	0.029 (2)	−0.003 (3)	0.005 (3)	0.008 (2)
Cl11	0.058 (3)	0.0403 (18)	0.0382 (14)	0.0123 (18)	0.0281 (13)	0.0128 (11)
Cl12	0.0287 (15)	0.0273 (13)	0.0359 (12)	0.0024 (10)	−0.0052 (11)	0.0095 (9)
Cl13	0.015 (2)	0.035 (3)	0.054 (5)	−0.005 (2)	0.004 (3)	0.016 (4)

C14	0.025 (4)	0.027 (4)	0.028 (4)	−0.001 (3)	0.008 (3)	0.001 (3)
C15	0.015 (3)	0.027 (3)	0.020 (3)	0.000 (2)	0.002 (2)	0.003 (2)
C16	0.036 (4)	0.029 (3)	0.018 (4)	0.005 (3)	0.011 (3)	0.007 (3)
C17	0.032 (8)	0.039 (7)	0.051 (10)	0.004 (5)	0.010 (7)	0.009 (6)
C18	0.042 (7)	0.041 (6)	0.058 (9)	0.002 (5)	0.019 (6)	0.010 (6)
C19	0.042 (8)	0.041 (5)	0.057 (11)	0.008 (4)	0.033 (7)	0.022 (5)
C20	0.041 (3)	0.035 (2)	0.061 (3)	0.007 (2)	0.030 (3)	0.013 (2)
C21	0.030 (2)	0.030 (2)	0.049 (3)	0.0014 (19)	0.022 (2)	0.001 (2)
C22	0.031 (2)	0.028 (2)	0.030 (2)	0.0048 (18)	0.0156 (19)	−0.0011 (18)
C23	0.034 (2)	0.033 (2)	0.028 (2)	0.0011 (19)	0.012 (2)	0.0007 (19)
C24	0.037 (3)	0.047 (3)	0.034 (3)	0.002 (2)	0.010 (2)	0.006 (2)
C25	0.035 (3)	0.047 (3)	0.052 (3)	0.009 (2)	0.016 (3)	0.017 (2)
O26	0.0293 (18)	0.0261 (17)	0.040 (2)	0.0027 (14)	0.0081 (15)	−0.0015 (15)
C27	0.030 (3)	0.038 (3)	0.035 (3)	0.002 (2)	0.010 (2)	−0.004 (2)
O28	0.037 (2)	0.0302 (18)	0.041 (2)	−0.0044 (15)	0.0062 (17)	−0.0065 (15)
C29	0.046 (3)	0.049 (3)	0.039 (3)	−0.015 (2)	0.011 (3)	−0.004 (2)
C30	0.061 (4)	0.042 (3)	0.050 (3)	−0.017 (3)	0.029 (3)	−0.005 (2)
O31	0.052 (3)	0.051 (3)	0.076 (3)	0.001 (2)	0.026 (2)	0.007 (2)
O32	0.110 (4)	0.066 (3)	0.050 (3)	−0.052 (3)	0.030 (3)	−0.011 (2)
C33	0.171 (10)	0.062 (4)	0.100 (7)	−0.063 (5)	0.081 (7)	−0.018 (4)
O34	0.06 (3)	0.21 (6)	0.04 (2)	0.000	0.015 (18)	0.000

Geometric parameters (Å, º)

Pt1A—N2	2.132 (5)	C17—H17A	0.9500
Pt1A—Cl11	2.288 (4)	C17—H17B	0.9500
Pt1A—Cl12	2.294 (3)	C17—C18	1.381 (12)
Pt1A—C14	2.124 (9)	C18—H18	1.0000
Pt1A—C15	2.187 (6)	C18—C19	1.508 (11)
Pt1B—N2	2.033 (6)	C19—H19A	0.9900
Pt1B—Cl10	2.291 (5)	C19—H19B	0.9900
Pt1B—Cl13	2.357 (7)	C19—C20	1.546 (11)
Pt1B—C17	2.20 (2)	C20—C21	1.407 (8)
Pt1B—C18	2.151 (18)	C20—C25	1.364 (9)
N2—H2AA	0.9100	C21—H21	0.9500
N2—H2AB	0.9100	C21—C22	1.386 (7)
N2—H2BC	0.9100	C22—C23	1.398 (7)
N2—H2BD	0.9100	C22—O26	1.369 (6)
N2—C3	1.450 (7)	C23—C24	1.381 (8)
C3—C4	1.370 (8)	C23—O28	1.374 (6)
C3—C8	1.384 (7)	C24—H24	0.9500
C4—H4	0.9500	C24—C25	1.385 (8)
C4—C5	1.374 (9)	C25—H25	0.9500
C5—H5	0.9500	O26—C27	1.422 (6)
C5—C6	1.386 (8)	C27—H27A	0.9800
C6—C7	1.370 (8)	C27—H27B	0.9800
C6—Cl9	1.741 (6)	C27—H27C	0.9800
C7—H7	0.9500	O28—C29	1.419 (7)

C7—C8	1.389 (7)	C29—H29A	0.9900
C8—H8	0.9500	C29—H29B	0.9900
C14—H14A	0.9500	C29—C30	1.530 (9)
C14—H14B	0.9500	C30—O31	1.218 (8)
C14—C15	1.383 (9)	C30—O32	1.332 (8)
C15—H15	1.0000	O32—C33	1.440 (9)
C15—C16	1.514 (8)	C33—H33A	0.9800
C16—H16A	0.9900	C33—H33B	0.9800
C16—H16B	0.9900	C33—H33C	0.9800
C16—C20	1.523 (8)		

N2—Pt1A—Cl11	86.8 (2)	H16A—C16—H16B	108.6
N2—Pt1A—Cl12	90.03 (16)	C20—C16—H16A	110.4
N2—Pt1A—C15	153.8 (2)	C20—C16—H16B	110.4
Cl11—Pt1A—Cl12	175.35 (16)	Pt1B—C17—H17A	115.8
C14—Pt1A—N2	168.7 (2)	Pt1B—C17—H17B	85.2
C14—Pt1A—Cl11	94.3 (3)	H17A—C17—H17B	120.0
C14—Pt1A—Cl12	88.2 (3)	C18—C17—Pt1B	69.4 (12)
C14—Pt1A—C15	37.4 (3)	C18—C17—H17A	120.0
C15—Pt1A—Cl11	87.2 (2)	C18—C17—H17B	120.0
C15—Pt1A—Cl12	97.1 (2)	Pt1B—C18—H18	111.2
N2—Pt1B—Cl10	91.2 (2)	C17—C18—Pt1B	73.6 (13)
N2—Pt1B—Cl13	88.5 (3)	C17—C18—H18	111.2
N2—Pt1B—C17	162.7 (5)	C17—C18—C19	129.1 (17)
N2—Pt1B—C18	160.0 (5)	C19—C18—Pt1B	114.6 (12)
Cl10—Pt1B—Cl13	168.6 (4)	C19—C18—H18	111.2
C17—Pt1B—Cl10	86.8 (6)	C18—C19—H19A	106.4
C17—Pt1B—Cl13	90.1 (6)	C18—C19—H19B	106.4
C18—Pt1B—Cl10	86.4 (6)	C18—C19—C20	123.8 (13)
C18—Pt1B—Cl13	97.6 (6)	H19A—C19—H19B	106.4
C18—Pt1B—C17	36.9 (4)	C20—C19—H19A	106.4
Pt1A—N2—H2AA	109.5	C20—C19—H19B	106.4
Pt1A—N2—H2AB	109.5	C21—C20—C16	122.4 (6)
Pt1B—N2—H2BC	110.2	C21—C20—C19	104.9 (8)
Pt1B—N2—H2BD	110.2	C25—C20—C16	118.1 (6)
H2AA—N2—H2AB	108.1	C25—C20—C19	133.4 (8)
H2BC—N2—H2BD	108.5	C25—C20—C21	119.3 (5)
C3—N2—Pt1A	110.5 (3)	C20—C21—H21	119.8
C3—N2—Pt1B	107.7 (3)	C22—C21—C20	120.4 (5)
C3—N2—H2AA	109.5	C22—C21—H21	119.8
C3—N2—H2AB	109.5	C21—C22—C23	119.3 (5)
C3—N2—H2BC	110.2	O26—C22—C21	124.6 (5)
C3—N2—H2BD	110.2	O26—C22—C23	116.1 (4)
C4—C3—N2	120.5 (5)	C24—C23—C22	119.7 (5)
C4—C3—C8	119.5 (5)	O28—C23—C22	115.1 (5)
C8—C3—N2	120.0 (5)	O28—C23—C24	125.2 (5)
C3—C4—H4	119.6	C23—C24—H24	119.7
C3—C4—C5	120.8 (6)	C23—C24—C25	120.6 (6)

C5—C4—H4	119.6	C25—C24—H24	119.7
C4—C5—H5	120.3	C20—C25—C24	120.7 (6)
C4—C5—C6	119.3 (6)	C20—C25—H25	119.7
C6—C5—H5	120.3	C24—C25—H25	119.7
C5—C6—Cl9	119.9 (5)	C22—O26—C27	117.5 (4)
C7—C6—C5	121.0 (6)	O26—C27—H27A	109.5
C7—C6—Cl9	119.1 (4)	O26—C27—H27B	109.5
C6—C7—H7	120.6	O26—C27—H27C	109.5
C6—C7—C8	118.9 (5)	H27A—C27—H27B	109.5
C8—C7—H7	120.6	H27A—C27—H27C	109.5
C3—C8—C7	120.5 (5)	H27B—C27—H27C	109.5
C3—C8—H8	119.7	C23—O28—C29	115.7 (4)
C7—C8—H8	119.7	O28—C29—H29A	110.4
Pt1A—C14—H14A	112.4	O28—C29—H29B	110.4
Pt1A—C14—H14B	84.2	O28—C29—C30	106.8 (5)
H14A—C14—H14B	120.0	H29A—C29—H29B	108.6
C15—C14—Pt1A	73.8 (4)	C30—C29—H29A	110.4
C15—C14—H14A	120.0	C30—C29—H29B	110.4
C15—C14—H14B	120.0	O31—C30—C29	125.9 (6)
Pt1A—C15—H15	113.4	O31—C30—O32	127.7 (6)
C14—C15—Pt1A	68.9 (5)	O32—C30—C29	105.7 (6)
C14—C15—H15	113.4	C30—O32—C33	115.0 (7)
C14—C15—C16	124.8 (6)	O32—C33—H33A	109.5
C16—C15—Pt1A	115.3 (5)	O32—C33—H33B	109.5
C16—C15—H15	113.4	O32—C33—H33C	109.5
C15—C16—H16A	110.4	H33A—C33—H33B	109.5
C15—C16—H16B	110.4	H33A—C33—H33C	109.5
C15—C16—C20	106.8 (5)	H33B—C33—H33C	109.5

Pt1A—N2—C3—C4	85.5 (5)	C18—C19—C20—C21	170.4 (16)
Pt1A—N2—C3—C8	−92.9 (5)	C18—C19—C20—C25	9 (3)
Pt1A—C14—C15—C16	−106.8 (7)	C19—C20—C21—C22	−165.6 (9)
Pt1A—C15—C16—C20	83.1 (6)	C19—C20—C25—C24	161.9 (12)
Pt1B—N2—C3—C4	76.9 (6)	C20—C21—C22—C23	−1.4 (8)
Pt1B—N2—C3—C8	−101.5 (5)	C20—C21—C22—O26	177.9 (5)
Pt1B—C17—C18—C19	109 (2)	C21—C20—C25—C24	2.1 (9)
Pt1B—C18—C19—C20	−65 (2)	C21—C22—C23—C24	1.9 (7)
N2—C3—C4—C5	−176.4 (5)	C21—C22—C23—O28	179.7 (4)
N2—C3—C8—C7	177.4 (5)	C21—C22—O26—C27	−2.8 (7)
C3—C4—C5—C6	−1.9 (10)	C22—C23—C24—C25	−0.5 (8)
C4—C3—C8—C7	−1.0 (8)	C22—C23—O28—C29	−179.6 (5)
C4—C5—C6—C7	0.9 (9)	C23—C22—O26—C27	176.5 (4)
C4—C5—C6—Cl9	179.6 (5)	C23—C24—C25—C20	−1.6 (9)
C5—C6—C7—C8	0.1 (8)	C23—O28—C29—C30	173.5 (4)
C6—C7—C8—C3	0.0 (8)	C24—C23—O28—C29	−2.0 (8)
C8—C3—C4—C5	2.0 (9)	C25—C20—C21—C22	−0.6 (8)
Cl9—C6—C7—C8	−178.7 (4)	O26—C22—C23—C24	−177.4 (5)
C14—C15—C16—C20	164.0 (7)	O26—C22—C23—O28	0.3 (6)

C15—C16—C20—C21	80.3 (8)	O28—C23—C24—C25	−178.0 (5)
C15—C16—C20—C25	−104.0 (7)	O28—C29—C30—O31	−23.3 (9)
C16—C20—C21—C22	175.0 (5)	O28—C29—C30—O32	165.6 (5)
C16—C20—C25—C24	−173.7 (6)	C29—C30—O32—C33	−179.7 (6)
C17—C18—C19—C20	−153 (2)	O31—C30—O32—C33	9.4 (11)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C20–C25 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*AA*···O26^{i}	0.91	2.45	3.027 (5)	122
N2—H2*AA*···O28^{i}	0.91	2.35	3.212 (6)	158
N2—H2*AB*···O31^{ii}	0.91	2.41	3.302 (3)	167
C16—H16*A*···Cl12	0.99	2.79	3.487 (10)	128
C16—H16*B*···Cl9^{iii}	0.99	2.76	3.472 (8)	129
C21—H21···Cl11^{iv}	0.95	2.82	3.726 (8)	159
C29—H29*B*···Cl12^{v}	0.99	2.80	3.651 (7)	145
C27—H27*B*···*Cg*1^{iv}	0.98	2.72	3.523 (6)	139

Symmetry codes: (i) *x*+1/2, *y*−1/2, *z*; (ii) −*x*+3/2, *y*−1/2, −*z*+3/2; (iii) *x*−1/2, *y*−1/2, *z*; (iv) −*x*+1, *y*, −*z*+3/2; (v) −*x*+3/2, −*y*+3/2, −*z*+2.

(II) *trans*-Dichlorido(4-chloroaniline-κ*N*){4-ethoxycarbonylmethoxy-3-methoxy-1-[(2,3-η)-prop-2-en-1-yl]benzene}platinum(II)

Crystal data

$[PtCl_2(C_6H_6ClN)(C_{14}H_{18}O_4)]$
M_r = 643.84
Triclinic, $P\overline{1}$
a = 9.9093 (3) Å
b = 10.0102 (3) Å
c = 11.1414 (4) Å
α = 97.302 (3)°
β = 99.706 (3)°
γ = 92.572 (2)°
V = 1078.01 (6) Å^3
Z = 2
F(000) = 624
D_x = 1.984 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 10730 reflections
θ = 3.2–29.0°
μ = 6.91 mm^{-1}
T = 100 K
Block, yellow
0.3 × 0.3 × 0.15 mm

Data collection

Agilent SuperNova diffractometer (single source at offset, Eos detector)
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 15.9631 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2012)
T_{min} = 0.547, T_{max} = 1.000
22329 measured reflections
4378 independent reflections
4177 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 26.4°, θ_{min} = 2.8°
h = −12→12
k = −12→12
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.057
S = 1.20
4378 reflections

292 parameters
264 restraints
Primary atom site location: iterative
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0056P)^2 + 3.1214P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.97$ e Å^{-3}
$\Delta\rho_{min} = -0.96$ e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Pt1A	0.69549 (11)	0.29586 (10)	0.25083 (7)	0.01218 (14)	0.872 (6)
Pt1B	0.6572 (11)	0.2618 (9)	0.2299 (6)	0.0263 (11)	0.128 (6)
N2	0.6352 (4)	0.3773 (4)	0.4142 (3)	0.0175 (7)	
H2AA	0.6687	0.4649	0.4346	0.021*	0.872 (6)
H2AB	0.5420	0.3754	0.4033	0.021*	0.872 (6)
H2BC	0.6834	0.4588	0.4258	0.021*	0.128 (6)
H2BD	0.5454	0.3921	0.4147	0.021*	0.128 (6)
C3	0.6861 (4)	0.3007 (4)	0.5131 (4)	0.0172 (9)	
C4	0.8223 (4)	0.3217 (4)	0.5704 (4)	0.0191 (9)	
H4	0.8815	0.3854	0.5446	0.023*	
C5	0.8722 (4)	0.2504 (4)	0.6650 (4)	0.0194 (9)	
H5	0.9653	0.2646	0.7049	0.023*	
C6	0.7836 (4)	0.1577 (4)	0.7002 (4)	0.0182 (9)	
C7	0.6483 (4)	0.1340 (4)	0.6433 (4)	0.0191 (9)	
H7	0.5897	0.0692	0.6685	0.023*	
C8	0.5994 (4)	0.2062 (4)	0.5490 (4)	0.0199 (9)	
H8	0.5065	0.1912	0.5088	0.024*	
Cl9	0.84620 (12)	0.06618 (11)	0.81957 (10)	0.0252 (2)	
Cl10	0.88980 (15)	0.4404 (2)	0.30141 (16)	0.0170 (4)	0.872 (6)
Cl11	0.4916 (2)	0.1647 (2)	0.20164 (18)	0.0173 (4)	0.872 (6)
Cl12	0.8689 (13)	0.377 (2)	0.2675 (13)	0.037 (3)	0.128 (6)
Cl13	0.4387 (19)	0.1586 (18)	0.1984 (16)	0.034 (3)	0.128 (6)
C14	0.7274 (5)	0.2580 (5)	0.0645 (4)	0.0236 (10)	
H14A	0.6473	0.2280	0.0057	0.028*	
H14B	0.7579	0.3509	0.0794	0.028*	
C15	0.8002 (5)	0.1655 (5)	0.1289 (4)	0.0242 (10)	
H15	0.9021	0.1839	0.1437	0.029*	0.872 (6)
H15A	0.9000	0.1894	0.1608	0.029*	0.128 (6)
C16	0.7539 (5)	0.0195 (4)	0.1067 (4)	0.0245 (10)	
H16A	0.8108	−0.0272	0.0517	0.029*	
H16B	0.6582	0.0106	0.0616	0.029*	
C17	0.7586 (5)	−0.0551 (4)	0.2180 (4)	0.0186 (9)	
C18	0.6816 (4)	−0.1797 (4)	0.1979 (4)	0.0187 (9)	

H18	0.6308	−0.2117	0.1184	0.022*
C19	0.6787 (4)	−0.2565 (4)	0.2923 (4)	0.0161 (8)
C20	0.7528 (4)	−0.2097 (4)	0.4101 (4)	0.0143 (8)
C21	0.8282 (4)	−0.0865 (4)	0.4312 (4)	0.0174 (9)
H21	0.8780	−0.0536	0.5108	0.021*
C22	0.8303 (4)	−0.0106 (4)	0.3335 (4)	0.0196 (9)
H22	0.8827	0.0736	0.3480	0.023*
O23	0.6053 (3)	−0.3770 (3)	0.2818 (3)	0.0183 (6)
C24	0.5250 (5)	−0.4260 (4)	0.1644 (4)	0.0241 (10)
H24A	0.5845	−0.4341	0.1023	0.036*
H24B	0.4549	−0.3629	0.1430	0.036*
H24C	0.4805	−0.5147	0.1672	0.036*
O25	0.7390 (3)	−0.2930 (3)	0.4975 (3)	0.0168 (6)
C26	0.8067 (4)	−0.2464 (4)	0.6172 (4)	0.0183 (9)
H26A	0.7842	−0.1526	0.6418	0.022*
H26B	0.9072	−0.2473	0.6214	0.022*
C27	0.7604 (4)	−0.3380 (4)	0.7025 (4)	0.0157 (8)
O28	0.6689 (3)	−0.4258 (3)	0.6725 (3)	0.0176 (6)
O29	0.8362 (3)	−0.3074 (3)	0.8142 (3)	0.0180 (6)
C30	0.8025 (5)	−0.3861 (5)	0.9070 (4)	0.0212 (10)
H30A	0.8025	−0.4837	0.8776	0.025*
H30B	0.7103	−0.3668	0.9249	0.025*
C31	0.9091 (4)	−0.3475 (4)	1.0205 (4)	0.0200 (9)
H31A	0.9993	−0.3714	1.0028	0.030*
H31B	0.8865	−0.3960	1.0864	0.030*
H31C	0.9112	−0.2501	1.0465	0.030*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1A	0.0123 (3)	0.0118 (2)	0.01192 (18)	−0.00266 (15)	0.00058 (15)	0.00299 (14)
Pt1B	0.030 (2)	0.030 (2)	0.0207 (16)	−0.0011 (19)	0.0073 (16)	0.0081 (15)
N2	0.0171 (17)	0.0194 (18)	0.0155 (19)	−0.0007 (14)	0.0029 (14)	0.0010 (14)
C3	0.020 (2)	0.017 (2)	0.015 (2)	0.0008 (16)	0.0050 (16)	0.0017 (16)
C4	0.021 (2)	0.020 (2)	0.016 (2)	−0.0049 (17)	0.0044 (17)	0.0020 (17)
C5	0.018 (2)	0.024 (2)	0.015 (2)	−0.0034 (17)	0.0022 (17)	0.0002 (18)
C6	0.025 (2)	0.018 (2)	0.012 (2)	0.0003 (16)	0.0033 (17)	0.0014 (17)
C7	0.022 (2)	0.017 (2)	0.019 (2)	−0.0041 (16)	0.0076 (17)	0.0024 (17)
C8	0.0146 (19)	0.026 (2)	0.019 (2)	−0.0033 (17)	0.0030 (17)	0.0048 (18)
Cl9	0.0379 (6)	0.0240 (6)	0.0123 (6)	−0.0029 (5)	0.0008 (5)	0.0041 (4)
Cl10	0.0148 (6)	0.0174 (8)	0.0176 (8)	−0.0065 (5)	0.0010 (5)	0.0032 (6)
Cl11	0.0124 (8)	0.0174 (7)	0.0201 (8)	−0.0054 (7)	0.0009 (7)	−0.0005 (5)
Cl12	0.034 (5)	0.049 (8)	0.026 (6)	−0.013 (5)	0.010 (4)	0.003 (5)
Cl13	0.033 (7)	0.036 (6)	0.034 (7)	−0.002 (6)	0.011 (6)	0.002 (5)
C14	0.030 (2)	0.025 (2)	0.017 (2)	0.0025 (19)	0.0043 (18)	0.0060 (18)
C15	0.028 (2)	0.025 (2)	0.022 (2)	−0.0012 (18)	0.0084 (19)	0.0056 (18)
C16	0.040 (3)	0.020 (2)	0.014 (2)	−0.0026 (19)	0.008 (2)	0.0022 (17)
C17	0.031 (2)	0.0151 (19)	0.012 (2)	0.0047 (17)	0.0083 (17)	0.0035 (16)

C18	0.027 (2)	0.018 (2)	0.011 (2)	0.0009 (17)	0.0024 (17)	0.0029 (16)
C19	0.018 (2)	0.0155 (19)	0.015 (2)	0.0009 (15)	0.0048 (16)	0.0033 (15)
C20	0.0158 (19)	0.0154 (19)	0.013 (2)	0.0009 (15)	0.0025 (15)	0.0052 (15)
C21	0.019 (2)	0.019 (2)	0.013 (2)	−0.0031 (16)	0.0016 (16)	0.0022 (16)
C22	0.024 (2)	0.015 (2)	0.020 (2)	−0.0035 (17)	0.0058 (17)	0.0041 (17)
O23	0.0226 (15)	0.0182 (15)	0.0127 (16)	−0.0043 (12)	−0.0018 (12)	0.0046 (12)
C24	0.034 (3)	0.020 (2)	0.016 (2)	−0.0050 (19)	−0.0040 (19)	0.0067 (18)
O25	0.0236 (15)	0.0160 (14)	0.0098 (15)	−0.0047 (12)	−0.0009 (12)	0.0054 (12)
C26	0.019 (2)	0.019 (2)	0.015 (2)	−0.0050 (17)	−0.0003 (16)	0.0048 (17)
C27	0.0174 (19)	0.016 (2)	0.014 (2)	0.0026 (16)	0.0029 (15)	0.0020 (16)
O28	0.0221 (15)	0.0177 (15)	0.0112 (16)	−0.0046 (12)	0.0005 (12)	0.0009 (12)
O29	0.0186 (15)	0.0225 (16)	0.0123 (15)	−0.0057 (12)	−0.0003 (12)	0.0063 (12)
C30	0.027 (2)	0.024 (2)	0.013 (2)	−0.0056 (18)	0.0030 (18)	0.0045 (18)
C31	0.025 (2)	0.023 (2)	0.012 (2)	−0.0006 (18)	0.0004 (17)	0.0040 (18)

Geometric parameters (Å, º)

Pt1A—N2	2.089 (4)	C16—H16A	0.9900
Pt1A—Cl10	2.3011 (14)	C16—H16B	0.9900
Pt1A—Cl11	2.3050 (15)	C16—C17	1.522 (6)
Pt1A—C14	2.142 (5)	C17—C18	1.406 (6)
Pt1A—C15	2.184 (5)	C17—C22	1.371 (6)
Pt1B—N2	2.273 (8)	C18—H18	0.9500
Pt1B—Cl12	2.297 (12)	C18—C19	1.382 (6)
Pt1B—Cl13	2.309 (14)	C19—C20	1.403 (6)
Pt1B—C14	2.073 (6)	C19—O23	1.362 (5)
Pt1B—C15	2.142 (6)	C20—C21	1.385 (6)
N2—H2AA	0.9100	C20—O25	1.380 (5)
N2—H2AB	0.9100	C21—H21	0.9500
N2—H2BC	0.9100	C21—C22	1.406 (6)
N2—H2BD	0.9100	C22—H22	0.9500
N2—C3	1.455 (5)	O23—C24	1.427 (5)
C3—C4	1.387 (6)	C24—H24A	0.9800
C3—C8	1.390 (6)	C24—H24B	0.9800
C4—H4	0.9500	C24—H24C	0.9800
C4—C5	1.383 (6)	O25—C26	1.399 (5)
C5—H5	0.9500	C26—H26A	0.9900
C5—C6	1.387 (6)	C26—H26B	0.9900
C6—C7	1.379 (6)	C26—C27	1.512 (5)
C6—Cl9	1.754 (4)	C27—O28	1.207 (5)
C7—H7	0.9500	C27—O29	1.332 (5)
C7—C8	1.384 (6)	O29—C30	1.449 (5)
C8—H8	0.9500	C30—H30A	0.9900
C14—H14A	0.9500	C30—H30B	0.9900
C14—H14B	0.9500	C30—C31	1.501 (6)
C14—C15	1.396 (6)	C31—H31A	0.9800
C15—H15	1.0000	C31—H31B	0.9800
C15—H15A	1.0000	C31—H31C	0.9800

C15—C16	1.489 (6)		
N2—Pt1A—Cl10	88.86 (10)	C14—C15—H15	114.2
N2—Pt1A—Cl11	88.77 (11)	C14—C15—H15A	117.2
N2—Pt1A—C14	163.99 (15)	C14—C15—C16	120.7 (4)
N2—Pt1A—C15	158.31 (16)	C16—C15—Pt1A	116.5 (3)
Cl10—Pt1A—Cl11	175.82 (7)	C16—C15—Pt1B	105.3 (4)
C14—Pt1A—Cl10	90.53 (14)	C16—C15—H15	114.2
C14—Pt1A—Cl11	90.80 (15)	C16—C15—H15A	117.2
C14—Pt1A—C15	37.62 (17)	C15—C16—H16A	107.9
C15—Pt1A—Cl10	89.13 (14)	C15—C16—H16B	107.9
C15—Pt1A—Cl11	94.33 (15)	C15—C16—C17	117.8 (4)
N2—Pt1B—Cl12	83.8 (4)	H16A—C16—H16B	107.2
N2—Pt1B—Cl13	93.1 (5)	C17—C16—H16A	107.9
Cl12—Pt1B—Cl13	176.1 (6)	C17—C16—H16B	107.9
C14—Pt1B—N2	149.1 (6)	C18—C17—C16	115.9 (4)
C14—Pt1B—Cl12	71.8 (5)	C22—C17—C16	125.5 (4)
C14—Pt1B—Cl13	110.3 (7)	C22—C17—C18	118.6 (4)
C14—Pt1B—C15	38.62 (18)	C17—C18—H18	119.6
C15—Pt1B—N2	143.8 (6)	C19—C18—C17	120.8 (4)
C15—Pt1B—Cl12	67.1 (6)	C19—C18—H18	119.6
C15—Pt1B—Cl13	116.7 (7)	C18—C19—C20	119.9 (4)
Pt1A—N2—H2AA	109.6	O23—C19—C18	124.8 (4)
Pt1A—N2—H2AB	109.6	O23—C19—C20	115.2 (3)
Pt1B—N2—H2BC	109.6	C21—C20—C19	119.7 (4)
Pt1B—N2—H2BD	109.6	O25—C20—C19	114.7 (3)
H2AA—N2—H2AB	108.1	O25—C20—C21	125.6 (4)
H2BC—N2—H2BD	108.2	C20—C21—H21	120.3
C3—N2—Pt1A	110.4 (3)	C20—C21—C22	119.4 (4)
C3—N2—Pt1B	110.1 (3)	C22—C21—H21	120.3
C3—N2—H2AA	109.6	C17—C22—C21	121.5 (4)
C3—N2—H2AB	109.6	C17—C22—H22	119.2
C3—N2—H2BC	109.6	C21—C22—H22	119.2
C3—N2—H2BD	109.6	C19—O23—C24	117.0 (3)
C4—C3—N2	119.5 (4)	O23—C24—H24A	109.5
C4—C3—C8	120.2 (4)	O23—C24—H24B	109.5
C8—C3—N2	120.4 (4)	O23—C24—H24C	109.5
C3—C4—H4	119.9	H24A—C24—H24B	109.5
C5—C4—C3	120.3 (4)	H24A—C24—H24C	109.5
C5—C4—H4	119.9	H24B—C24—H24C	109.5
C4—C5—H5	120.7	C20—O25—C26	116.1 (3)
C4—C5—C6	118.6 (4)	O25—C26—H26A	110.0
C6—C5—H5	120.7	O25—C26—H26B	110.0
C5—C6—Cl9	118.9 (3)	O25—C26—C27	108.3 (3)
C7—C6—C5	122.1 (4)	H26A—C26—H26B	108.4
C7—C6—Cl9	119.0 (3)	C27—C26—H26A	110.0
C6—C7—H7	120.6	C27—C26—H26B	110.0
C6—C7—C8	118.7 (4)	O28—C27—C26	124.6 (4)

C8—C7—H7	120.6	O28—C27—O29	125.8 (4)
C3—C8—H8	119.9	O29—C27—C26	109.7 (3)
C7—C8—C3	120.1 (4)	C27—O29—C30	116.1 (3)
C7—C8—H8	119.9	O29—C30—H30A	110.2
Pt1A—C14—H14A	115.0	O29—C30—H30B	110.2
Pt1A—C14—H14B	82.6	O29—C30—C31	107.6 (3)
H14A—C14—H14B	120.0	H30A—C30—H30B	108.5
C15—C14—Pt1A	72.9 (3)	C31—C30—H30A	110.2
C15—C14—Pt1B	73.4 (3)	C31—C30—H30B	110.2
C15—C14—H14A	120.0	C30—C31—H31A	109.5
C15—C14—H14B	120.0	C30—C31—H31B	109.5
Pt1A—C15—H15	114.2	C30—C31—H31C	109.5
Pt1B—C15—H15A	117.2	H31A—C31—H31B	109.5
C14—C15—Pt1A	69.5 (3)	H31A—C31—H31C	109.5
C14—C15—Pt1B	68.0 (3)	H31B—C31—H31C	109.5
Pt1A—N2—C3—C4	78.3 (4)	C16—C17—C22—C21	179.8 (4)
Pt1A—N2—C3—C8	−101.0 (4)	C17—C18—C19—C20	0.3 (6)
Pt1A—C14—C15—C16	109.4 (4)	C17—C18—C19—O23	178.8 (4)
Pt1A—C15—C16—C17	−56.7 (5)	C18—C17—C22—C21	0.0 (7)
Pt1B—N2—C3—C4	91.5 (5)	C18—C19—C20—C21	0.2 (6)
Pt1B—N2—C3—C8	−87.8 (5)	C18—C19—C20—O25	178.3 (4)
Pt1B—C14—C15—C16	95.3 (6)	C18—C19—O23—C24	−0.5 (6)
Pt1B—C15—C16—C17	−64.4 (5)	C19—C20—C21—C22	−0.6 (6)
N2—C3—C4—C5	179.7 (4)	C19—C20—O25—C26	−177.2 (3)
N2—C3—C8—C7	−179.8 (4)	C20—C19—O23—C24	178.1 (4)
C3—C4—C5—C6	0.3 (7)	C20—C21—C22—C17	0.5 (7)
C4—C3—C8—C7	0.9 (7)	C20—O25—C26—C27	170.4 (3)
C4—C5—C6—C7	0.6 (7)	C21—C20—O25—C26	0.7 (6)
C4—C5—C6—Cl9	179.7 (3)	C22—C17—C18—C19	−0.4 (6)
C5—C6—C7—C8	−0.7 (7)	O23—C19—C20—C21	−178.5 (4)
C6—C7—C8—C3	0.0 (7)	O23—C19—C20—O25	−0.4 (5)
C8—C3—C4—C5	−1.0 (7)	O25—C20—C21—C22	−178.4 (4)
Cl9—C6—C7—C8	−179.8 (3)	O25—C26—C27—O28	−7.9 (6)
C14—C15—C16—C17	−137.6 (5)	O25—C26—C27—O29	171.8 (3)
C15—C16—C17—C18	163.5 (4)	C26—C27—O29—C30	179.3 (3)
C15—C16—C17—C22	−16.3 (7)	C27—O29—C30—C31	173.4 (4)
C16—C17—C18—C19	179.8 (4)	O28—C27—O29—C30	−1.1 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*AA*···O23^{i}	0.91	2.49	3.025 (5)	118
N2—H2*AA*···O25^{i}	0.91	2.47	3.377 (5)	174
N2—H2*AB*···O28^{ii}	0.91	2.22	3.085 (5)	158
C26—H26*A*···Cl9	0.99	2.73	3.581 (4)	144

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*+1, −*y*, −*z*+1.