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Mixed natural arylolefin–quinoline platinum(II) complexes: synthesis, structural characterization and *in vitro* cytotoxicity studies

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Five new platinum(II) complexes bearing a eugenol and a quinoline derivative, namely [η^2 -4-allyl-2-methoxy-1-(propoxycarbonylmethoxy)benzene]-*trans*-dichlorido(quinoline- κ N)platinum(II), [PtCl₂(C₁₅H₂₀O₄)(C₉H₇N)], (**2**), [η^2 -4-allyl-2-methoxy-1-[(propan-2-yloxy)carbonylmethoxy]benzene]-*trans*-dichlorido(quinoline- κ N)platinum(II), [PtCl₂(C₁₅H₁₉O₄)(C₉H₇N)], (**3**), [η^2 -4-allyl-2-methoxy-1-(propoxycarbonylmethoxy)benzene]chlorido(quinolin-8-olato- κ^2 N,*O*)platinum(II), [Pt(C₉H₆NO)Cl(C₁₅H₂₀O₄)], (**4**), [η^2 -4-allyl-2-methoxy-1-[(propan-2-yloxy)carbonylmethoxy]benzene]chlorido(quinolin-8-olato- κ^2 N,*O*)platinum(II), [Pt(C₉H₆NO)Cl(C₁₅H₂₀O₄)], (**5**), and [η^2 -4-allyl-2-methoxy-1-(propoxycarbonylmethoxy)benzene]chlorido(quinolin-2-carboxylato- κ^2 N,*O*)platinum(II), [Pt(C₁₀H₆NO₂)Cl(C₁₅H₂₀O₄)], (**6**), have been synthesized and fully characterized spectroscopically. A single-crystal X-ray diffraction study was carried out for complexes (**2**) and (**4**)–(**6**). PrEug [or 4-allyl-2-methoxy-1-(propoxycarbonylmethoxy)benzene] in (**2**), (**4**) and (**6**), and ¹PrEug (the propan-2-yloxy analogue of PrEug) in (**3**) and (**5**) coordinate with Pt^{II} at the ethylenic double bond of the allyl group. In (**2**)–(**6**), the donor N atom of the amine group occupies a *trans* position with respect to the double bond. A comparison of the IC₅₀ values of 0.38–29.23 μ M for (**2**)–(**6**) with cisplatin, as well as other platinum(II) complexes, indicates an excellent *in vitro* cytotoxicity against the KB, LU, Hep-G2 and MCF-7 cancer cell lines, with the highest cytotoxic effect (IC₅₀ = 0.38–1.99 μ M) being for complexes (**4**) and (**5**) bearing a quinolin-8-olate ligand.

1. Introduction

Although metal-containing drugs form only a small portion of the approved clinical drugs, platinum-based drugs, such as cisplatin, carboplatin and oxaliplatin, are still essential anticancer agents in cancer chemotherapy (Johnstone *et al.*, 2014). Nevertheless, the unwanted side effects and the evolution of drug resistance during therapy of these drugs has been stimulating chemists to develop less toxic, more effective and target-specific metal-based anticancer drugs (Luo *et al.*, 2014). Therefore, numerous platinum(II) complexes bearing natural bioactive ligands, such as safrole (Da *et al.*, 2015), caffeine (Pneumatikakis, 1984; Shahabadi & Moeini, 2015), derivatives of caffeine (Romerosa *et al.*, 2004; Zhang *et al.*, 2015), oleanolic acid (Fang *et al.*, 2016), propyl gallate (Massoni *et al.*, 2017) and peptides (Johnstone *et al.*, 2016), were synthesized and demonstrated antitumour activities.

Eugenol or 4-allyl-2-methoxyphenol [part (a) in Scheme 1] is a major constituent of a number of medicinal plants, such as clove (*Syzygium aromaticum*) and tulsi (*Ocimum sanctum* L.).

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Eugenol possesses various interesting activities, such as anti-viral (Tragoolpua & Jatisatienr, 2007), antibacterial (Gill & Holley, 2004), antifungal (Chami *et al.*, 2004), anti-inflammatory and anesthetic properties (Pramod *et al.*, 2013). Thus, eugenol has been recognized as a potent pharmacological phytochemical and is applied in the fragrance and flavouring industries (Pramod *et al.*, 2013). Recently, eugenol and its derivatives [Meug and EtEug; part (a) in Scheme 1] have been introduced into the coordination entity of platinum(II) in series of complexes bearing amines (Chi *et al.*, 2017a,b; Da *et al.*, 2015). Most of these complexes bearing quinoline or a chelator derived from quinolin-8-ol exhibit significant inhibitory activities on the tested human cancer cells, especially on the KB and Hep-G2 cell lines, with $IC_{50} = 0.43\text{--}9.58\text{ }\mu\text{M}$. However, crystal data for these complexes are very limited, some examples being the crystal structures of [PtCl(Cl-QO)(Eug)] (Chi *et al.*, 2017a) and [Pt(EtEug-1H)(Qui-COO)] (Da *et al.*, 2015). Moreover, complexes bearing propyl eugenoxycetate (PrEug) or isopropyl eugenoxycetate (ⁱPrEug) [part (a) in Scheme 1] and amines have not been studied so far.

In continuation of promising results on complexes containing derivatives of eugenol and quinoline, we report herein the synthesis and solution structure of five platinum(II) complexes bearing PrEug or ⁱPrEug (AlkEug) and quinolines [part (b) in Scheme 1], as well as their *in vitro* cytotoxicity on the human cancer cell lines KB, Lu, Hep-G2 and MCF-7. In addition, the crystal structures of four of the five complexes have been investigated.

2. Experimental

Unless otherwise noted, all operations were performed without taking precautions to exclude air and moisture. All solvents and chemicals were used as received without further treatment if not noted otherwise. Amines were purchased from Sigma–Aldrich. *Ocimum sanctum* L. oil, extracted from tulsi plants and bearing about 70% eugenol, was purchased

from the Essential Oils & Aroma Joint Stock Company – Vietnam Academy of Science and Technology.

Pt was analyzed according to the weight method (Ghelman *et al.*, 1949) and C, H and N were analyzed on a LECO CHNS model 932 elemental analyzer. ESI–MS spectra were recorded on an 1100 LC-MSD-Trap-SL instrument. IR spectra were recorded on an IMPACK-410 NICOLET spectrometer in the range 400–4000 cm^{−1}. ¹H NMR spectra were recorded on a Bruker AVANCE 500 MHz at 298–300 K, and the chemical shifts (δ) were internally referenced by the residual solvent signals relative to tetramethylsilane (TMS). The ESI mass spectra (Fig. S1, S6, S10–S13, S17 and S18) and the ¹H NMR spectra (Fig. S2–S5, S7–S9, S14–S16 and S19–S24) are given in the supporting information.

2.1. Synthesis and crystallization

2.1.1. Synthesis of AlkEug (PrEug and ⁱPrEug). A mixture of eugenoxycetic acid [2.22 g, 10 mmol; prepared from *Ocimum sanctum* L. oil according to the synthetic protocol of Labarrios *et al.* (1999)] in propan-1-ol (30 ml) (for PrEug) or propan-2-ol (for ⁱPrEug) and H₂SO₄ (0.5 ml) was refluxed for 20 h. The reaction solution was concentrated to ~5 ml under reduced pressure and was then neutralized with an Na₂CO₃ solution. The resulting mixture was extracted and washed with warm water (5 × 5 ml) to afford the product as a yellowish oil after drying under vacuum for 2 h.

PrEug: yield 1.11 g (42%). IR (cm^{−1}, ν): 3060, 2972, 2840 (CH); 1758 (C=O); 1640, 1590, 1520 (C=C). ¹H NMR (500 Hz, CD₃COCD₃, ppm): δ 6.86 (*d*, ³*J* = 8.0 Hz, 1H, Ar-*H*), 6.84 (*d*, ⁴*J* = 1.5 Hz, 1H, Ar-*H*), 6.68 (*dd*, ³*J* = 8.0, ⁴*J* = 1.5 Hz, 1H, Ar-*H*), 5.96 (*m*, 1H, CH=CH₂), 5.07 (*dd*, ³*J* = 15.0, ²*J* = 1.5 Hz, 1H, CH=CH₂), 5.01 (*dd*, ³*J* = 10.0, ²*J* = 1.5 Hz, 1H, CH=CH₂), 4.65 (*s*, 2H, OCH₂), 4.10 (*t*, ³*J* = 7.0 Hz, 2H, CH₂CH₂CH₃), 3.82 (*s*, 3H, OCH₃), 3.32 (*d*, ³*J* = 7.0 Hz, 1H, CH₂-CH), 1.67 (*m*, 2H, CH₂CH₂CH₃), 0.91 (*t*, ³*J* = 7.0 Hz, 3H, CH₂CH₂CH₃).

ⁱPrEug: yield 1.19 g (45%). IR (cm^{−1}, ν): 3050, 2968, 2835 (CH); 1760 (C=O); 1640, 1593, 1515 (C=C). ¹H NMR (500 Hz, CD₃COCD₃, ppm): δ 6.85–6.84 (*ov*, 2H, Ar-*H*), 6.69 (*dd*, ³*J* = 8.0, ⁴*J* = 1.5 Hz, 1H, Ar-*H*), 5.96 (*m*, 1H, CH=CH₂), 5.09–5.00 (*ov*, 3H, CH=CH₂, OCH), 4.61 (*s*, 2H, OCH₂), 3.81 (*s*, 3H, OCH₃), 3.32 (*d*, ³*J* = 7.0 Hz, 2H, CH₂-CH), 1.23 [*d*, ³*J* = 6.5 Hz, 6H, CH(CH₃)₂].

2.1.2. Synthesis of K[PtCl₃(PrEug)], (1a), and K[PtCl₃(ⁱPrEug)], (1b). PrEug [for (1a)] or ⁱPrEug [for (1b)] (2.90 g, 11.0 mmol) was mixed with Zeise's salt {K[PtCl₃(C₂H₄)]·H₂O; 3.86 g, 10.0 mmol}. The reaction mixture was stirred thoroughly for 1 h at ambient temperature until it began to transform into a viscous state and was then washed with diethyl ether (3 × 5 ml). The product was obtained as a yellow powder. The yield was 562 mg (93%) for (1a) and 574 mg (95%) for (1b). The ESI–MS, IR and ¹H NMR spectra of (1a) and (1b) have been described by Chi *et al.* (2013) and Thong & Chi (2014), respectively.

2.1.3. Synthesis of *trans*-[PtCl₂(PrEug)(Qui)], (2). A solution of quinoline (130 μl, 1.1 mmol) in ethanol (5 ml) was

added slowly with stirring at room temperature to a suspension of (**1a**) (604 mg, 1.0 mmol) in ethanol (10 ml) for 1 h. The reaction mixture was stirred for a further 2 h and then filtered through Celite to give a clear light-yellow solution. Slow evaporation of the solvent of the obtained solution under ambient conditions over a period of 8 h afforded yellow crystals, which were suitable for X-ray diffraction and other analyses. The yield was 592 mg (90%). Analysis calculated for $C_{24}H_{27}Cl_2NO_4Pt$: Pt 29.64, C 43.77, H 4.10, N 2.13; found: Pt 30.14, C 43.92, H 3.98, N 2.24%. ESI-MS (m/z , intensity), –MS: 1023, 100%, $[2(M - Qui - HCl) + Cl]^-$; 567, 55%, $[M - Qui + Cl]^-$. IR (cm^{-1} , ν): 3054, 2961, 2930 (CH); 1751 (C=O); 1590, 1511, 1460 (C=C, C=N). 1H NMR (500 Hz, CD_3COCD_3 , ppm): δ 9.03 (d , $^3J = 5.0$ Hz, 1H, Ar-*H*), 8.82 (br , 1H, Ar-*H*), 8.68 (d , $^3J = 8.0$ Hz, 1H, Ar-*H*), 8.15 (d , $^3J = 8.0$ Hz, 1H, Ar-*H*), 7.89 (t , $^3J = 8.0$ Hz, 1H, Ar-*H*), 7.82 (dd , $^3J = 5.0$; 8.0 Hz, 1H, Ar-*H*), 7.78 (t , $^3J = 8.0$ Hz, 1H, Ar-*H*), 7.29 (d , $^4J = 1.5$ Hz, 1H, Ar-*H*), 7.11 (dd , $^3J = 8.0$, $^4J = 1.5$ Hz, 1H, Ar-*H*), 7.03 (d , $^3J = 8.0$ Hz, 1H, Ar-*H*), 5.91 (m , $^2J_{Pt-H} = 70$ Hz, 1H, CH=CH₂), 4.83 (dd , $^3J = 14.0$, $^2J = 1.5$, $^2J_{Pt-H} = 70$ Hz, 1H, CH=CH₂), 4.80 (s , 2H, OCH₂), 4.72 (dd , $^3J = 8.0$, $^2J = 1.5$, $^2J_{Pt-H} = 70$ Hz, 1H, CH=CH₂), 4.15 (t , $^3J = 7.0$ Hz, 2H, CH₂CH₂CH₃), 3.79 (s , 3H, OCH₃), 3.61 (dd , $^2J = 15$, $^3J = 9.5$ Hz, 1H, CH₂-CH), 3.31 (dd , $^2J = 15$, $^3J = 5.0$ Hz, 1H, CH₂-CH), 1.67 (m , 2H, CH₂CH₂CH₃), 0.93 (t , $^3J = 7.0$ Hz, 3H, CH₂CH₂CH₃).

2.1.4. Synthesis of *trans*-[PtCl₂(ⁱPrEug)(Qui)], (3**).** Complex (**3**) was prepared starting from (**1b**) (604 mg, 1.0 mmol) and quinoline (130 μ l, 1.1 mmol), according to the procedure for the preparation of (**2**). The yield was 599 mg (91%) as small yellow crystals. Analysis calculated for $C_{24}H_{27}Cl_2NO_4Pt$: Pt 29.64, C 43.77, H 4.10, N 2.13; found: Pt 30.08, C 43.56, H 4.18, N 2.02%. ESI-MS (m/z , intensity), –MS: 1022, 100%, $[2(M - Qui - HCl) + Cl]^-$; 528, 30%, $[M - Qui - HCl + Cl]^-$. IR (cm^{-1}): 3054, 2951, 2930 (CH); 1751 (C=O); 1590, 1511, 1460 (C=C, C=N). 1H NMR (500 Hz, CD_3COCD_3 , ppm): δ 9.02 (d , $^3J = 5.0$ Hz, 1H, Ar-*H*), 8.82 (br , 1H, Ar-*H*), 8.68 (d , $^3J = 8.0$ Hz, 1H, Ar-*H*), 8.14 (d , $^3J = 8.0$ Hz, 1H, Ar-*H*), 7.89 (t , $^3J = 8.0$ Hz, 1H, Ar-*H*), 7.82 (dd , $^3J = 5.0$; 8.0 Hz, 1H, Ar-*H*), 7.77 (t , $^3J = 8.0$ Hz, 1H, Ar-*H*), 7.28 (d , $^4J = 1.5$ Hz, 1H, Ar-*H*), 7.11 (dd , $^3J = 8.0$, $^4J = 1.5$ Hz, 1H, Ar-*H*), 7.01 (d , $^3J = 8.0$ Hz, 1H, Ar-*H*), 5.91 (m , $^2J_{Pt-H} = 70$ Hz, 1H, CH=CH₂), 5.10 (m , 1H, OCH), 4.83 (dd , $^3J = 14$, $^2J = 1.5$, $^2J_{Pt-H} = 70$ Hz, 1H, CH=CH₂), 4.74 (s , 2H, OCH₂), 4.72 (dd , $^3J = 8.5$, $^2J = 1.5$, $^2J_{Pt-H} = 70$ Hz, 1H, CH=CH₂), 3.79 (s , 3H, OCH₃), 3.61 (dd , $^2J = 15$, $^3J = 9.0$ Hz, 1H, CH₂-CH), 3.31 (dd , $^2J = 15$, $^3J = 5.0$, $^3J_{Pt-H} = 50$ Hz, 1H, CH₂-CH), 1.26 [d , $^3J = 6.5$ Hz, 6H, CH(CH₃)₂].

2.1.5. Synthesis of [PtCl(Qui-O)(PrEug)], (4**).** Complex (**4**) was prepared starting from (**1a**) (604 mg, 1.0 mmol) and quinolin-8-ol (145 mg, 1.0 mmol), according to the procedure for the preparation of (**2**). The yield was 587 mg (92%) of orange-yellow crystals which were suitable for X-ray diffraction and other analyses. Analysis calculated for $C_{24}H_{26}ClNO_5Pt$: Pt 30.56, C 45.14, H 4.08, N 2.19; found: Pt 30.94, C 45.32, H 4.23, N 2.29%. ESI-MS (m/z , intensity), +MS: 640, 50%, $[M + H]^+$; 603, 100%, $[M - Cl]^+$; –MS: 637, 45%, $[M -$

$H]^-$; 596, 100%, $[M - C_3H_7]^-$; 409, 25%, $[M - PrEug + Cl]^-$. The data for the IR and 1H NMR spectra of (**4**) have been described by Chi *et al.* (2014).

2.1.6. Synthesis of [PtCl(Qui-O)(ⁱPrEug)], (5**).** Complex (**5**) was prepared starting from (**1b**) (604 mg, 1.0 mmol) and quinolin-8-ol (145 mg, 1.0 mmol), according to the procedure for the preparation of (**2**). The yield was 574 mg (90%) of orange-yellow crystals which were suitable for X-ray diffraction and other analyses. Analysis calculated (%) for $C_{24}H_{26}ClNO_5Pt$: Pt 30.56, C 45.14, H 4.08, N 2.19; found: Pt 30.69, C 45.01, H 4.19, N 2.26%. ESI-MS (m/z , intensity), +MS: 640, 35%, $[M + H]^+$; 603, 100%, $[M - Cl]^+$; 561, 30%, $[M - Cl]^+$; –MS: 637, 100%, $[M - H]^-$; 596, 15%, $[M - C_3H_7]^-$; 409, 75%, $[M - PrEug + Cl]^-$. IR (cm^{-1} , ν): 3075, 2933, 2850 (CH); 1753 (C=O); 1583, 1500; 1462 (C=C, C=N). 1H NMR (500 Hz, CD_3COCD_3 , ppm): δ 9.07 (d , $^3J = 5.0$, $^3J_{Pt-H} = 34$ Hz, 1H, Ar-*H*), 8.76 (d , $^3J = 8.0$ Hz, 1H, Ar-*H*), 7.82 (dd , $^3J = 5.0$, 8.0 Hz, 1H, Ar-*H*), 7.51 (t , $^3J = 8.0$ Hz, 1H, Ar-*H*), 7.23 (d , $^3J = 8.0$ Hz, 1H, Ar-*H*), 7.15 (d , $^4J = 1.5$ Hz, 1H, Ar-*H*), 7.06 (d , $^3J = 8.0$ Hz, 1H, Ar-*H*), 6.92 (dd , $^3J = 8.0$, $^4J = 1.5$ Hz, 1H, Ar-*H*), 6.81 (d , $^3J = 8.0$ Hz, 1H, Ar-*H*), 5.61 (m , $^2J_{Pt-H} = 70$ Hz, 1H, CH=CH₂), 5.00 (m , 1H, OCH), 4.76 (d , $^3J = 14$, $^2J_{Pt-H} = 70$ Hz, 1H, CH=CH₂), 4.74 (d , $^3J = 9.0$, $^2J_{Pt-H} = 70$ Hz, 1H, CH=CH₂), 4.57 (s , 2H, OCH₂), 3.60 (dd , $^2J = 15$, $^3J = 7.5$ Hz, 1H, CH₂-CH), 3.49 (s , 3H, OCH₃), 3.27 (dd , $^2J = 15$, $^3J = 6.0$, $^3J_{Pt-H} = 50$ Hz, 1H, CH₂-CH), 1.19 [d , $^3J = 6.0$ Hz, 6H, CH(CH₃)₂].

2.1.7. Synthesis of [PtCl(Qui-COO)(PrEug)], (6**).** Complex (**6**) was prepared starting from (**1a**) (604 mg, 1.0 mmol) with quinoline-2-carboxylic acid (173 mg, 1.0 mmol) in ethanol (10 ml) at room temperature, according to the procedure for the preparation of **2**. The yield was 593 mg (89%) of small yellow crystals. Single crystals suitable for X-ray diffraction were obtained by slow evaporation within 10 h from a concentrated chloroform solution at ambient temperature. Analysis calculated (%) for $C_{25}H_{26}ClNO_6Pt$: Pt 29.28, C 45.05, H 3.90, N 2.10; found: Pt 29.46, C 45.22, H 3.82, N 2.18. ESI-MS (m/z , intensity), +MS: 667, 25%, $[M + H]^+$; 631, 100%, $[M - Cl]^+$; –MS: 702, 100%, $[M + Cl]^-$; 666, 10%, $[M - H]^-$; 438, 25%, $[M - PrEug + Cl]^-$. IR (cm^{-1} , ν): 3101, 2950 and 2936 (CH); 1751; 1674 (C=O); 1597, 1512 and 1458 (C=C, C=N). 1H NMR (500 Hz, $CDCl_3$, ppm): δ 9.58 (d , $^3J = 8.5$ Hz, 1H, Ar-*H*), 8.68 (d , $^3J = 8.5$ Hz, 1H, Ar-*H*), 8.24 (d , $^3J = 8.5$ Hz, 1H, Ar-*H*), 8.01 (d , $^3J = 8.5$ Hz, 1H, Ar-*H*), 7.94 (t - d , $^3J = 8.5$, $^4J = 1.5$ Hz, 1H, Ar-*H*), 7.80 (t , $^3J = 8.5$ Hz, 1H, Ar-*H*), 6.95 (s , 1H, Ar-*H*), 6.88 (d , $^3J = 8.0$ Hz, 1H, Ar-*H*), 6.78 (d , $^3J = 8.0$ Hz, 1H, Ar-*H*), 5.90 (m , $^2J_{Pt-H} = 70$ Hz, 1H, CH=CH₂), 4.88–4.91 (ov , 2H, CH=CH₂), 4.64 (s , 2H, OCH₂), 4.13 (t , $^3J = 7.0$ Hz, 2H, CH₂CH₂CH₃), 3.83 (s , 3H, OCH₃), 3.57 (br , 1H, CH₂-CH), 3.22 (br , 1H, CH₂-CH), 1.64 (m , 2H, CH₂CH₂CH₃), 0.89 (t , $^3J = 7.0$ Hz, 3H, CH₂CH₂CH₃).

2.2. Refinement

Crystal data, data collection and structure refinement details for (**2**), (**4**), (**5**) and (**6**) are summarized in Table 1. The structures were solved by direct methods using the program SHELXS (Sheldrick, 2008) and were refined with the

Table 1
Experimental details.

	(2)	(4)	(5)	(6)
Crystal data				
Chemical formula	[PtCl ₂ (C ₁₅ H ₂₀ O ₄)(C ₉ H ₇ N)]	[Pt(C ₉ H ₆ NO)Cl(C ₁₅ H ₂₀ O ₄)]	[Pt(C ₉ H ₆ NO)Cl(C ₁₅ H ₂₀ O ₄)]	[Pt(C ₁₀ H ₆ O ₂)Cl-(C ₁₅ H ₂₀ O ₄)]
M_r	659.45	639.00	639.00	667.01
Crystal system, space group	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/c$
Temperature (K)	100	100	200	100
a, b, c (Å)	8.1252 (3), 11.7042 (4), 13.7340 (5)	8.3447 (2), 11.9191 (4), 12.9315 (5)	9.7858 (3), 11.0447 (2), 11.8117 (3)	15.6457 (13), 9.7291 (4), 16.6062 (8)
α, β, γ (°)	65.864 (4), 84.716 (3), 88.191 (3)	63.296 (4), 84.618 (3), 76.484 (3)	85.059 (2), 73.685 (3), 71.139 (2)	90, 111.150 (8), 90
V (Å ³)	1186.82 (9)	1117.09 (7)	1159.41 (6)	2357.5 (3)
Z	2	2	2	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm ⁻¹)	6.17	6.44	6.20	6.11
Crystal size (mm)	0.35 × 0.10 × 0.10	0.25 × 0.25 × 0.10	0.30 × 0.25 × 0.15	0.30 × 0.15 × 0.10
Data collection				
Diffractometer	Agilent SuperNova Dual Source diffractometer with an Eos detector	Agilent SuperNova Dual Source diffractometer with an Eos detector	Agilent SuperNova Dual Source diffractometer with an Eos detector	Agilent SuperNova Dual Source diffractometer with an Eos detector
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2013)	Multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2013)	Multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2013)	Multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2013)
$T_{\min}, T_{\max}$	0.432, 1.000	0.411, 1.000	0.369, 1.000	0.522, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19752, 4867, 4458	18255, 4564, 4417	47800, 4738, 4534	21714, 4030, 3348
R_{int}	0.036	0.029	0.037	0.066
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.625	0.625	0.625	0.588
Refinement				
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.036, 0.073, 1.12	0.021, 0.048, 1.09	0.017, 0.041, 1.10	0.038, 0.086, 1.08
No. of reflections	4867	4564	4738	4030
No. of parameters	337	291	292	316
No. of restraints	14	0	0	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	3.21, -1.79	2.18, -1.45	1.46, -1.01	2.22, -1.14

Computer programs: *CrysAlis PRO* (Agilent, 2013), *SHELXS97* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

SHELXL (Sheldrick, 2015) refinement package using full-matrix least-squares minimization. These programs were implemented within the *OLEX2* package (Dolomanov *et al.*, 2009). H atoms were placed in calculated positions and refined using a riding model, with C—H = 0.95 (aromatic) and 0.98 Å (CH₃), and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2U_{\text{eq}}(\text{C})$ otherwise.

In complex (2), atoms Pt1, Cl2, Cl3, C14 and C15 are disordered, with occupancies converging to 0.656 (8) and 0.344 (8) for the two positions (*A* and *B*). The distances C14—C15 and C15—C16 for both sets were restrained to be equal (SADI command in *SHELXL*), and atoms C14*B* and C15*B* were restrained to approximate isotropic behaviour (ISOR command in *SHELXL*). In complex (6), atoms Pt1 and Cl2 show disorder, with occupancies of 0.930 (1) and 0.070 (1) for the two positions (*A* and *B*). The same anisotropic displacement parameters were used for atoms Pt1*A/B* and Cl2*A/B* (EADP command in *SHELXL*).

2.3. In vitro cell tests

An MTT assay was used to determine the cytotoxic activity of compounds (2)–(6) with human cancer cell lines (KB, LU-1,

Hep-G2 and MCF-7) acquired from the American Type Culture Collection (ATCC, Manassas, VA). Cells were cultured in medium RPMI 1640 supplemented with 10% FBS (Fetal bovine serum) under a humidified atmosphere of 5% CO₂ at 37 °C.

Compounds (2)–(6) were dissolved in DMSO at a concentration of 20 mg ml⁻¹. A series of dilutions for each compound was prepared to final concentrations of 128, 32, 8, 2 and 0.5 µg ml⁻¹. Samples (100 µl) of the complexes with different concentrations were added to the wells on 96-well plates. Cells were separated with trypsin and EDTA, and seeded in each well with 3×10^4 cells per well. An MTT solution (20 µl, 4 mg ml⁻¹) of phosphate buffer saline (8 g NaCl, 0.2 g KCl, 1.44 g Na₂HPO₄ and 0.24 g KH₂PO₄ per l) was added to each well after being incubated for 48 h. The cells were further incubated for 4 h and a purple formazan precipitate was formed, which was separated by centrifugation. The precipitate was dissolved by adding DMSO (100 µl) to each well. The optical density of the solution was determined by a plate reader (TECAN) at 540 nm. The inhibition ratio was achieved on the basis of the optical densities from the calculation of three replicate tests.

3. Results and discussion

3.1. Synthesis and structure of complexes (1)–(6)

Complexes $K[PtCl_3(AlkEug)]$ [$AlkEug$: $PrEug$ (**1a**) or $iPrEug$ (**1b**)] were synthesized by the reaction between Zeise's salt and either $PrEug$ or $iPrEug$, respectively (Chi *et al.*, 2013; Thong & Chi, 2014). The reactions were carried out at 313–318 K in propan-1-ol for (**1a**) and in an acetone–propan-2-ol (1:1 *v/v*) mixture for (**1b**) in 2–3 h with high yields (92–95%). Encouraged by the effective synthetic procedure of $K[PtCl_3(eugenol)]$ by the interaction between Zeise's salt and eugenol without solvent at room temperature (Chi *et al.*, 2017b), we applied this protocol for producing (**1a**) and (**1b**) in this research and obtained the products with the same yields (93–95%).

Complexes (**2**)–(**6**) were prepared as shown in Scheme 2 in good yields (89–92%). The reactions were carried out at 298–303 K in ethanol with a $K[PtCl_3(AlkEug)]$ –amine molar ratio of 1:1.1, with the amine being quinoline (Qui), and a 1:1 molar

ratio in the case of quinolin-8-ol (Qui-OH) and quinoline-2-carboxylic acid (Qui-COOH). The neutral complexes (**2**)–(**6**) were obtained easily as crystals by evaporation of the reaction solvent at room temperature. The crystals of compounds (**2**), (**4**) and (**5**) were suitable for X-ray diffraction. For (**6**), suitable crystals were obtained from a concentrated chloroform solution at room temperature. Despite numerous efforts, we were unable to obtain suitable crystals of (**3**). The complexes are well soluble in $CHCl_3$, $(CH_3)_2CO$ and DMSO, but insoluble in water and Et_2O . Complexes (**2**), (**5**) and (**6**) are yellow crystals, while (**3**) and (**4**) are orange–yellow crystals. Surprisingly, our attempt to synthesize the pure complex $[PtCl(Qui-COO)(iPrEug)]$ using the same procedure as for the preparation of (**4**)–(**6**) was unsuccessful. The product was a mixture of three complexes, namely $[PtCl(Qui-COO)(iPrEug)]$, *trans*- $[Pt(Qui-COO)_2]$ and *cis*- $[Pt(Qui-COO)_2]$, with a molar ratio of 1:0.15:0.05 (determined by 1H NMR spectroscopy). The desired complex could not be isolated from the mixture despite many trials. The synthetic method for (**4**) was different from the previously reported route by which (**4**) was obtained in powder form and not as single crystals (Chi *et al.*, 2014).

Based on the analysis of the IR, ESI–MS, NMR and XRD spectra which is presented below, the structures of the examined complexes were determined as displayed in Scheme 2. It can be observed from Scheme 2 that for the reaction of quinoline with (**1a**)/(**1b**), two complexes, namely *trans*- $[PtCl_2(AlkEug)(Qui)]$, (**2**) and (**3**), were obtained by replacement of the Cl ligand, which is in a *trans* position to the $AlkEug$ in $K[PtCl_3(AlkEug)]$, by the quinoline ligand. However, the interaction between $K[PtCl_3(AlkEug)]$ and the two amines Qui-OH and Qui-COOH gave no *trans*- $[PtCl_2(AlkEug)(amine)]$, but $[PtCl(amine-1H)(AlkEug)]$, *i.e.* (**4**)–(**6**), in which the amines (Qui-OH and Qui-COOH) are deprotonated and coordinate with Pt^{II} *via* both the N and O atoms, as displayed in Scheme 2. The analogous coordination of Qui-OH and Qui-COOH with Pt^{II} was also observed when they were reacted with $K[PtCl_3(L)]$ (L is safrole, eugenol, methyleugenol or piperidine) (Chi *et al.*, 2014, 2017a; Da *et al.*, 2015).

Some ions detected by the ESI mass spectra of (**2**)–(**6**) are listed in Table 2. The isotopic envelopes match with the calculated patterns, as illustrated in Fig. S25 of the supporting information using the zoom scan spectrum of the $[(6)-Cl]^+$ fragment as an example. The partial negative spectra of (**3**)

Table 2

Cations and anions detected by ESI mass spectroscopy (*m/z*, %) for complexes (**2**)–(**6**) and several other platinum(II) complexes.

Complexes	$[M - Cl]^+$	$[M + H]^+$	$[M - H]^-$	$[M - AlkEug + Cl]^-$	$[2(M - Qui - HCl) + Cl]^-$
$[PtCl_2(PrEug)(Qui)]$ (2)	–	–	–	–	1022 (100)
$[PtCl_2(iPrEug)(Qui)]$ (3)	–	–	–	–	1022 (100)
$[PtCl(Qui-O)(PrEug)]$ (4)	603 (100)	640 (50)	637 (45)	409 (40)	–
$[PtCl(Qui-O)(iPrEug)]$ (5)	603 (100)	640 (35)	637 (100)	409 (75)	–
$[PtCl(Qui-COO)(PrEug)]$ (6)	631 (100)	667 (25)	666 (10)	438 (25)	–
$[PtCl(Qui-O)(Eug)]^a$	503 (100)	540 (25)	–	–	–
$[PtCl(MeQui-O)(Eug)]^b$	517 (100)	553 (10)	–	–	–
$[PtCl(NO_2Qui-O)(Eug)]^b$	548 (100)	584 (80)	–	–	–
$[PtCl(ClQui-O)(Eug)]^b$	571 (100)	607 (20)	–	–	–

References: (a) Chi *et al.* (2017a); (b) Chi *et al.* (2017b).

and (6), and the partial positive mass spectrum of (5) are shown in Fig. 1 as representatives.

The data in Table 2 show that base peaks with a relative intensity of 100% at m/z 1022 au (Fig. 1a), consistent with pseudomolecular anions $[2(M - \text{Qui} - \text{HCl}) + \text{Cl}]^-$, i.e. $[\text{Pt}_2\text{Cl}_3(\text{AlkEug-1H})_2]^-$, were observed in the ESI mass spectra of complexes (2)–(3). This provides evidence for the proposed quinoline coordination. For (4)–(6), the pseudomolecular cations $[M - \text{Cl}]^+$, with a relative intensity of 100%, i.e. $[\text{Pt}(\text{amine})(\text{AlkEug})]^+$ (Fig. 1b), and $[M - \text{AlkEug} + \text{Cl}]^-$ peaks (25–75%), i.e. $[\text{PtCl}_2(\text{amine})]^-$ (Fig. 1c), were detected in the ESI mass spectra, showing the presence of AlkEug and the amines in these complexes.

In addition, the assigned results have established two unambiguous rules for the formation of pseudomolecular ions in the mass spectra of (2)–(6). Specifically, in the negative-ion mode, complexes (2) and (3), bearing the monodentate amine (Qui), tend to combine together to create the dimeric complexes $[\text{Pt}_2\text{Cl}_2(\text{AlkEug-1H})_2]$. These dimers further combine with Cl^- to form the pseudomolecular anions $[\text{Pt}_2\text{Cl}_3(\text{AlkEug-1H})_2]^-$ with the highest intensity in the negative-mode mass spectra (see Scheme 3). The formation of the analogous pseudomolecular ion, $[\text{Pt}_2\text{Cl}_3(\text{Eug-1H})_2]^-$, was also observed in the negative mode ESI–MS of $[\text{Pt}_2\text{Cl}_2(\text{Eug-1H})_2]$ (Chi *et al.*, 2018).

Scheme 3

Unlike (2) and (3), complexes (4)–(6), containing the chelating ligand Qui-O or Qui-COO, have no tendency to create pseudomolecular $[\text{Pt}_2\text{Cl}_3(\text{AlkEug-1H})_2]^-$ peaks in the –MS spectra, but form $[M - \text{H}]^-$ and $[M - \text{AlkEug} + \text{Cl}]^-$ peaks with intensities of 25–75%. Base peaks for the $[M - \text{Cl}]^+$ cations and peaks with different intensities for the $[M + \text{H}]^+$ cations were observed in all the +MS spectra of (4)–(6), as well as of their analogues (Table 2). This is associated with the reactions shown in Scheme 4.

The strong absorption band for $\nu_{\text{C=O}}$ at 1762–1751 cm^{-1} in the IR spectra of (2)–(6) shows the presence of AlkEug in the coordination sphere. Moreover, the absence of a band at 1640 cm^{-1} for $\nu_{(\text{C}=\text{C} \text{ allyl})}$ indicates that the allyl group in (2)–(6) has coordinated with Pt^{II} in a η^2 manner. Besides, in the IR spectra of (4)–(6), there is no evidence for a ν_{OH} band, indi-

cating that quinolin-8-ol and quinoline-2-carboxylic acid have been deprotonated and coordinate to Pt^{II} via the N and O atoms.

These deprotonation and coordination of Qui-OH and Qui-COOH in (4)–(6) are not only observed in analogous platinum(II) complexes (Chi *et al.*, 2017a,b; Da *et al.*, 2015), but also in other platinum(II) complexes (Kato *et al.*, 2002; Fang *et al.*, 2016).

Scheme 4

The proton signals are assigned based on their chemical shift (δ), intensity, shape and spin–spin splitting pattern. The results (see *Experimental*) demonstrate fully the proton signals of AlkEug and the amines present in (2)–(6). To elucidate the coordination of the ligands with Pt^{II} in the examined complexes, the signals of the allyl protons of AlkEug, as well as H12 and H18 of the amines in (2)–(6), are listed in Table 3.

For free AlkEug, two H8 protons give rise to a doublet at 3.32 ppm, but in the spectra of (2)–(6), there are two separate signals (in the form of a doublet of doublets) for H8a and H8b. Moreover, the resonances of the ethylenic protons (H9 and H10) shift upfield in comparison to those of noncoordinated AlkEug and their ^{195}Pt satellites are clear ($^2J_{\text{Pt-H}} = 70 \text{ Hz}$). All these observations are in good agreement with the observations in the spectra of complexes containing similar allyl-benzenes ($\text{Ar}-\text{CH}_2-\text{CH}=\text{CH}_2$) (Chi *et al.*, 2017a,b; Da *et al.*, 2015) and indicate that AlkEug in (2)–(6) have coordinated with Pt^{II} via the allyl group as a η^2 ligand. Fig. 2 presents

Figure 1

A partial negative mass spectra of (a) (3) and (c) (6), and a partial positive spectrum of (b) (5).

Table 3

Chemical shift (ppm), multiplicity and coupling constant $J_{\text{Pt-H}}$ (Hz) of atoms H8, H9, H10, H12 and H18 in free AlkEug and in (1)–(6)^a.

Compound	H8a	H8b	H9	H10 _{trans}	H10 _{cis}	H12	H18
Free PrEug	3.32 <i>d</i>		5.96 <i>m</i>	5.06 <i>dd</i>	5.01 <i>dd</i>		
Free ¹ PrEug	3.32 <i>d</i>		5.96 <i>m</i>	5.08–5.00 <i>ov</i>			
(1a) ^b	2.98 <i>dd</i>	3.49 <i>dd</i>	5.05 <i>m</i> ² $J_{\text{Pt-H}}$ 70	4.30 <i>dd</i> ² $J_{\text{Pt-H}}$ 70	4.13 <i>ov</i>		
(1b) ^c	2.87 <i>dd</i>	3.48 <i>dd</i>	5.00 <i>m</i> ² $J_{\text{Pt-H}}$ 70	4.27 <i>dd</i> ² $J_{\text{Pt-H}}$ 70	4.10 <i>dd</i> ² $J_{\text{Pt-H}}$ 70		
(2)	3.31 <i>dd</i>	3.61 <i>dd</i>	5.91 <i>m</i> ² $J_{\text{Pt-H}}$ 70	4.83 <i>dd</i> ² $J_{\text{Pt-H}}$ 70	4.72 <i>dd</i> ² $J_{\text{Pt-H}}$ 70	9.03 <i>d</i>	8.82 <i>br</i>
(3)	3.31 <i>dd</i> ³ $J_{\text{Pt-H}}$ 50	3.61 <i>dd</i>	5.91 <i>m</i> ² $J_{\text{Pt-H}}$ 70	4.83 <i>dd</i> ² $J_{\text{Pt-H}}$ 70	4.72 <i>dd</i> ² $J_{\text{Pt-H}}$ 70	9.02 <i>d</i>	8.82 <i>br</i>
(4) ^d	3.27 <i>dd</i> ³ $J_{\text{Pt-H}}$ 50	3.59 <i>dd</i>	5.59 <i>m</i> ² $J_{\text{Pt-H}}$ 70	4.76 <i>d</i> ² $J_{\text{Pt-H}}$ 70	4.73 <i>d</i> ² $J_{\text{Pt-H}}$ 70	9.07 <i>d</i> ³ $J_{\text{Pt-H}}$ 34	
(5)	3.27 <i>dd</i> ³ $J_{\text{Pt-H}}$ 50	3.60 <i>dd</i>	5.61 <i>m</i> ² $J_{\text{Pt-H}}$ 70	4.76 <i>d</i> ² $J_{\text{Pt-H}}$ 70	4.74 <i>d</i> ² $J_{\text{Pt-H}}$ 70	9.07 <i>d</i> ³ $J_{\text{Pt-H}}$ 34	
(6) ^e	3.22 <i>br</i>	3.57 <i>br</i>	5.90 <i>m</i> ² $J_{\text{Pt-H}}$ 70	4.88–4.91 <i>ov</i>	4.88–4.91 <i>ov</i>		9.58 <i>d</i>

Notes/references: (a) acetone-*d*₆; (b) Chi *et al.* (2013); (c) Thong & Chi (2014); (d) Chi *et al.* (2014); (e) chloroform-*d*₁.

the signals of the allyl protons and H12 and H18 in (3) as an example.

Upon coordination of the amines with Pt^{II}, all the resonances of the ethylenic protons of AlkEug shift remarkably downfield compared to the parent complex (1a) [for (2), (4) and (6)] and (1b) [for (3) and (5)] (Table 3). Two ¹⁹⁵Pt satellites in the doublet at 9.07 ppm from H12 of Qui-O in (4) and (5) are clear, with a ³ $J_{\text{Pt-H}}$ value of 34 Hz [for (2) and (3), the ¹⁹⁵Pt satellites in the signal of H12 are broadened beyond detection (Fig. 2)]. This value is comparable in magnitude to ³ $J_{\text{Pt-H}}$ in analogous platinum(II) complexes (Chi *et al.*, 2017a,b; Da *et al.*, 2015). The signal of H18 in (2) and (3) becomes broadened (Fig. 2). This may be due to the anisotropic effect of the Pt—(C=C_{allyl}) bond on the quinoline ligand, depending on the orientation of the quinoline plane with respect to the coordination plane of Pt^{II}. In addition, the signal at 9.58 ppm of H18 in (6) is significantly downfield compared to quinoline-2-carboxylic acid (8.01 ppm).

In order to confirm the configuration of the examined complexes and to determine concretely the position of the donor N atom of the quinoline derivatives in the coordination entity, as well as the molecular arrangement of the complexes, single-crystal X-ray diffraction was initiated.

Figure 2

A partial ¹H NMR spectrum of (3); ¹⁹⁵Pt satellites are indicated by asterisks (*).

3.2. Crystal structures of complexes (2), (4)–(6)

Complexes (2), (4) and (5) crystallize in the triclinic space group $P\bar{1}$, whereas complex (6) crystallizes in the monoclinic space group $P2_1/c$. The central Pt^{II} atom in (2) displays a distorted square-planar coordination with a *trans* positioning of the two Cl atoms (Fig. 3). The coordination is further completed by the N atom of quinoline and the C=C double bond of PrEug. Part of the complex (atoms Pt1, Cl2, Cl3, C14 and C15) is disordered, with population parameters of 0.656 (8) and 0.344 (8) for positions *A* and *B*, respectively. The dihedral angle between the best planes through the quinoline and phenyl rings is 74.4 (2)°. An intramolecular C—H... π interaction is present (Fig. 3 and Table 4) and the packing is built up by C—H...O (Table 4) and π – π interactions

Figure 3

The molecular structure of complex (2), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. The fragment with a population parameter of 0.341 (8) is shown in blue and the intramolecular C—H... π interaction is shown as a grey dotted line.

Figure 4

Packing diagram for (2), showing the C—H...O (red dashed lines), π — π (black) and C=O... π (black) interactions. [Symmetry codes: (i) $-x + 2, -y + 2, -z + 1$; (ii) $-x + 1, -y + 1, -z + 1$.]

($Cg1 \cdots Cg1^i = 3.557(3) \text{ \AA}$; $Cg1$ is the centroid of ring C8–C13; symmetry code: (i) $-x + 2, -y + 2, -z + 1$; Fig. 4). Atom O28 interacts with the phenyl ring of PrEug [$O28 \cdots Cg2^{ii} = 3.978(4) \text{ \AA}$; $Cg2$ is the centroid of ring C17–C22; symmetry code: (ii) $-x + 1, -y + 1, -z + 1$; Fig. 4].

In complex (4), the quinoline ligand is now replaced by quinolin-8-ol. The crystal structure determination confirms the deprotonation of quinolin-8-ol and the Pt^{II} coordination consisting of a Cl atom, the C=C double bond of PrEug and the N and O atoms of quinolin-8-olate (with the C=C double bond and N atom *trans* with respect to each other) (Fig. 5). The dihedral angle between the best planes through the quinoline and phenyl rings is $78.70(14)^\circ$. Centrosymmetric dimers are formed at one end by ring–metal interactions

Figure 5

The molecular structure of complex (4), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Intramolecular C—H...O interactions are shown as red dotted lines and the intramolecular C—H... π interaction is shown as a grey dotted line.

Table 4

Hydrogen-bond geometry ($\text{\AA}, ^\circ$) for (2).

$Cg1$ is the centroid of ring C17–C22.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C6-H6 \cdots O28^{ii}$	0.95	2.47	3.404 (7)	169
$C7-H7 \cdots O23^{ii}$	0.95	2.39	3.324 (7)	168
$C24-H24B \cdots O23^{iii}$	0.98	2.53	3.287 (6)	134
$C12-H12 \cdots Cg1$	0.95	2.93	3.732 (6)	142

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

[$Cg1 \cdots Pt1^i = 3.985 \text{ \AA}$, $Cg1$ is the centroid of ring C6–C11; symmetry code: (i) $-x, -y + 2, -z + 1$] and C—H... π interactions (Table 5), and at the other end by C—H... π inter-

Figure 6

Packing diagram for (4), showing dimer formation at both ends of the complex through C—H... π interactions (grey dotted lines). Parallel chains interact through C—H...O interaction (red dotted line). Symmetry codes are as given in Table 5.

Figure 7

The molecular structure of complex (5), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. An intramolecular C—H...O interaction is shown as a red dotted line and the intramolecular C—H... π interaction is shown as a grey dotted line.

actions (Table 5). Neighbouring chains interact *via* C—H...O interactions (Table 5 and Fig. 6).

The molecular structure of (5) is very similar to that of complex (4) (Fig. 7). Fitting both structures, omitting the propyl groups, gives an r.m.s. deviation of 0.137 Å. The dihedral angle between the best planes through the quinoline and phenyl rings is 75.37 (13)°. Similar centrosymmetric dimers are formed in the crystal packing (Fig. 8 and Table 6). However, no ring–metal interaction is present as the two Pt^{II} ends in the dimer are shifted compared to complex (4). A further consequence of this shifting is that only one of the vinyl H atoms is involved in a C—H... π interaction and that

Table 5

Hydrogen-bond geometry (Å, °) for (4).

Cg1 is the centroid of ring C6–C11, Cg2 is the centroid of ring N2/C3–C6/C11 and Cg3 is the centroid of ring C17–C22.

<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>
C16—H16B...O12	0.99	2.45	3.070 (4)	120
C18—H18...O12	0.95	2.57	3.352 (5)	140
C4—H4...O12 ⁱ	0.95	2.57	3.488 (4)	163
C14—H14A...Cg2 ⁱⁱ	0.93	2.94	3.581 (4)	127
C14—H14B...Cg1 ⁱⁱ	0.93	2.88	3.493 (4)	125
C24—H24C...Cg1	0.98	2.91	3.513 (5)	121
C32—H32A...Cg3 ⁱⁱⁱ	0.98	2.84	3.655 (5)	141

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

Table 6

Hydrogen-bond geometry (Å, °) for (5).

Cg1 is the centroid of ring N2/C3–C6/C11, Cg2 is the centroid of ring C6–C11 and Cg3 is the centroid of ring C17–C22.

<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>
C5—H5...O23 ⁱ	0.95	2.46	3.073 (4)	122
C16—H16A...O12	0.99	2.40	3.051 (4)	123
C14—H14B...Cg1 ⁱⁱ	0.99	2.94	3.454 (4)	114
C24—H24B...Cg2	0.98	2.93	3.564 (4)	124
C30—H30...Cg3 ⁱⁱⁱ	1.00	2.96	3.827 (4)	145

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

the C—H...O interactions between neighbouring chains are now through atom O23 and not O12 as in (4).

In complex (6), the quinoline ligand is replaced by quino-line-2-carboxylic acid which is deprotonated and coordinates to Pt^{II} through the N and O atoms (Fig. 9). The Pt^{II} coordi-

Figure 8

Packing diagram for (5), showing dimer formation at both ends of the complex through C—H... π interactions (grey dotted lines). Parallel chains interact through C—H...O interactions (red dotted line). Symmetry codes are as given in Table 6.

Table 7
Hydrogen-bond geometry (Å, °) for (6).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C11-H11\cdots Cl2A$	0.95	2.34	3.211 (8)	153
$C11-H11\cdots Cl2B$	0.95	2.81	3.59 (3)	140
$C16-H16A\cdots O30^i$	0.95	2.55	3.452 (9)	159
$C20-H20\cdots O30^i$	0.95	2.59	3.524 (9)	167
$C28-H28B\cdots Cl2A^{ii}$	0.99	2.64	3.473 (7)	142
$C32-H32A\cdots O30^{iii}$	0.99	2.52	3.459 (10)	158

Symmetry codes: (i) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (ii) $x, -y + \frac{5}{2}, z + \frac{1}{2}$; (iii) $-x + 2, -y + 2, -z + 3$.

nation is completed by a Cl atom and the C=C double bond of PrEug (with the C=C double bond and N atom *trans* with respect to each other). Part of the complex (atoms Pt1 and Cl2) is disordered, with population parameters of 0.930 (1) and 0.070 (1) for positions *A* and *B*, respectively. Both Cl atoms are involved in an intramolecular C—H $\cdots$ Cl interaction (Fig. 9 and Table 7). The dihedral angle between the best planes through the quinoline and phenyl rings is 70.6 (3)°. The packing is built up by C—H $\cdots$ O and C—H $\cdots$ Cl interactions (Fig. 10 and Table 7), and π – π interactions [$Cg1\cdots Cg3^i = 3.807$ (5) Å, $Cg1\cdots Cg1^{iv} = 3.942$ (4) Å and $Cg1\cdots Cg2^{iv} = 3.683$ (5) Å; $Cg1$, $Cg2$ and $Cg3$ are the centroids of rings N3/C4–C7/C12, C7–C12 and C19–C24, respectively; symmetry codes: (i) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (iv) $-x + 1, -y + 2, -z + 1$; Fig. 10].

3.3. *In vitro* cytotoxicity of the examined complexes (2)–(6)

The *in vitro* cytotoxicity of (2)–(6) against the four human tumour cell lines KB (Human epidemic carcinoma), Hep-G2

Figure 9
The molecular structure of complex (6), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. The fragment with a population parameter of 0.094 (7) is shown in blue and the intramolecular C—H $\cdots$ Cl interactions are shown as dotted lines.

(Hepatocellular carcinoma), LU (Human lung carcinoma) and MCF-7 (Human breast carcinoma) were assessed by the MTT method. The IC_{50} values are listed in Table 8, together with literature data for some other platinum(II) complexes.

The reported complexes (2)–(6) have notably high activities against the four cancer cell lines, with IC_{50} values of 0.38–29.23 μM . A comparison among complexes (2)–(6) shows a clear trend on all four tested cell lines, with increasing IC_{50} values in the order from (4) and (5) (0.38–1.99 μM) via (2) and (3) (4.27–7.02 μM) to (6) (7.27–29.23 μM). In other words, the *in vitro* cytotoxicities of the complexes bearing quinolin-8-olate are the highest, followed by the complexes containing quinoline and finally the quinoline-2-carboxylate complex (Fig. 11). Moreover, comparisons between complexes (3) and

Figure 10
Packing diagram for (6), showing the C—H $\cdots$ O (red dashed lines), C—H $\cdots$ Cl (green) and π – π (black) interactions. Symmetry codes are as given in Table 7 and the text.

Table 8

Cytotoxic effects of the examined compounds (IC_{50}^a in μM) and some reference compounds.

Values highlighted in bold are the lowest values.

Compound	KB	LU	Hep-G2	MCF-7
<i>trans</i> -[PtCl ₂ (Preug)(Qui)], (2)	4.27±0.09	7.02±0.28	6.64±0.20	6.47±0.32
<i>trans</i> -[PtCl ₂ (¹ Preug)(Qui)], (3)	5.09±0.18	4.64±0.12	5.96±0.30	5.93±0.12
[PtCl(Qui-O)(Preug)], (4)	0.39 ±0.02	1.25 ±0.05	1.99 ±0.10	1.55 ±0.06
[PtCl(Qui-O)(¹ Preug)], (5)	0.41 ±0.01	0.44 ±0.02	0.38 ±0.01	0.61 ±0.03
[PtCl(Qui-COO)(Preug)], (6)	7.27±0.32	18.60±0.37	14.68±0.45	29.23±1.24
Ellipticine	1.26±0.03	1.42±0.07	2.15±0.09	1.83±0.06
[PtCl(Qui-O)(olefin)] ^b	0.43–1.39	2.95–8.17	5.29–9.58	1.84–9.04
Other Pt ^{II}	5.98–22.54 ^c		3.4–85.37 ^d	4.65–90.79 ^e
Qui-OH ^f	37.89	62.96	43.54	40.37
Cisplatin ^g	15.2	42.9	13.3	45.7

Notes: (a) IC_{50} is the concentration of the compound required to inhibit cell growth by 50%. Mean values of IC_{50} (in μM) $\pm$ S.D. from three experiments are presented. References: (b) Chi *et al.* (2017a) and Da *et al.* (2015); (c) Li *et al.* (2013); (d) Qin *et al.* (2015), Liu *et al.* (2014), Fang *et al.* (2016) and Meng *et al.* (2016); (e) Nakatake *et al.* (2011), Liu *et al.* (2014) and Abu-Safieh *et al.* (2016); (f) Da *et al.* (2015); (g) Chi *et al.* (2017a).

(5), and between (2) and (4), which differ solely in the amine group, reveal a trend that the complexes bearing Qui-O, *i.e.* (4) and (5), display a higher cytotoxicity on the tested cell lines (except the KB cell line) than the complexes containing Qui, *i.e.* (2) and (3) (Fig. 11).

Compared to analogs [PtCl(Qui-O)(olefin)] (olefin is eugenol or methyleugenol) (Da *et al.*, 2015; Chi *et al.*, 2017a) and other Pt^{II} complexes (Li *et al.*, 2013; Qin *et al.*, 2015; Liu *et al.*, 2014; Fang *et al.*, 2016; Abu-Safieh *et al.*, 2016; Meng *et al.*, 2016; Nakatake *et al.*, 2011), complexes (4) and (5) show better antitumour activities (Table 8). It is noteworthy that free Qui-OH causes only a weak inhibition of the growth of the four cancer cell lines. This indicates that the *N,O*-chelated hydroxyquinolate ligand coordination causes a significant increase in the cytotoxicity of complexes (4) and (5), as well as of complexes [PtCl(Qui-O)(olefin)] (Fig. 12). The IC_{50} value of (5) for the Lu cell line is approximately 143 times lower than Qui-OH. In comparison with cisplatin, the IC_{50} values of complexes (4) and (5) are markedly lower, especially for the Lu and MCF-7 cell lines (approximately 30 times lower than cisplatin; Fig. 12).

4. Conclusions

In our search for more effective platinum-based anticancer drugs, we have synthesized five new Pt^{II} complexes of type *trans*-[PtCl₂(AlkEug)(Qui)], (2) and (3), and [PtCl(amine)-(AlkEug)], (4)–(6), in excellent yields ($\geq 89\%$) by replacement of one Cl ligand in K[PtCl₃(AlkEug)], (1), with quinoline, or of two Cl ligands with quinolin-8-ol or quinoline-2-carboxylic acid. The Pt^{II} coordination was explored by NMR spectroscopy, IR spectroscopy, ESI mass spectroscopy and single-crystal X-ray diffraction studies. The *in vitro* cytotoxicity of compounds (2)–(6), as well as of reference compounds, against the four human cancer cell lines KB, LU, Hep-G2 and MCF-7 was evaluated using the MTT assay. The results indicate that the excellent cytotoxicity (the IC_{50} values of 0.38–29.23 μM) depends on the amine ligand and increases in the order quinoline-2-carboxylate complex (6) < quinoline complexes (2) and (3) < quinolin-8-olate complexes (4) and (5). The IC_{50}

Figure 11
The cytotoxic effects (IC_{50} values) of complexes (2)–(6) against the KB, LU, Hep-G2 and MCF-7 cell lines.

Figure 12
The cytotoxic effects (IC_{50} values) of complexes (4), (5) and cisplatin against the KB, LU, Hep-G2 and MCF-7 cell lines.

values of the most promising complex, *i.e.* (**5**), is at least 30 times lower than that of cisplatin. The significant inhibiting abilities on the four human cancer cell lines of these new complexes, as well as the unambiguous trend on the influence of the amine on the cytotoxicity, requires in a next phase a study of the anticancer mechanism of the complexes and the structure–function relationship.

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supporting information

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Mixed natural arylolefin–quinoline platinum(II) complexes: synthesis, structural characterization and *in vitro* cytotoxicity studies

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Computing details

For all structures, data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO* (Agilent, 2013); data reduction: *CrysAlis PRO* (Agilent, 2013); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

[η^2 -4-Allyl-2-methoxy-1-(propoxycarbonylmethoxy)benzene]-*trans*-dichlorido(quinoline- κ N)platinum(II) (chi29)

Crystal data

[PtCl₂(C₁₅H₂₀O₄)(C₉H₇N)]

$M_r = 659.45$

Triclinic, $P\bar{1}$

$a = 8.1252$ (3) Å

$b = 11.7042$ (4) Å

$c = 13.7340$ (5) Å

$\alpha = 65.864$ (4)°

$\beta = 84.716$ (3)°

$\gamma = 88.191$ (3)°

$V = 1186.82$ (9) Å³

$Z = 2$

$F(000) = 644$

$D_x = 1.845$ Mg m⁻³

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

Cell parameters from 9524 reflections

$\theta = 3.1$ – 28.7°

$\mu = 6.17$ mm⁻¹

$T = 100$ K

Needle, yellow

$0.35 \times 0.1 \times 0.1$ mm

Data collection

Agilent SuperNova Dual Source

diffractometer with an 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, 2013)

$T_{\min} = 0.432$, $T_{\max} = 1.000$

19752 measured reflections

4867 independent reflections

4458 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -10 \rightarrow 10$

$k = -14 \rightarrow 14$

$l = -16 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.073$

$S = 1.12$

4867 reflections

337 parameters

14 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0079P)^2 + 5.6087P]$

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

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

$\Delta\rho_{\max} = 3.21$ e Å⁻³

$\Delta\rho_{\min} = -1.79$ 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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Pt1A	0.7798 (3)	1.14396 (15)	0.16089 (7)	0.0218 (2)	0.656 (8)
Pt1B	0.8263 (6)	1.1211 (3)	0.15616 (15)	0.0265 (4)	0.344 (8)
Cl2A	0.5445 (3)	1.2493 (3)	0.1821 (2)	0.0266 (6)	0.656 (8)
Cl2B	0.5661 (6)	1.1993 (8)	0.1688 (4)	0.0363 (13)	0.344 (8)
Cl3A	1.0244 (5)	1.0451 (3)	0.1445 (2)	0.0277 (6)	0.656 (8)
Cl3B	1.0943 (11)	1.0535 (7)	0.1458 (5)	0.0387 (15)	0.344 (8)
N4	0.8817 (5)	1.1787 (4)	0.2779 (3)	0.0304 (9)	
C5	0.9845 (6)	1.2744 (4)	0.2488 (4)	0.0270 (10)	
H5	1.017631	1.317137	0.174624	0.032*	
C6	1.0480 (6)	1.3173 (5)	0.3183 (4)	0.0291 (11)	
H6	1.121358	1.387069	0.292850	0.035*	
C7	0.9996 (6)	1.2538 (5)	0.4266 (4)	0.0331 (12)	
H7	1.038101	1.280591	0.477129	0.040*	
C8	0.8923 (5)	1.1485 (4)	0.4616 (4)	0.0220 (9)	
C9	0.8457 (6)	1.0762 (5)	0.5707 (4)	0.0329 (12)	
H9	0.886544	1.098149	0.623483	0.039*	
C10	0.7439 (6)	0.9763 (5)	0.6016 (4)	0.0360 (12)	
H10	0.711827	0.929103	0.675353	0.043*	
C11	0.6863 (6)	0.9429 (5)	0.5240 (4)	0.0292 (11)	
H11	0.614478	0.872448	0.546956	0.035*	
C12	0.7277 (5)	1.0061 (4)	0.4171 (4)	0.0263 (10)	
H12	0.687704	0.980387	0.366333	0.032*	
C13	0.8345 (6)	1.1133 (5)	0.3841 (4)	0.0266 (10)	
C14A	0.7271 (13)	1.1640 (9)	0.0050 (8)	0.027 (2)	0.656 (8)
H14A	0.818330	1.150443	−0.037382	0.033*	0.656 (8)
H14B	0.699529	1.246656	−0.002897	0.033*	0.656 (8)
C14B	0.783 (3)	1.1440 (12)	−0.0069 (16)	0.025 (5)	0.344 (8)
H14C	0.682405	1.183980	−0.033108	0.030*	0.344 (8)
H14D	0.883222	1.190307	−0.027753	0.030*	0.344 (8)
C15A	0.6335 (8)	1.0627 (6)	0.0787 (5)	0.0219 (17)	0.656 (8)
H15A	0.514099	1.084817	0.083641	0.026*	0.656 (8)
C15B	0.7818 (15)	1.0182 (12)	0.0618 (10)	0.030 (4)	0.344 (8)
H15B	0.885328	0.976909	0.047701	0.036*	0.344 (8)
C16	0.6538 (8)	0.9333 (5)	0.1026 (4)	0.0433 (15)	
H16A	0.764296	0.922215	0.070763	0.052*	0.656 (8)
H16B	0.571023	0.909066	0.065743	0.052*	0.656 (8)
H16C	0.658121	0.882998	0.059340	0.052*	0.344 (8)
H16D	0.549857	0.981538	0.089099	0.052*	0.344 (8)
C17	0.6386 (7)	0.8423 (5)	0.2189 (4)	0.0303 (11)	

C18	0.7735 (6)	0.7702 (4)	0.2630 (4)	0.0263 (10)
H18	0.873913	0.778617	0.219332	0.032*
C19	0.7647 (6)	0.6864 (4)	0.3692 (4)	0.0247 (10)
C20	0.6174 (6)	0.6750 (4)	0.4348 (4)	0.0259 (10)
C21	0.4818 (6)	0.7449 (5)	0.3906 (4)	0.0306 (11)
H21	0.380501	0.735833	0.433631	0.037*
C22	0.4930 (7)	0.8286 (5)	0.2830 (4)	0.0347 (12)
H22	0.399386	0.876730	0.253642	0.042*
O23	0.8917 (4)	0.6111 (3)	0.4178 (3)	0.0280 (7)
C24	1.0443 (6)	0.6212 (5)	0.3527 (4)	0.0331 (12)
H24A	1.024473	0.600999	0.292203	0.050*
H24B	1.124805	0.562539	0.395878	0.050*
H24C	1.087552	0.706805	0.325834	0.050*
O25	0.6212 (4)	0.5923 (3)	0.5400 (3)	0.0294 (8)
C26	0.4797 (6)	0.5859 (5)	0.6092 (4)	0.0271 (10)
H26A	0.385482	0.550928	0.589158	0.032*
H26B	0.449664	0.670725	0.604002	0.032*
C27	0.5177 (6)	0.5029 (4)	0.7221 (4)	0.0269 (10)
O28	0.6508 (4)	0.4610 (3)	0.7501 (3)	0.0340 (8)
O29	0.3804 (4)	0.4862 (3)	0.7874 (3)	0.0296 (8)
C30	0.3997 (6)	0.4167 (5)	0.9005 (4)	0.0313 (11)
H30A	0.497099	0.447884	0.920848	0.038*
H30B	0.415443	0.326622	0.917035	0.038*
C31	0.2440 (6)	0.4356 (5)	0.9611 (4)	0.0334 (12)
H31A	0.229895	0.526173	0.943080	0.040*
H31B	0.255733	0.392959	1.038969	0.040*
C32	0.0907 (6)	0.3855 (5)	0.9357 (4)	0.0331 (12)
H32A	0.076437	0.429307	0.859105	0.050*
H32B	−0.006417	0.399117	0.977384	0.050*
H32C	0.103443	0.295626	0.954158	0.050*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1A	0.0224 (5)	0.0218 (4)	0.02258 (19)	0.0050 (3)	−0.0097 (2)	−0.00915 (19)
Pt1B	0.0303 (10)	0.0276 (6)	0.0235 (4)	0.0092 (6)	−0.0126 (5)	−0.0109 (4)
Cl2A	0.0234 (10)	0.0243 (13)	0.0346 (11)	0.0062 (9)	−0.0088 (8)	−0.0136 (10)
Cl2B	0.034 (2)	0.040 (3)	0.035 (2)	0.010 (2)	−0.0070 (17)	−0.015 (2)
Cl3A	0.0237 (15)	0.0344 (12)	0.0284 (11)	0.0061 (13)	−0.0057 (12)	−0.0161 (9)
Cl3B	0.034 (4)	0.053 (3)	0.036 (2)	0.012 (3)	−0.010 (3)	−0.024 (2)
N4	0.027 (2)	0.033 (2)	0.031 (2)	0.0013 (18)	−0.0066 (18)	−0.0131 (19)
C5	0.025 (2)	0.025 (3)	0.028 (2)	−0.004 (2)	−0.001 (2)	−0.008 (2)
C6	0.027 (3)	0.026 (3)	0.038 (3)	0.003 (2)	−0.008 (2)	−0.016 (2)
C7	0.028 (3)	0.036 (3)	0.044 (3)	0.009 (2)	−0.009 (2)	−0.024 (3)
C8	0.016 (2)	0.026 (2)	0.026 (2)	0.0102 (18)	−0.0037 (18)	−0.014 (2)
C9	0.030 (3)	0.038 (3)	0.026 (3)	0.014 (2)	0.000 (2)	−0.011 (2)
C10	0.031 (3)	0.038 (3)	0.032 (3)	0.013 (2)	0.003 (2)	−0.009 (2)
C11	0.019 (2)	0.027 (3)	0.036 (3)	0.006 (2)	−0.002 (2)	−0.008 (2)

C12	0.019 (2)	0.027 (3)	0.029 (2)	0.0057 (19)	−0.0062 (19)	−0.007 (2)
C13	0.021 (2)	0.031 (3)	0.027 (2)	0.013 (2)	−0.0087 (19)	−0.010 (2)
C14A	0.035 (6)	0.035 (5)	0.015 (4)	−0.001 (4)	0.000 (4)	−0.013 (4)
C14B	0.028 (8)	0.032 (8)	0.013 (7)	−0.010 (6)	0.001 (6)	−0.007 (6)
C15A	0.022 (4)	0.024 (4)	0.022 (3)	0.000 (3)	−0.011 (3)	−0.009 (3)
C15B	0.035 (7)	0.038 (7)	0.022 (6)	0.003 (5)	−0.008 (5)	−0.017 (5)
C16	0.078 (4)	0.025 (3)	0.027 (3)	−0.005 (3)	−0.020 (3)	−0.006 (2)
C17	0.043 (3)	0.021 (3)	0.028 (3)	−0.003 (2)	−0.011 (2)	−0.008 (2)
C18	0.033 (3)	0.021 (2)	0.024 (2)	0.000 (2)	−0.002 (2)	−0.010 (2)
C19	0.027 (2)	0.021 (2)	0.027 (2)	0.0047 (19)	−0.0043 (19)	−0.010 (2)
C20	0.023 (2)	0.021 (2)	0.030 (3)	0.0009 (19)	0.0007 (19)	−0.008 (2)
C21	0.024 (2)	0.023 (3)	0.041 (3)	0.004 (2)	−0.003 (2)	−0.009 (2)
C22	0.035 (3)	0.026 (3)	0.045 (3)	0.008 (2)	−0.017 (2)	−0.014 (2)
O23	0.0241 (17)	0.0315 (19)	0.0235 (17)	0.0103 (14)	0.0027 (13)	−0.0079 (15)
C24	0.026 (3)	0.040 (3)	0.028 (3)	0.006 (2)	0.006 (2)	−0.011 (2)
O25	0.0275 (18)	0.0244 (18)	0.0228 (17)	0.0054 (14)	0.0111 (14)	0.0009 (14)
C26	0.019 (2)	0.024 (3)	0.034 (3)	0.0021 (19)	0.0087 (19)	−0.010 (2)
C27	0.027 (3)	0.019 (2)	0.033 (3)	−0.004 (2)	0.007 (2)	−0.010 (2)
O28	0.0217 (18)	0.036 (2)	0.035 (2)	0.0053 (15)	0.0056 (15)	−0.0076 (16)
O29	0.0236 (17)	0.037 (2)	0.0259 (17)	0.0019 (15)	0.0049 (14)	−0.0126 (15)
C30	0.024 (2)	0.037 (3)	0.029 (3)	0.005 (2)	0.001 (2)	−0.011 (2)
C31	0.025 (3)	0.044 (3)	0.030 (3)	0.001 (2)	0.006 (2)	−0.015 (2)
C32	0.031 (3)	0.034 (3)	0.032 (3)	0.001 (2)	0.005 (2)	−0.013 (2)

Geometric parameters (Å, °)

PT1Aa—C12A	2.303 (2)	C12—C13	1.437 (7)
PT1Bb—C12B	2.298 (5)	C16—H16A	0.9900
PT1Aa—C13A	2.307 (3)	C16—H16B	0.9900
PT1Bb—C13B	2.305 (6)	C16—H16C	0.9900
PT1Aa—N4	2.058 (4)	C16—H16D	0.9900
PT1Bb—N4	2.129 (5)	C16—C17	1.510 (7)
PT1Aa—C14A	2.139 (11)	C17—C18	1.388 (7)
C14Aa—H14A	0.9500	C17—C22	1.381 (8)
C14Aa—H14B	0.9500	C18—H18	0.9500
PT1Bb—C14B	2.20 (2)	C18—C19	1.382 (6)
C14Bb—H14C	0.9500	C19—C20	1.406 (7)
C14Bb—H14D	0.9500	C19—O23	1.369 (5)
C14Aa—C15A	1.394 (9)	C20—C21	1.382 (7)
PT1Aa—C15A	2.188 (6)	C20—O25	1.374 (6)
C15Aa—H15A	1.0000	C21—H21	0.9500
PT1Bb—C15B	2.157 (13)	C21—C22	1.396 (7)
C14Bb—C15B	1.386 (11)	C22—H22	0.9500
C15Bb—H15B	1.0000	O23—C24	1.438 (5)
C15Bb—C16	1.373 (10)	C24—H24A	0.9800
C15Aa—C16	1.420 (8)	C24—H24B	0.9800
N4—C5	1.320 (6)	C24—H24C	0.9800
N4—C13	1.365 (6)	O25—C26	1.406 (5)

C5—H5	0.9500	C26—H26A	0.9900
C5—C6	1.389 (7)	C26—H26B	0.9900
C6—H6	0.9500	C26—C27	1.510 (7)
C6—C7	1.388 (7)	C27—O28	1.203 (6)
C7—H7	0.9500	C27—O29	1.332 (6)
C7—C8	1.419 (7)	O29—C30	1.450 (6)
C8—C9	1.409 (7)	C30—H30A	0.9900
C8—C13	1.408 (6)	C30—H30B	0.9900
C9—H9	0.9500	C30—C31	1.511 (6)
C9—C10	1.350 (8)	C31—H31A	0.9900
C10—H10	0.9500	C31—H31B	0.9900
C10—C11	1.398 (7)	C31—C32	1.521 (7)
C11—H11	0.9500	C32—H32A	0.9800
C11—C12	1.361 (7)	C32—H32B	0.9800
C12—H12	0.9500	C32—H32C	0.9800
C14Aa—C15Aa—Pt1A	69.3 (6)	C15Bb—C16—H16D	107.1
C15Aa—C14Aa—Pt1A	73.1 (5)	H16Cb—C16—H16D	106.8
C5—N4—Pt1A	118.8 (3)	C15Aa—C16—C17	117.9 (5)
C5—N4—Pt1B	116.7 (3)	C15Bb—C16—C17	121.0 (7)
C5—N4—C13	119.0 (4)	C18—C17—C16	119.7 (5)
C13—N4—Pt1A	121.9 (3)	C22—C17—C16	121.6 (5)
C13—N4—Pt1B	123.7 (3)	C22—C17—C18	118.7 (5)
N4—C5—H5	117.5	C17—C18—H18	119.3
C14Bb—C15Bb—Pt1B	73.4 (11)	C19—C18—C17	121.4 (5)
C15Bb—C14Bb—Pt1B	69.6 (10)	C19—C18—H18	119.3
C15Aa—PT1Aa—Cl2A	87.0 (2)	C18—C19—C20	119.6 (4)
C14Aa—PT1Aa—Cl2A	92.7 (3)	O23—C19—C18	124.7 (4)
C15Bb—PT1Bb—Cl2B	99.5 (5)	O23—C19—C20	115.8 (4)
C14Bb—PT1Bb—Cl2B	87.8 (5)	C21—C20—C19	119.2 (4)
C15Aa—PT1Aa—Cl3A	96.6 (2)	O25—C20—C19	115.7 (4)
CL2Aa—PT1Aa—Cl3A	176.37 (10)	O25—C20—C21	125.1 (4)
C14Aa—PT1Aa—Cl3A	90.0 (3)	C20—C21—H21	119.9
CL2Bb—PT1Bb—Cl3B	176.1 (2)	C20—C21—C22	120.3 (5)
C14Bb—PT1Bb—Cl3B	94.2 (5)	C22—C21—H21	119.9
C15Bb—PT1Bb—Cl3B	84.1 (5)	C17—C22—C21	120.8 (5)
C15Aa—C14Aa—H14A	120.0	C17—C22—H22	119.6
PT1Aa—C14Aa—H14A	115.0	C21—C22—H22	119.6
H14Aa—C14Aa—H14B	120.0	C19—O23—C24	117.0 (4)
C15Aa—C14Aa—H14B	120.0	O23—C24—H24A	109.5
PT1Aa—C14Aa—H14B	82.4	N4—PT1Aa—Cl2A	90.11 (14)
C15Bb—PT1Bb—C14B	37.0 (4)	N4—PT1Bb—Cl2B	86.73 (18)
C15Bb—C14Bb—H14C	120.0	N4—PT1Aa—Cl3A	86.51 (14)
PT1Bb—C14Bb—H14C	116.1	N4—PT1Bb—Cl3B	90.1 (2)
PT1Bb—C14Bb—H14D	84.8	N4—PT1Aa—C14A	159.7 (3)
C15Bb—C14Bb—H14D	120.0	N4—PT1Bb—C14B	156.6 (4)
N4—C5—C6	125.1 (5)	N4—PT1Aa—C15A	162.7 (2)
C6—C5—H5	117.5	N4—PT1Bb—C15B	166.1 (4)

C5—C6—H6	121.5	C16—C15Aa—Pt1A	117.7 (4)
C7—C6—C5	117.0 (5)	C16—C15Bb—Pt1B	115.1 (8)
C7—C6—H6	121.5	C16—C15Bb—C14B	130.5 (14)
C6—C7—H7	120.1	C16—C15Aa—H15A	111.4
C6—C7—C8	119.7 (5)	C16—C15Bb—H15B	110.6
C8—C7—H7	120.1	O23—C24—H24B	109.5
C9—C8—C7	122.4 (5)	O23—C24—H24C	109.5
C13—C8—C7	118.5 (4)	H24A—C24—H24B	109.5
C13—C8—C9	119.0 (5)	H24A—C24—H24C	109.5
C8—C9—H9	119.5	H24B—C24—H24C	109.5
C10—C9—C8	121.1 (5)	C20—O25—C26	116.9 (4)
C10—C9—H9	119.5	O25—C26—H26A	110.1
C9—C10—H10	120.3	O25—C26—H26B	110.1
C9—C10—C11	119.4 (5)	O25—C26—C27	108.2 (4)
C11—C10—H10	120.3	H26A—C26—H26B	108.4
C10—C11—H11	118.4	C27—C26—H26A	110.1
C12—C11—C10	123.3 (5)	C27—C26—H26B	110.1
C12—C11—H11	118.4	O28—C27—C26	126.1 (4)
C11—C12—H12	121.3	O28—C27—O29	124.9 (5)
C11—C12—C13	117.4 (5)	O29—C27—C26	109.0 (4)
C13—C12—H12	121.3	C27—O29—C30	115.7 (4)
N4—C13—C8	120.6 (5)	O29—C30—H30A	110.3
N4—C13—C12	119.5 (4)	O29—C30—H30B	110.3
C8—C13—C12	119.9 (4)	O29—C30—C31	107.1 (4)
C17—C16—H16A	107.8	H30A—C30—H30B	108.6
C17—C16—H16B	107.8	C31—C30—H30A	110.3
C17—C16—H16C	107.1	C31—C30—H30B	110.3
C17—C16—H16D	107.1	C30—C31—H31A	109.1
H14Cb—C14Bb—H14D	120.0	C30—C31—H31B	109.1
C14Aa—Pt1Aa—C15A	37.6 (3)	C30—C31—C32	112.6 (4)
C14Aa—C15Aa—H15A	111.4	H31A—C31—H31B	107.8
Pt1Aa—C15Aa—H15A	111.4	C32—C31—H31A	109.1
C14Bb—C15Bb—H15B	110.6	C32—C31—H31B	109.1
Pt1Bb—C15Bb—H15B	110.6	C31—C32—H32A	109.5
C14Aa—C15Aa—C16	128.8 (7)	C31—C32—H32B	109.5
C15Aa—C16—H16A	107.8	C31—C32—H32C	109.5
C15Aa—C16—H16B	107.8	H32A—C32—H32B	109.5
H16Aa—C16—H16B	107.2	H32A—C32—H32C	109.5
C15Bb—C16—H16C	107.1	H32B—C32—H32C	109.5
Pt1Aa—N4—C5—C6	172.5 (4)	C10—C11—C12—C13	−0.9 (7)
Pt1Bb—N4—C5—C6	−173.3 (4)	C11—C12—C13—N4	179.0 (4)
Pt1Aa—N4—C13—C8	−172.7 (3)	C11—C12—C13—C8	0.3 (7)
Pt1Bb—C14Bb—C15Bb—C16	109.1 (16)	C13—N4—C5—C6	−1.5 (8)
Pt1Bb—N4—C13—C8	172.2 (4)	C13—C8—C9—C10	−1.6 (7)
Pt1Aa—N4—C13—C12	8.6 (6)	C16—C17—C18—C19	179.7 (4)
Pt1Bb—N4—C13—C12	−6.4 (6)	C16—C17—C22—C21	−179.4 (5)
C15Bb—C16—C17—C18	−51.0 (10)	C17—C18—C19—C20	−1.1 (7)

PT1Aa—C14Aa—C15Aa—C16	−109.6 (7)	C17—C18—C19—O23	179.1 (4)
PT1Aa—C15Aa—C16—C17	51.4 (7)	C18—C17—C22—C21	0.7 (7)
C14Bb—C15Bb—C16—C17	−136.9 (16)	C18—C19—C20—C21	2.3 (7)
C14Aa—C15Aa—C16—C17	136.3 (9)	C18—C19—C20—O25	−178.1 (4)
PT1Bb—C15Bb—C16—C17	−47.8 (11)	C18—C19—O23—C24	0.1 (7)
C15Aa—C16—C17—C18	−117.4 (6)	C19—C20—C21—C22	−2.1 (7)
N4—C5—C6—C7	0.3 (8)	C19—C20—O25—C26	175.4 (4)
C5—N4—C13—C8	1.0 (7)	C20—C19—O23—C24	−179.7 (4)
C5—N4—C13—C12	−177.6 (4)	C20—C21—C22—C17	0.6 (8)
C5—C6—C7—C8	1.2 (7)	C20—O25—C26—C27	−172.9 (4)
C6—C7—C8—C9	176.6 (5)	C21—C20—O25—C26	−5.0 (7)
C6—C7—C8—C13	−1.5 (7)	C22—C17—C18—C19	−0.4 (7)
C7—C8—C9—C10	−179.7 (5)	O23—C19—C20—C21	−177.8 (4)
C7—C8—C13—N4	0.4 (7)	O23—C19—C20—O25	1.8 (6)
C7—C8—C13—C12	179.1 (4)	O25—C20—C21—C22	178.4 (5)
C8—C9—C10—C11	1.1 (7)	O25—C26—C27—O28	7.9 (7)
C9—C8—C13—N4	−177.8 (4)	O25—C26—C27—O29	−174.2 (4)
C9—C8—C13—C12	0.9 (6)	C26—C27—O29—C30	−175.1 (4)
C9—C10—C11—C12	0.2 (8)	C27—O29—C30—C31	166.3 (4)
C15Bb—C16—C17—C22	129.1 (9)	O28—C27—O29—C30	2.9 (7)
C15Aa—C16—C17—C22	62.7 (7)	O29—C30—C31—C32	61.8 (6)

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of ring C17—C22.

<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>
C6—H6···O28 ⁱⁱ	0.95	2.47	3.404 (7)	169
C7—H7···O23 ⁱⁱ	0.95	2.39	3.324 (7)	168
C24—H24B···O23 ⁱⁱⁱ	0.98	2.53	3.287 (6)	134
C12—H12···Cg1	0.95	2.93	3.732 (6)	142

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

[η^2 -4-Allyl-2-methoxy-1-(propoxycarbonylmethoxy)benzene]chlorido(quinolin-8-olato- κ^2N,O)platinum(II) (chi30)

Crystal data

[Pt(C₉H₆NO)Cl(C₁₅H₂₀O₄)]

M_r = 639.00

Triclinic, *P*1

a = 8.3447 (2) Å

b = 11.9191 (4) Å

c = 12.9315 (5) Å

α = 63.296 (4)°

β = 84.618 (3)°

γ = 76.484 (3)°

V = 1117.09 (7) Å³

Z = 2

F(000) = 624

D_x = 1.900 Mg m^{−3}

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 12015 reflections

θ = 3.0–29.0°

μ = 6.44 mm^{−1}

T = 100 K

Block, orange

0.25 × 0.25 × 0.1 mm

Data collection

Agilent SuperNova Dual Source
diffractometer with an 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, 2013)

$T_{\min} = 0.411$, $T_{\max} = 1.000$
18255 measured reflections
4564 independent reflections
4417 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
 $\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 2.8^\circ$
 $h = -10 \rightarrow 10$
 $k = -14 \rightarrow 14$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.021$
 $wR(F^2) = 0.048$
 $S = 1.09$
4564 reflections
291 parameters
0 restraints

Primary atom site location: heavy-atom method
Hydrogen site location: mixed
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0163P)^2 + 2.8225P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 2.18 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.45 \text{ e } \text{\AA}^{-3}$

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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Pt1	0.04044 (2)	0.99699 (2)	0.32891 (2)	0.01151 (5)
Cl13	0.16523 (10)	1.14992 (8)	0.18856 (7)	0.01867 (17)
O12	-0.0616 (3)	0.8637 (2)	0.4578 (2)	0.0154 (5)
O23	0.2621 (3)	0.5145 (2)	0.3564 (2)	0.0176 (5)
O25	0.2664 (3)	0.5075 (2)	0.1596 (2)	0.0146 (5)
O28	0.4923 (3)	0.3181 (3)	0.1420 (2)	0.0255 (6)
O29	0.3771 (3)	0.3538 (2)	-0.02330 (19)	0.0153 (5)
N2	0.2441 (3)	0.9061 (2)	0.4345 (2)	0.0112 (5)
C3	0.3926 (4)	0.9321 (3)	0.4188 (3)	0.0146 (7)
H3	0.4123	1.0059	0.3522	0.017*
C4	0.5220 (4)	0.8532 (3)	0.4986 (3)	0.0154 (7)
H4	0.6274	0.8743	0.4859	0.018*
C5	0.4963 (4)	0.7459 (3)	0.5946 (3)	0.0136 (7)
H5	0.5837	0.6924	0.6485	0.016*
C6	0.3385 (4)	0.7147 (3)	0.6136 (3)	0.0123 (6)
C7	0.2995 (4)	0.6068 (3)	0.7088 (3)	0.0151 (7)
H7	0.3812	0.5480	0.7655	0.018*
C8	0.1415 (4)	0.5875 (3)	0.7187 (3)	0.0179 (7)
H8	0.1156	0.5142	0.7830	0.022*
C9	0.0163 (4)	0.6730 (3)	0.6365 (3)	0.0167 (7)
H9	-0.0917	0.6570	0.6465	0.020*

C10	0.0502 (4)	0.7797 (3)	0.5419 (3)	0.0125 (6)
C11	0.2137 (4)	0.7999 (3)	0.5310 (3)	0.0112 (6)
C14	−0.1965 (4)	1.1023 (3)	0.2518 (3)	0.0168 (7)
H14A	−0.2815	1.0850	0.3047	0.020*
H14B	−0.1540	1.1746	0.2327	0.020*
C15	−0.1322 (4)	1.0206 (3)	0.2011 (3)	0.0145 (7)
H15	−0.0979	1.0643	0.1209	0.017*
C16	−0.1942 (4)	0.9026 (3)	0.2278 (3)	0.0160 (7)
H16A	−0.2944	0.9280	0.1802	0.019*
H16B	−0.2267	0.8654	0.3100	0.019*
C17	−0.0716 (4)	0.7992 (3)	0.2064 (3)	0.0136 (7)
C18	0.0381 (4)	0.7055 (3)	0.2943 (3)	0.0144 (7)
H18	0.0358	0.7070	0.3673	0.017*
C19	0.1504 (4)	0.6104 (3)	0.2758 (3)	0.0132 (7)
C20	0.1528 (4)	0.6070 (3)	0.1684 (3)	0.0116 (6)
C21	0.0445 (4)	0.6995 (3)	0.0812 (3)	0.0140 (7)
H21	0.0452	0.6976	0.0085	0.017*
C22	−0.0659 (4)	0.7957 (3)	0.1008 (3)	0.0144 (7)
H22	−0.1385	0.8602	0.0402	0.017*
C24	0.2638 (5)	0.5115 (4)	0.4676 (3)	0.0289 (9)
H24A	0.3460	0.4367	0.5173	0.043*
H24B	0.1547	0.5054	0.5022	0.043*
H24C	0.2919	0.5902	0.4598	0.043*
C26	0.2514 (4)	0.4874 (3)	0.0616 (3)	0.0146 (7)
H26A	0.2601	0.5658	−0.0102	0.018*
H26B	0.1429	0.4673	0.0611	0.018*
C27	0.3883 (4)	0.3763 (3)	0.0677 (3)	0.0134 (7)
C30	0.5000 (5)	0.2451 (3)	−0.0251 (3)	0.0227 (8)
H30A	0.4733	0.1632	0.0331	0.027*
H30B	0.6105	0.2487	−0.0065	0.027*
C31	0.4988 (5)	0.2527 (4)	−0.1449 (3)	0.0252 (8)
H31A	0.3863	0.2547	−0.1651	0.030*
H31B	0.5313	0.3327	−0.2023	0.030*
C32	0.6175 (5)	0.1375 (4)	−0.1479 (4)	0.0294 (9)
H32A	0.7285	0.1359	−0.1276	0.044*
H32B	0.6177	0.1431	−0.2259	0.044*
H32C	0.5833	0.0588	−0.0922	0.044*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.01206 (7)	0.01043 (7)	0.01114 (7)	0.00036 (5)	−0.00234 (5)	−0.00484 (5)
Cl13	0.0219 (4)	0.0151 (4)	0.0148 (4)	−0.0047 (3)	−0.0009 (3)	−0.0023 (3)
O12	0.0083 (11)	0.0158 (12)	0.0217 (13)	−0.0014 (9)	−0.0011 (9)	−0.0082 (10)
O23	0.0211 (12)	0.0163 (12)	0.0153 (12)	0.0041 (10)	−0.0066 (10)	−0.0094 (10)
O25	0.0152 (11)	0.0143 (11)	0.0150 (12)	0.0034 (9)	−0.0024 (9)	−0.0097 (10)
O28	0.0191 (13)	0.0301 (15)	0.0315 (15)	0.0090 (11)	−0.0115 (11)	−0.0217 (13)
O29	0.0192 (12)	0.0137 (11)	0.0117 (12)	0.0025 (9)	−0.0004 (9)	−0.0074 (9)

N2	0.0153 (13)	0.0102 (13)	0.0099 (13)	−0.0015 (11)	0.0012 (11)	−0.0068 (11)
C3	0.0163 (16)	0.0157 (16)	0.0138 (17)	−0.0052 (13)	0.0020 (13)	−0.0078 (14)
C4	0.0112 (15)	0.0200 (17)	0.0183 (18)	−0.0039 (13)	0.0015 (13)	−0.0113 (14)
C5	0.0122 (15)	0.0149 (16)	0.0144 (17)	0.0028 (13)	−0.0034 (13)	−0.0090 (13)
C6	0.0155 (16)	0.0113 (15)	0.0121 (16)	0.0004 (12)	−0.0016 (12)	−0.0082 (13)
C7	0.0202 (17)	0.0131 (16)	0.0108 (16)	−0.0003 (13)	−0.0024 (13)	−0.0054 (13)
C8	0.0253 (18)	0.0150 (16)	0.0125 (17)	−0.0065 (14)	0.0029 (14)	−0.0048 (14)
C9	0.0168 (16)	0.0188 (17)	0.0161 (17)	−0.0062 (14)	0.0031 (13)	−0.0085 (14)
C10	0.0144 (15)	0.0127 (15)	0.0120 (16)	−0.0006 (12)	0.0002 (12)	−0.0078 (13)
C11	0.0139 (15)	0.0120 (15)	0.0108 (16)	−0.0022 (12)	0.0011 (12)	−0.0081 (13)
C14	0.0139 (16)	0.0171 (17)	0.0195 (18)	0.0022 (13)	−0.0071 (13)	−0.0095 (14)
C15	0.0115 (15)	0.0162 (16)	0.0143 (17)	0.0014 (13)	−0.0057 (13)	−0.0063 (14)
C16	0.0114 (15)	0.0185 (17)	0.0169 (17)	0.0014 (13)	−0.0015 (13)	−0.0085 (14)
C17	0.0099 (15)	0.0116 (15)	0.0199 (18)	−0.0019 (12)	0.0000 (13)	−0.0076 (14)
C18	0.0147 (16)	0.0158 (16)	0.0157 (17)	−0.0031 (13)	−0.0003 (13)	−0.0094 (14)
C19	0.0117 (15)	0.0114 (15)	0.0173 (17)	−0.0024 (12)	−0.0013 (13)	−0.0067 (13)
C20	0.0102 (14)	0.0095 (15)	0.0152 (17)	−0.0028 (12)	0.0030 (12)	−0.0056 (13)
C21	0.0143 (15)	0.0151 (16)	0.0126 (16)	−0.0032 (13)	0.0010 (13)	−0.0063 (13)
C22	0.0125 (15)	0.0109 (15)	0.0167 (17)	−0.0007 (12)	−0.0022 (13)	−0.0037 (13)
C24	0.035 (2)	0.030 (2)	0.021 (2)	0.0109 (18)	−0.0132 (17)	−0.0170 (17)
C26	0.0141 (16)	0.0143 (16)	0.0141 (17)	0.0002 (13)	−0.0007 (13)	−0.0065 (14)
C27	0.0122 (15)	0.0121 (15)	0.0163 (17)	−0.0036 (13)	0.0020 (13)	−0.0065 (13)
C30	0.0223 (18)	0.0186 (18)	0.027 (2)	−0.0013 (15)	0.0014 (15)	−0.0112 (16)
C31	0.0216 (19)	0.029 (2)	0.030 (2)	−0.0067 (16)	0.0041 (16)	−0.0184 (18)
C32	0.028 (2)	0.030 (2)	0.037 (2)	−0.0081 (17)	0.0065 (18)	−0.0201 (19)

Geometric parameters (Å, °)

Pt1—Cl13	2.2935 (8)	C14—H14B	0.9296
Pt1—O12	2.003 (2)	C14—C15	1.389 (5)
Pt1—N2	2.042 (3)	C15—H15	0.9789
Pt1—C14	2.136 (3)	C15—C16	1.495 (5)
Pt1—C15	2.174 (3)	C16—H16A	0.9900
O12—C10	1.353 (4)	C16—H16B	0.9900
O23—C19	1.370 (4)	C16—C17	1.519 (4)
O23—C24	1.423 (4)	C17—C18	1.398 (5)
O25—C20	1.376 (4)	C17—C22	1.380 (5)
O25—C26	1.413 (4)	C18—H18	0.9500
O28—C27	1.198 (4)	C18—C19	1.388 (5)
O29—C27	1.334 (4)	C19—C20	1.405 (5)
O29—C30	1.461 (4)	C20—C21	1.383 (4)
N2—C3	1.323 (4)	C21—H21	0.9500
N2—C11	1.376 (4)	C21—C22	1.397 (5)
C3—H3	0.9500	C22—H22	0.9500
C3—C4	1.406 (5)	C24—H24A	0.9800
C4—H4	0.9500	C24—H24B	0.9800
C4—C5	1.369 (5)	C24—H24C	0.9800
C5—H5	0.9500	C26—H26A	0.9900

C5—C6	1.421 (5)	C26—H26B	0.9900
C6—C7	1.404 (5)	C26—C27	1.510 (4)
C6—C11	1.413 (4)	C30—H30A	0.9900
C7—H7	0.9500	C30—H30B	0.9900
C7—C8	1.376 (5)	C30—C31	1.511 (5)
C8—H8	0.9500	C31—H31A	0.9900
C8—C9	1.413 (5)	C31—H31B	0.9900
C9—H9	0.9500	C31—C32	1.508 (5)
C9—C10	1.378 (5)	C32—H32A	0.9800
C10—C11	1.423 (4)	C32—H32B	0.9800
C14—H14A	0.9291	C32—H32C	0.9800
O12—Pt1—Cl13	176.98 (7)	C15—C16—H16B	108.6
O12—Pt1—N2	82.92 (10)	C15—C16—C17	114.8 (3)
O12—Pt1—C14	90.86 (12)	H16A—C16—H16B	107.5
O12—Pt1—C15	92.59 (11)	C17—C16—H16A	108.6
N2—Pt1—Cl13	94.62 (8)	C17—C16—H16B	108.6
N2—Pt1—C14	166.29 (12)	C18—C17—C16	120.0 (3)
N2—Pt1—C15	154.39 (11)	C22—C17—C16	121.1 (3)
C14—Pt1—Cl13	91.17 (10)	C22—C17—C18	118.9 (3)
C14—Pt1—C15	37.59 (13)	C17—C18—H18	119.8
C15—Pt1—Cl13	90.38 (9)	C19—C18—C17	120.5 (3)
C10—O12—Pt1	111.51 (19)	C19—C18—H18	119.8
C19—O23—C24	118.0 (3)	O23—C19—C18	124.8 (3)
C20—O25—C26	116.5 (2)	O23—C19—C20	115.3 (3)
C27—O29—C30	114.8 (3)	C18—C19—C20	119.9 (3)
C3—N2—Pt1	129.5 (2)	O25—C20—C19	115.4 (3)
C3—N2—C11	119.8 (3)	O25—C20—C21	124.8 (3)
C11—N2—Pt1	110.6 (2)	C21—C20—C19	119.8 (3)
N2—C3—H3	119.2	C20—C21—H21	120.2
N2—C3—C4	121.5 (3)	C20—C21—C22	119.5 (3)
C4—C3—H3	119.2	C22—C21—H21	120.2
C3—C4—H4	120.0	C17—C22—C21	121.4 (3)
C5—C4—C3	120.0 (3)	C17—C22—H22	119.3
C5—C4—H4	120.0	C21—C22—H22	119.3
C4—C5—H5	120.1	O23—C24—H24A	109.5
C4—C5—C6	119.9 (3)	O23—C24—H24B	109.5
C6—C5—H5	120.1	O23—C24—H24C	109.5
C7—C6—C5	124.3 (3)	H24A—C24—H24B	109.5
C7—C6—C11	118.8 (3)	H24A—C24—H24C	109.5
C11—C6—C5	116.9 (3)	H24B—C24—H24C	109.5
C6—C7—H7	120.5	O25—C26—H26A	110.1
C8—C7—C6	119.1 (3)	O25—C26—H26B	110.1
C8—C7—H7	120.5	O25—C26—C27	108.0 (3)
C7—C8—H8	118.9	H26A—C26—H26B	108.4
C7—C8—C9	122.2 (3)	C27—C26—H26A	110.1
C9—C8—H8	118.9	C27—C26—H26B	110.1
C8—C9—H9	119.8	O28—C27—O29	125.1 (3)

C10—C9—C8	120.3 (3)	O28—C27—C26	125.3 (3)
C10—C9—H9	119.8	O29—C27—C26	109.6 (3)
O12—C10—C9	123.7 (3)	O29—C30—H30A	110.1
O12—C10—C11	118.5 (3)	O29—C30—H30B	110.1
C9—C10—C11	117.7 (3)	O29—C30—C31	108.1 (3)
N2—C11—C6	121.8 (3)	H30A—C30—H30B	108.4
N2—C11—C10	116.2 (3)	C31—C30—H30A	110.1
C6—C11—C10	121.9 (3)	C31—C30—H30B	110.1
Pt1—C14—H14A	112.7	C30—C31—H31A	109.8
Pt1—C14—H14B	84.8	C30—C31—H31B	109.8
H14A—C14—H14B	120.0	H31A—C31—H31B	108.2
C15—C14—Pt1	72.67 (19)	C32—C31—C30	109.5 (3)
C15—C14—H14A	120.4	C32—C31—H31A	109.8
C15—C14—H14B	119.7	C32—C31—H31B	109.8
Pt1—C15—H15	114.1	C31—C32—H32A	109.5
C14—C15—Pt1	69.75 (19)	C31—C32—H32B	109.5
C14—C15—H15	114.2	C31—C32—H32C	109.5
C14—C15—C16	122.6 (3)	H32A—C32—H32B	109.5
C16—C15—Pt1	114.4 (2)	H32A—C32—H32C	109.5
C16—C15—H15	114.2	H32B—C32—H32C	109.5
C15—C16—H16A	108.6		
Pt1—O12—C10—C9	−175.2 (3)	C8—C9—C10—O12	177.9 (3)
Pt1—O12—C10—C11	3.0 (3)	C8—C9—C10—C11	−0.3 (5)
Pt1—N2—C3—C4	−175.9 (2)	C9—C10—C11—N2	178.9 (3)
Pt1—N2—C11—C6	175.2 (2)	C9—C10—C11—C6	−0.1 (5)
Pt1—N2—C11—C10	−3.8 (3)	C11—N2—C3—C4	0.4 (5)
Pt1—C14—C15—C16	106.6 (3)	C11—C6—C7—C8	−0.1 (5)
Pt1—C15—C16—C17	−75.3 (3)	C14—C15—C16—C17	−156.0 (3)
O12—C10—C11—N2	0.6 (4)	C15—C16—C17—C18	88.9 (4)
O12—C10—C11—C6	−178.4 (3)	C15—C16—C17—C22	−91.0 (4)
O23—C19—C20—O25	0.3 (4)	C16—C17—C18—C19	179.9 (3)
O23—C19—C20—C21	179.9 (3)	C16—C17—C22—C21	−178.8 (3)
O25—C20—C21—C22	179.7 (3)	C17—C18—C19—O23	−179.8 (3)
O25—C26—C27—O28	−1.3 (5)	C17—C18—C19—C20	−0.8 (5)
O25—C26—C27—O29	179.5 (3)	C18—C17—C22—C21	1.3 (5)
O29—C30—C31—C32	−176.7 (3)	C18—C19—C20—O25	−178.7 (3)
N2—C3—C4—C5	0.5 (5)	C18—C19—C20—C21	0.8 (5)
C3—N2—C11—C6	−1.7 (5)	C19—C20—C21—C22	0.2 (5)
C3—N2—C11—C10	179.3 (3)	C20—O25—C26—C27	179.0 (3)
C3—C4—C5—C6	−0.1 (5)	C20—C21—C22—C17	−1.3 (5)
C4—C5—C6—C7	179.7 (3)	C22—C17—C18—C19	−0.3 (5)
C4—C5—C6—C11	−1.1 (5)	C24—O23—C19—C18	0.1 (5)
C5—C6—C7—C8	179.1 (3)	C24—O23—C19—C20	−178.9 (3)
C5—C6—C11—N2	2.0 (5)	C26—O25—C20—C19	168.6 (3)
C5—C6—C11—C10	−179.0 (3)	C26—O25—C20—C21	−10.9 (4)
C6—C7—C8—C9	−0.3 (5)	C27—O29—C30—C31	−166.0 (3)
C7—C6—C11—N2	−178.7 (3)	C30—O29—C27—O28	2.8 (5)

C7—C6—C11—C10	0.3 (5)	C30—O29—C27—C26	−178.0 (3)
C7—C8—C9—C10	0.5 (5)		

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of ring C6—C11, Cg2 is the centroid of ring N2/C3—C6/C11 and Cg3 is the centroid of ring C17—C22.

<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>
C16—H16B $\cdots$ O12	0.99	2.45	3.070 (4)	120
C18—H18 $\cdots$ O12	0.95	2.57	3.352 (5)	140
C4—H4 $\cdots$ O12 ⁱ	0.95	2.57	3.488 (4)	163
C14—H14A $\cdots$ Cg2 ⁱⁱ	0.93	2.94	3.581 (4)	127
C14—H14B $\cdots$ Cg1 ⁱⁱ	0.93	2.88	3.493 (4)	125
C24—H24C $\cdots$ Cg1	0.98	2.91	3.513 (5)	121
C32—H32A $\cdots$ Cg3 ⁱⁱⁱ	0.98	2.84	3.655 (5)	141

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

{ η^2 -4-Allyl-2-methoxy-1-[(propan-2-yloxy)carbonyl]methoxy]benzene}chlorido(quinolin-8-olato- κ^2N,O)platinum(II) (chi9)

Crystal data

[Pt(C₉H₆NO)Cl(C₁₅H₂₀O₄)]

$M_r = 639.00$

Triclinic, $P\bar{1}$

$a = 9.7858$ (3) Å

$b = 11.0447$ (2) Å

$c = 11.8117$ (3) Å

$\alpha = 85.059$ (2)°

$\beta = 73.685$ (3)°

$\gamma = 71.139$ (2)°

$V = 1159.41$ (6) Å³

$Z = 2$

$F(000) = 624$

$D_x = 1.830$ Mg m^{−3}

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

Cell parameters from 30804 reflections

$\theta = 3.3$ – 29.2°

$\mu = 6.20$ mm^{−1}

$T = 200$ K

Block, yellow

$0.3 \times 0.25 \times 0.15$ mm

Data collection

Agilent SuperNova Dual Source

diffractometer with an 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, 2013)

$T_{\min} = 0.369$, $T_{\max} = 1.000$

47800 measured reflections

4738 independent reflections

4534 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

$\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 2.7^\circ$

$h = -12 \rightarrow 12$

$k = -13 \rightarrow 13$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.017$

$wR(F^2) = 0.041$

$S = 1.10$

4738 reflections

292 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0139P)^2 + 1.3246P]$

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

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

$\Delta\rho_{\max} = 1.46$ e Å^{−3}

$\Delta\rho_{\min} = -1.01$ 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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C3	−0.1859 (3)	0.5736 (3)	0.8919 (3)	0.0312 (6)
H3	−0.136026	0.551246	0.952579	0.037*
C4	−0.1698 (3)	0.6780 (3)	0.8191 (3)	0.0371 (7)
H4	−0.109806	0.725613	0.831437	0.044*
C5	−0.2395 (3)	0.7118 (3)	0.7307 (3)	0.0325 (6)
H5	−0.228789	0.782996	0.681875	0.039*
C6	−0.3279 (3)	0.6399 (3)	0.7125 (2)	0.0291 (6)
C7	−0.4021 (4)	0.6640 (3)	0.6226 (3)	0.0375 (7)
H7	−0.392972	0.730819	0.567552	0.045*
C8	−0.4877 (4)	0.5894 (3)	0.6156 (3)	0.0428 (8)
H8	−0.538702	0.606963	0.555603	0.051*
C9	−0.5029 (4)	0.4884 (3)	0.6935 (3)	0.0391 (7)
H9	−0.563451	0.439284	0.685632	0.047*
C10	−0.4298 (3)	0.4602 (3)	0.7819 (2)	0.0283 (6)
C11	−0.3416 (3)	0.5375 (2)	0.7905 (2)	0.0241 (5)
C14	−0.3857 (4)	0.2014 (3)	1.0626 (3)	0.0399 (7)
H14A	−0.378315	0.190373	1.144981	0.048*
H14B	−0.482399	0.198555	1.054109	0.048*
C15	−0.2573 (4)	0.1376 (3)	0.9756 (3)	0.0346 (7)
H15	−0.168809	0.090147	1.005924	0.042*
C16	−0.2630 (3)	0.0802 (3)	0.8671 (3)	0.0365 (7)
H16A	−0.351713	0.134864	0.842030	0.044*
H16B	−0.276076	−0.005014	0.886936	0.044*
C17	−0.1239 (3)	0.0657 (3)	0.7646 (3)	0.0311 (6)
C18	−0.1177 (3)	0.1623 (3)	0.6802 (3)	0.0325 (6)
H18	−0.201221	0.237708	0.687036	0.039*
C19	0.0092 (3)	0.1488 (3)	0.5867 (2)	0.0300 (6)
C20	0.1327 (3)	0.0372 (3)	0.5753 (2)	0.0289 (6)
C21	0.1276 (3)	−0.0571 (3)	0.6586 (3)	0.0342 (6)
H21	0.210996	−0.132599	0.652078	0.041*
C22	−0.0004 (4)	−0.0419 (3)	0.7529 (3)	0.0354 (7)
H22	−0.002276	−0.107384	0.810518	0.042*
C24	−0.0978 (4)	0.3521 (3)	0.5056 (3)	0.0555 (10)
H24A	−0.073160	0.405287	0.436914	0.083*
H24B	−0.117973	0.399543	0.577958	0.083*
H24C	−0.186798	0.329817	0.505151	0.083*
C26	0.3687 (3)	−0.0846 (3)	0.4582 (3)	0.0316 (6)
H26A	0.329614	−0.150676	0.439842	0.038*
H26B	0.404777	−0.111460	0.529549	0.038*

C27	0.4958 (3)	−0.0715 (3)	0.3562 (3)	0.0294 (6)
C30	0.7357 (3)	−0.1960 (3)	0.2374 (3)	0.0379 (7)
H30	0.772178	−0.124178	0.248467	0.046*
C31	0.7087 (4)	−0.1866 (4)	0.1172 (3)	0.0512 (9)
H31A	0.803987	−0.198775	0.056507	0.077*
H31B	0.639097	−0.102057	0.108053	0.077*
H31C	0.665597	−0.252856	0.108640	0.077*
C32	0.8458 (4)	−0.3219 (3)	0.2587 (4)	0.0555 (10)
H32A	0.815462	−0.392474	0.240074	0.083*
H32B	0.847282	−0.327029	0.341567	0.083*
H32C	0.946136	−0.327789	0.208108	0.083*
Cl13	−0.14543 (9)	0.33203 (8)	1.08003 (7)	0.04446 (19)
N2	−0.2692 (2)	0.5055 (2)	0.87781 (19)	0.0254 (5)
O12	−0.4363 (2)	0.36373 (18)	0.85739 (18)	0.0314 (4)
O23	0.0252 (2)	0.23816 (19)	0.50069 (18)	0.0411 (5)
O25	0.2535 (2)	0.03400 (18)	0.47921 (18)	0.0354 (5)
O28	0.5090 (3)	0.0266 (2)	0.3106 (2)	0.0453 (6)
O29	0.5949 (2)	−0.18764 (18)	0.32815 (18)	0.0323 (4)
Pt1	−0.29907 (2)	0.34304 (2)	0.96161 (2)	0.02646 (4)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C3	0.0306 (15)	0.0285 (14)	0.0353 (16)	−0.0075 (12)	−0.0114 (12)	−0.0024 (12)
C4	0.0318 (16)	0.0302 (15)	0.0499 (19)	−0.0122 (13)	−0.0086 (14)	−0.0014 (13)
C5	0.0315 (15)	0.0225 (14)	0.0339 (16)	−0.0042 (12)	0.0009 (12)	0.0019 (11)
C6	0.0298 (14)	0.0228 (13)	0.0235 (13)	0.0014 (11)	−0.0005 (11)	−0.0017 (10)
C7	0.0478 (19)	0.0263 (15)	0.0299 (15)	0.0003 (13)	−0.0120 (14)	0.0033 (12)
C8	0.050 (2)	0.0377 (17)	0.0386 (18)	0.0019 (15)	−0.0258 (16)	−0.0024 (14)
C9	0.0384 (17)	0.0368 (17)	0.0458 (19)	−0.0071 (14)	−0.0209 (15)	−0.0047 (14)
C10	0.0250 (14)	0.0243 (14)	0.0309 (15)	−0.0011 (11)	−0.0071 (11)	−0.0020 (11)
C11	0.0217 (13)	0.0198 (12)	0.0241 (13)	0.0002 (10)	−0.0024 (10)	−0.0034 (10)
C14	0.0438 (18)	0.0311 (16)	0.0331 (16)	−0.0125 (14)	0.0061 (14)	0.0092 (13)
C15	0.0405 (17)	0.0235 (14)	0.0291 (15)	−0.0068 (12)	0.0012 (13)	0.0080 (11)
C16	0.0381 (17)	0.0280 (15)	0.0395 (17)	−0.0132 (13)	−0.0015 (14)	0.0031 (12)
C17	0.0365 (16)	0.0249 (14)	0.0298 (15)	−0.0122 (12)	−0.0025 (12)	−0.0010 (11)
C18	0.0339 (16)	0.0245 (14)	0.0315 (15)	−0.0041 (12)	−0.0025 (12)	−0.0013 (11)
C19	0.0344 (15)	0.0239 (14)	0.0250 (14)	−0.0040 (12)	−0.0040 (12)	0.0008 (11)
C20	0.0315 (15)	0.0267 (14)	0.0236 (14)	−0.0054 (12)	−0.0038 (11)	−0.0014 (11)
C21	0.0393 (17)	0.0234 (14)	0.0335 (16)	−0.0037 (12)	−0.0072 (13)	0.0013 (12)
C22	0.0471 (18)	0.0239 (14)	0.0315 (15)	−0.0127 (13)	−0.0044 (13)	0.0046 (12)
C24	0.047 (2)	0.0341 (18)	0.055 (2)	0.0089 (15)	0.0041 (17)	0.0179 (16)
C26	0.0308 (15)	0.0239 (14)	0.0321 (15)	−0.0009 (12)	−0.0045 (12)	−0.0012 (11)
C27	0.0280 (14)	0.0255 (14)	0.0327 (15)	−0.0040 (11)	−0.0090 (12)	−0.0045 (12)
C30	0.0269 (15)	0.0352 (16)	0.0465 (18)	−0.0092 (13)	0.0004 (13)	−0.0089 (14)
C31	0.043 (2)	0.063 (2)	0.0398 (19)	−0.0156 (17)	0.0024 (15)	−0.0077 (17)
C32	0.0304 (18)	0.046 (2)	0.079 (3)	−0.0011 (15)	−0.0075 (18)	−0.0070 (19)
Cl13	0.0453 (4)	0.0485 (5)	0.0394 (4)	−0.0074 (4)	−0.0220 (4)	0.0084 (3)

N2	0.0240 (11)	0.0230 (11)	0.0254 (11)	−0.0037 (9)	−0.0051 (9)	−0.0001 (9)
O12	0.0292 (10)	0.0289 (10)	0.0366 (11)	−0.0113 (8)	−0.0084 (9)	0.0047 (8)
O23	0.0392 (12)	0.0298 (11)	0.0312 (11)	0.0048 (9)	0.0052 (9)	0.0103 (9)
O25	0.0327 (11)	0.0249 (10)	0.0319 (11)	0.0027 (8)	0.0027 (9)	0.0035 (8)
O28	0.0419 (13)	0.0243 (11)	0.0556 (15)	−0.0047 (9)	0.0018 (11)	0.0018 (10)
O29	0.0286 (10)	0.0247 (10)	0.0363 (11)	−0.0037 (8)	−0.0018 (9)	−0.0033 (8)
Pt1	0.02589 (6)	0.02385 (6)	0.02392 (6)	−0.00394 (4)	−0.00313 (4)	0.00299 (4)

Geometric parameters (Å, °)

C3—H3	0.9500	C18—C19	1.387 (4)
C3—C4	1.401 (4)	C19—C20	1.404 (4)
C3—N2	1.323 (3)	C19—O23	1.367 (3)
C4—H4	0.9500	C20—C21	1.374 (4)
C4—C5	1.365 (4)	C20—O25	1.383 (3)
C5—H5	0.9500	C21—H21	0.9500
C5—C6	1.416 (4)	C21—C22	1.397 (4)
C6—C7	1.410 (4)	C22—H22	0.9500
C6—C11	1.413 (4)	C24—H24A	0.9800
C7—H7	0.9500	C24—H24B	0.9800
C7—C8	1.372 (5)	C24—H24C	0.9800
C8—H8	0.9500	C24—O23	1.424 (4)
C8—C9	1.403 (5)	C26—H26A	0.9900
C9—H9	0.9500	C26—H26B	0.9900
C9—C10	1.385 (4)	C26—C27	1.505 (4)
C10—C11	1.423 (4)	C26—O25	1.411 (3)
C10—O12	1.335 (3)	C27—O28	1.196 (3)
C11—N2	1.370 (3)	C27—O29	1.336 (3)
C14—H14A	0.9900	C30—H30	1.0000
C14—H14B	0.9900	C30—C31	1.505 (5)
C14—C15	1.400 (4)	C30—C32	1.510 (5)
C14—Pt1	2.134 (3)	C30—O29	1.470 (3)
C15—H15	1.0000	C31—H31A	0.9800
C15—C16	1.501 (4)	C31—H31B	0.9800
C15—Pt1	2.172 (3)	C31—H31C	0.9800
C16—H16A	0.9900	C32—H32A	0.9800
C16—H16B	0.9900	C32—H32B	0.9800
C16—C17	1.520 (4)	C32—H32C	0.9800
C17—C18	1.400 (4)	Cl13—Pt1	2.2947 (8)
C17—C22	1.378 (4)	N2—Pt1	2.039 (2)
C18—H18	0.9500	O12—Pt1	2.0135 (19)
C4—C3—H3	119.3	C20—C21—H21	120.1
N2—C3—H3	119.3	C20—C21—C22	119.9 (3)
N2—C3—C4	121.5 (3)	C22—C21—H21	120.1
C3—C4—H4	119.7	C17—C22—C21	121.6 (3)
C5—C4—C3	120.5 (3)	C17—C22—H22	119.2
C5—C4—H4	119.7	C21—C22—H22	119.2

C4—C5—H5	120.3	H24A—C24—H24B	109.5
C4—C5—C6	119.4 (3)	H24A—C24—H24C	109.5
C6—C5—H5	120.3	H24B—C24—H24C	109.5
C7—C6—C5	124.4 (3)	O23—C24—H24A	109.5
C7—C6—C11	118.5 (3)	O23—C24—H24B	109.5
C11—C6—C5	117.1 (3)	O23—C24—H24C	109.5
C6—C7—H7	120.5	H26A—C26—H26B	108.3
C8—C7—C6	119.0 (3)	C27—C26—H26A	109.8
C8—C7—H7	120.5	C27—C26—H26B	109.8
C7—C8—H8	118.7	O25—C26—H26A	109.8
C7—C8—C9	122.7 (3)	O25—C26—H26B	109.8
C9—C8—H8	118.7	O25—C26—C27	109.3 (2)
C8—C9—H9	119.9	O28—C27—C26	125.9 (3)
C10—C9—C8	120.2 (3)	O28—C27—O29	125.6 (3)
C10—C9—H9	119.9	O29—C27—C26	108.4 (2)
C9—C10—C11	117.6 (3)	C31—C30—H30	109.5
O12—C10—C9	123.4 (3)	C31—C30—C32	113.5 (3)
O12—C10—C11	118.9 (2)	C32—C30—H30	109.5
C6—C11—C10	122.0 (2)	O29—C30—H30	109.5
N2—C11—C6	122.0 (2)	O29—C30—C31	109.4 (3)
N2—C11—C10	116.0 (2)	O29—C30—C32	105.4 (3)
H14A—C14—H14B	113.3	C30—C31—H31A	109.5
C15—C14—H14A	116.3	C30—C31—H31B	109.5
C15—C14—H14B	116.3	C30—C31—H31C	109.5
C15—C14—Pt1	72.51 (16)	H31A—C31—H31B	109.5
Pt1—C14—H14A	116.3	H31A—C31—H31C	109.5
Pt1—C14—H14B	116.3	H31B—C31—H31C	109.5
C14—C15—H15	114.5	C30—C32—H32A	109.5
C14—C15—C16	123.1 (3)	C30—C32—H32B	109.5
C14—C15—Pt1	69.57 (16)	C30—C32—H32C	109.5
C16—C15—H15	114.5	H32A—C32—H32B	109.5
C16—C15—Pt1	112.57 (19)	H32A—C32—H32C	109.5
Pt1—C15—H15	114.5	H32B—C32—H32C	109.5
C15—C16—H16A	108.8	C3—N2—C11	119.5 (2)
C15—C16—H16B	108.8	C3—N2—Pt1	129.50 (19)
C15—C16—C17	113.6 (3)	C11—N2—Pt1	110.82 (17)
H16A—C16—H16B	107.7	C10—O12—Pt1	111.41 (16)
C17—C16—H16A	108.8	C19—O23—C24	118.1 (2)
C17—C16—H16B	108.8	C20—O25—C26	115.3 (2)
C18—C17—C16	120.7 (3)	C27—O29—C30	117.6 (2)
C22—C17—C16	121.0 (3)	C14—Pt1—C15	37.92 (11)
C22—C17—C18	118.3 (3)	C14—Pt1—Cl13	92.02 (10)
C17—C18—H18	119.7	C15—Pt1—Cl13	90.47 (9)
C19—C18—C17	120.6 (3)	N2—Pt1—C14	166.07 (11)
C19—C18—H18	119.7	N2—Pt1—C15	153.86 (10)
C18—C19—C20	120.2 (3)	N2—Pt1—Cl13	94.65 (7)
O23—C19—C18	124.5 (3)	O12—Pt1—C14	90.51 (11)
O23—C19—C20	115.3 (2)	O12—Pt1—C15	92.84 (10)

C21—C20—C19	119.4 (3)	O12—Pt1—Cl13	176.69 (6)
C21—C20—O25	125.2 (3)	O12—Pt1—N2	82.43 (8)
O25—C20—C19	115.4 (2)		
C3—C4—C5—C6	−0.4 (4)	C17—C18—C19—C20	0.5 (4)
C4—C3—N2—C11	−0.1 (4)	C17—C18—C19—O23	−179.8 (3)
C4—C3—N2—Pt1	174.8 (2)	C18—C17—C22—C21	−1.3 (4)
C4—C5—C6—C7	−178.5 (3)	C18—C19—C20—C21	−1.2 (4)
C4—C5—C6—C11	1.5 (4)	C18—C19—C20—O25	−179.7 (3)
C5—C6—C7—C8	−178.4 (3)	C18—C19—O23—C24	−1.3 (5)
C5—C6—C11—C10	178.8 (2)	C19—C20—C21—C22	0.6 (4)
C5—C6—C11—N2	−2.1 (4)	C19—C20—O25—C26	−171.4 (2)
C6—C7—C8—C9	−1.0 (5)	C20—C19—O23—C24	178.4 (3)
C6—C11—N2—C3	1.3 (4)	C20—C21—C22—C17	0.7 (5)
C6—C11—N2—Pt1	−174.45 (19)	C21—C20—O25—C26	10.1 (4)
C7—C6—C11—C10	−1.2 (4)	C22—C17—C18—C19	0.7 (4)
C7—C6—C11—N2	178.0 (2)	C26—C27—O29—C30	−174.5 (2)
C7—C8—C9—C10	−0.1 (5)	C27—C26—O25—C20	−176.6 (2)
C8—C9—C10—C11	0.5 (4)	C31—C30—O29—C27	−79.9 (3)
C8—C9—C10—O12	−178.4 (3)	C32—C30—O29—C27	157.7 (3)
C9—C10—C11—C6	0.1 (4)	N2—C3—C4—C5	−0.4 (5)
C9—C10—C11—N2	−179.1 (2)	O12—C10—C11—C6	179.1 (2)
C9—C10—O12—Pt1	174.3 (2)	O12—C10—C11—N2	−0.1 (4)
C10—C11—N2—C3	−179.5 (2)	O23—C19—C20—C21	179.1 (3)
C10—C11—N2—Pt1	4.7 (3)	O23—C19—C20—O25	0.5 (4)
C11—C6—C7—C8	1.6 (4)	O25—C20—C21—C22	179.0 (3)
C11—C10—O12—Pt1	−4.7 (3)	O25—C26—C27—O28	10.2 (4)
C14—C15—C16—C17	156.2 (3)	O25—C26—C27—O29	−172.3 (2)
C15—C16—C17—C18	−92.4 (3)	O28—C27—O29—C30	3.0 (4)
C15—C16—C17—C22	86.9 (3)	Pt1—C14—C15—C16	−104.3 (3)
C16—C17—C18—C19	−180.0 (3)	Pt1—C15—C16—C17	76.6 (3)
C16—C17—C22—C21	179.4 (3)		

Hydrogen-bond geometry ($\text{\AA}$, $^\circ$)

Cg1 is the centroid of ring N2/C3—C6/C11, Cg2 is the centroid of ring C6—C11 and Cg3 is the centroid of ring C17—C22.

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
C5—H5 $\cdots$ O23 ⁱ	0.95	2.46	3.073 (4)	122
C16—H16A $\cdots$ O12	0.99	2.40	3.051 (4)	123
C14—H14B $\cdots$ Cg1 ⁱⁱ	0.99	2.94	3.454 (4)	114
C24—H24B $\cdots$ Cg2	0.98	2.93	3.564 (4)	124
C30—H30 $\cdots$ Cg3 ⁱⁱⁱ	1.00	2.96	3.827 (4)	145

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

[η^2 -4-Allyl-2-methoxy-1-(propoxycarbonylmethoxy)benzene]chlorido(quinolin-2-carboxylato- κ^2N,O)platinum(II) (chi33)

Crystal data

[Pt(C₁₀H₆O₂)Cl(C₁₅H₂₀O₄)]

$M_r = 667.01$

Monoclinic, $P2_1/c$

$a = 15.6457(13) \text{ \AA}$

$b = 9.7291(4) \text{ \AA}$

$c = 16.6062(8) \text{ \AA}$

$\beta = 111.150(8)^\circ$

$V = 2357.5(3) \text{ \AA}^3$

$Z = 4$

$F(000) = 1304$

$D_x = 1.879 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 6260 reflections

$\theta = 3.4\text{--}28.0^\circ$

$\mu = 6.11 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Needle, yellow

$0.3 \times 0.15 \times 0.10 \text{ mm}$

Data collection

Agilent SuperNova Dual Source

diffractometer with an Eos detector

Radiation source: SuperNova (Mo) X-ray
Source

Mirror monochromator

Detector resolution: $15.9631 \text{ pixels mm}^{-1}$

ω scans

Absorption correction: multi-scan
(CrysAlis PRO; Agilent, 2013)

$T_{\min} = 0.522$, $T_{\max} = 1.000$

21714 measured reflections

4030 independent reflections

3348 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.066$

$\theta_{\max} = 24.7^\circ$, $\theta_{\min} = 2.8^\circ$

$h = -18 \rightarrow 18$

$k = -11 \rightarrow 11$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.086$

$S = 1.08$

4030 reflections

316 parameters

0 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0209P)^2 + 13.4203P]$

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

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

$\Delta\rho_{\max} = 2.22 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -1.13 \text{ e \AA}^{-3}$

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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Pt1A	0.69372 (3)	0.90310 (4)	0.69364 (2)	0.02742 (15)	0.9298 (13)
Pt1B	0.6573 (5)	0.9379 (6)	0.7023 (3)	0.02742 (15)	0.0702 (13)
Cl2A	0.74945 (19)	1.1196 (2)	0.69048 (14)	0.0519 (7)	0.9298 (13)
Cl2B	0.710 (3)	1.143 (4)	0.711 (2)	0.0519 (7)	0.0702 (13)
N3	0.6096 (4)	0.8677 (6)	0.5632 (3)	0.0261 (13)	
C4	0.5626 (5)	0.7531 (7)	0.5569 (4)	0.0281 (16)	
C5	0.5000 (5)	0.7022 (8)	0.4798 (4)	0.0380 (18)	
H5	0.466660	0.620352	0.479342	0.046*	

C6	0.4873 (6)	0.7711 (9)	0.4056 (5)	0.045 (2)	
H6	0.444434	0.738369	0.352463	0.054*	
C7	0.5374 (5)	0.8902 (8)	0.4075 (5)	0.0399 (19)	
C8	0.5288 (6)	0.9618 (9)	0.3313 (5)	0.049 (2)	
H8	0.486090	0.930261	0.277779	0.058*	
C9	0.5800 (6)	1.0743 (10)	0.3325 (5)	0.052 (2)	
H9	0.573686	1.121077	0.280497	0.063*	
C10	0.6428 (6)	1.1212 (8)	0.4123 (5)	0.048 (2)	
H10	0.678626	1.200557	0.413662	0.058*	
C11	0.6532 (6)	1.0544 (8)	0.4881 (5)	0.0403 (19)	
H11	0.696339	1.087252	0.541004	0.048*	
C12	0.6004 (5)	0.9381 (7)	0.4874 (4)	0.0302 (16)	
C13	0.5797 (5)	0.6706 (8)	0.6392 (4)	0.0326 (17)	
O14	0.6441 (4)	0.7167 (5)	0.7062 (3)	0.0403 (13)	
O15	0.5356 (4)	0.5679 (5)	0.6383 (3)	0.0402 (13)	
C16	0.8065 (5)	0.8737 (8)	0.8114 (4)	0.0360 (18)	
H16A	0.820957	0.779283	0.823459	0.043*	
H16B	0.839552	0.927213	0.784616	0.043*	
C17	0.7365 (5)	0.9339 (8)	0.8331 (4)	0.041 (2)	
H17	0.747581	1.031930	0.852165	0.049*	0.9298 (13)
H17A	0.752705	1.027924	0.858348	0.049*	0.0702 (13)
C18	0.6843 (6)	0.8543 (9)	0.8744 (5)	0.047 (2)	
H18A	0.688324	0.755037	0.863072	0.057*	
H18B	0.618940	0.881693	0.850753	0.057*	
C19	0.7245 (5)	0.8821 (9)	0.9717 (4)	0.041 (2)	
C20	0.7935 (5)	0.7966 (8)	1.0248 (4)	0.0373 (18)	
H20	0.814797	0.721662	1.000530	0.045*	
C21	0.8313 (5)	0.8211 (8)	1.1136 (4)	0.0323 (17)	
C22	0.7985 (5)	0.9311 (7)	1.1495 (4)	0.0304 (17)	
C23	0.7315 (5)	1.0157 (8)	1.0962 (4)	0.0358 (17)	
H23	0.710572	1.092086	1.119598	0.043*	
C24	0.6942 (5)	0.9891 (8)	1.0073 (4)	0.0396 (19)	
H24	0.646899	1.046700	0.971174	0.047*	
O25	0.8981 (3)	0.7447 (5)	1.1711 (3)	0.0414 (13)	
C26	0.9278 (6)	0.6241 (9)	1.1385 (5)	0.054 (2)	
H26A	0.949783	0.650355	1.092396	0.081*	
H26B	0.876367	0.560041	1.115666	0.081*	
H26C	0.977560	0.579745	1.185385	0.081*	
O27	0.8385 (3)	0.9431 (5)	1.2376 (3)	0.0336 (12)	
C28	0.8073 (5)	1.0523 (7)	1.2750 (4)	0.0345 (18)	
H28A	0.739919	1.046870	1.258444	0.041*	
H28B	0.822518	1.141173	1.254417	0.041*	
C29	0.8532 (5)	1.0422 (8)	1.3717 (4)	0.0305 (16)	
O30	0.8787 (4)	0.9389 (5)	1.4110 (3)	0.0367 (12)	
O31	0.8578 (3)	1.1679 (5)	1.4060 (3)	0.0366 (12)	
C32	0.8972 (5)	1.1747 (8)	1.4997 (4)	0.0414 (19)	
H32A	0.952958	1.116983	1.521270	0.050*	
H32B	0.852620	1.139311	1.524470	0.050*	

C33	0.9208 (6)	1.3209 (8)	1.5269 (5)	0.050 (2)
H33A	0.866320	1.380139	1.500989	0.060*
H33B	0.969642	1.353675	1.506787	0.060*
C34	0.9536 (7)	1.3289 (11)	1.6247 (5)	0.066 (3)
H34A	0.972162	1.423355	1.643341	0.099*
H34B	1.005973	1.267105	1.649891	0.099*
H34C	0.903806	1.301305	1.643904	0.099*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1A	0.0359 (3)	0.0302 (2)	0.01614 (15)	0.00021 (17)	0.00946 (13)	0.00123 (13)
Pt1B	0.0359 (3)	0.0302 (2)	0.01614 (15)	0.00021 (17)	0.00946 (13)	0.00123 (13)
Cl2A	0.0799 (19)	0.0368 (13)	0.0309 (12)	-0.0187 (12)	0.0103 (11)	0.0034 (9)
Cl2B	0.0799 (19)	0.0368 (13)	0.0309 (12)	-0.0187 (12)	0.0103 (11)	0.0034 (9)
N3	0.030 (3)	0.034 (4)	0.017 (3)	0.006 (3)	0.012 (2)	0.001 (2)
C4	0.031 (4)	0.036 (4)	0.020 (3)	0.004 (3)	0.011 (3)	0.001 (3)
C5	0.039 (4)	0.053 (5)	0.021 (4)	-0.007 (4)	0.010 (3)	-0.009 (3)
C6	0.057 (5)	0.055 (6)	0.022 (4)	0.008 (4)	0.012 (4)	-0.004 (4)
C7	0.051 (5)	0.052 (5)	0.025 (4)	0.018 (4)	0.023 (4)	0.002 (3)
C8	0.072 (6)	0.058 (6)	0.020 (4)	0.015 (5)	0.022 (4)	0.009 (4)
C9	0.072 (6)	0.067 (6)	0.028 (4)	0.031 (5)	0.030 (4)	0.016 (4)
C10	0.061 (6)	0.042 (5)	0.053 (5)	0.010 (4)	0.033 (5)	0.019 (4)
C11	0.054 (5)	0.043 (5)	0.028 (4)	0.010 (4)	0.020 (4)	0.007 (3)
C12	0.036 (4)	0.038 (4)	0.021 (4)	0.010 (3)	0.015 (3)	0.006 (3)
C13	0.037 (4)	0.041 (5)	0.022 (4)	0.000 (4)	0.013 (3)	0.002 (3)
O14	0.064 (4)	0.041 (3)	0.013 (2)	-0.013 (3)	0.010 (2)	0.004 (2)
O15	0.051 (3)	0.048 (3)	0.025 (3)	-0.022 (3)	0.018 (2)	-0.005 (2)
C16	0.043 (4)	0.041 (5)	0.022 (4)	0.004 (4)	0.009 (3)	0.004 (3)
C17	0.056 (5)	0.049 (5)	0.010 (3)	0.003 (4)	0.003 (3)	-0.002 (3)
C18	0.050 (5)	0.062 (6)	0.030 (4)	-0.013 (4)	0.016 (4)	-0.008 (4)
C19	0.047 (5)	0.059 (6)	0.019 (4)	-0.013 (4)	0.015 (4)	0.002 (4)
C20	0.048 (5)	0.042 (5)	0.031 (4)	-0.013 (4)	0.026 (4)	-0.013 (3)
C21	0.034 (4)	0.038 (4)	0.029 (4)	-0.005 (3)	0.015 (3)	-0.003 (3)
C22	0.037 (4)	0.037 (4)	0.019 (3)	-0.012 (3)	0.013 (3)	0.000 (3)
C23	0.040 (4)	0.042 (5)	0.026 (4)	-0.001 (4)	0.013 (3)	0.003 (3)
C24	0.041 (5)	0.055 (5)	0.020 (4)	-0.005 (4)	0.009 (3)	-0.001 (3)
O25	0.049 (3)	0.048 (3)	0.030 (3)	0.005 (3)	0.017 (3)	-0.009 (2)
C26	0.066 (6)	0.054 (6)	0.046 (5)	0.011 (5)	0.027 (5)	-0.009 (4)
O27	0.041 (3)	0.036 (3)	0.022 (2)	0.001 (2)	0.009 (2)	-0.005 (2)
C28	0.052 (5)	0.033 (4)	0.016 (3)	0.000 (3)	0.009 (3)	-0.001 (3)
C29	0.035 (4)	0.030 (4)	0.031 (4)	-0.002 (3)	0.017 (3)	-0.003 (3)
O30	0.053 (3)	0.032 (3)	0.023 (3)	0.000 (2)	0.011 (2)	-0.001 (2)
O31	0.056 (3)	0.030 (3)	0.020 (2)	0.003 (2)	0.010 (2)	-0.003 (2)
C32	0.048 (5)	0.053 (5)	0.022 (4)	0.003 (4)	0.012 (4)	-0.004 (3)
C33	0.067 (6)	0.045 (5)	0.032 (4)	0.012 (4)	0.008 (4)	-0.018 (4)
C34	0.067 (7)	0.085 (7)	0.039 (5)	0.011 (5)	0.011 (5)	-0.023 (5)

Geometric parameters (Å, °)

PT1Aa—Cl2A	2.287 (2)	C17—C18	1.464 (11)
PT1Bb—Cl2B	2.14 (3)	C18—H18A	0.9900
PT1Aa—N3	2.118 (5)	C18—H18B	0.9900
PT1Bb—N3	2.262 (7)	C18—C19	1.533 (10)
PT1Aa—O14	2.013 (5)	C19—C20	1.396 (11)
PT1Bb—O14	2.166 (7)	C19—C24	1.363 (11)
PT1Bb—C16	2.464 (9)	C20—H20	0.9500
PT1Aa—C16	2.128 (7)	C20—C21	1.397 (9)
PT1Aa—C17	2.186 (6)	C21—C22	1.409 (10)
PT1Bb—C17	2.077 (8)	C21—O25	1.355 (8)
N3—C4	1.320 (9)	C22—C23	1.374 (10)
N3—C12	1.393 (8)	C22—O27	1.373 (7)
C4—C5	1.392 (9)	C23—H23	0.9500
C4—C13	1.522 (9)	C23—C24	1.402 (9)
C5—H5	0.9500	C24—H24	0.9500
C5—C6	1.353 (10)	O25—C26	1.437 (9)
C6—H6	0.9500	C26—H26A	0.9800
C6—C7	1.393 (11)	C26—H26B	0.9800
C7—C8	1.408 (10)	C26—H26C	0.9800
C7—C12	1.416 (10)	O27—C28	1.405 (8)
C8—H8	0.9500	C28—H28A	0.9900
C8—C9	1.352 (12)	C28—H28B	0.9900
C9—H9	0.9500	C28—C29	1.508 (9)
C9—C10	1.411 (12)	C29—O30	1.186 (8)
C10—H10	0.9500	C29—O31	1.340 (8)
C10—C11	1.372 (10)	O31—C32	1.453 (8)
C11—H11	0.9500	C32—H32A	0.9900
C11—C12	1.399 (10)	C32—H32B	0.9900
C13—O14	1.283 (8)	C32—C33	1.498 (11)
C13—O15	1.212 (8)	C33—H33A	0.9900
C16—H16A	0.9500	C33—H33B	0.9900
C16—H16B	0.9500	C33—C34	1.518 (10)
C16—C17	1.399 (10)	C34—H34A	0.9800
C17—H17	1.0000	C34—H34B	0.9800
C17—H17A	1.0000	C34—H34C	0.9800
CL2Bb—PT1Bb—N3	108.9 (9)	C17—PT1Bb—N3	156.2 (5)
CL2Bb—PT1Bb—O14	163.9 (12)	C17—PT1Bb—O14	88.7 (3)
CL2Bb—PT1Bb—C16	87.0 (10)	C17—PT1Bb—C16	34.6 (3)
PT1Aa—C16—H16A	112.3	C18—C17—Pt1A	114.5 (5)
PT1Aa—C16—H16B	84.7	C18—C17—Pt1B	106.1 (5)
H16Aa—C16—H16B	120.0	C18—C17—H17	114.7
PT1Aa—C17—H17	114.7	C18—C17—H17A	112.8
PT1Bb—C17—H17A	112.8	C17—C18—H18A	110.0
N3—PT1Aa—Cl2A	103.13 (16)	C17—C18—H18B	110.0
N3—PT1Bb—C16	123.4 (4)	C17—C18—C19	108.3 (6)

N3—PT1Aa—C16	157.1 (2)	H18A—C18—H18B	108.4
N3—PT1Aa—C17	161.0 (3)	C19—C18—H18A	110.0
C4—N3—Pt1A	109.9 (4)	C19—C18—H18B	110.0
C4—N3—Pt1B	107.7 (4)	C20—C19—C18	119.4 (7)
C4—N3—C12	118.1 (6)	C24—C19—C18	121.2 (7)
C12—N3—Pt1A	131.9 (5)	C24—C19—C20	119.5 (7)
C12—N3—Pt1B	131.5 (5)	C19—C20—H20	120.0
N3—C4—C5	124.0 (6)	C19—C20—C21	120.1 (7)
N3—C4—C13	117.5 (6)	C21—C20—H20	120.0
C5—C4—C13	118.4 (7)	C20—C21—C22	119.7 (7)
C4—C5—H5	120.5	O25—C21—C20	125.1 (7)
C6—C5—C4	119.0 (8)	O25—C21—C22	115.2 (6)
C6—C5—H5	120.5	C23—C22—C21	119.5 (6)
C5—C6—H6	120.2	O27—C22—C21	114.8 (6)
C5—C6—C7	119.6 (7)	O27—C22—C23	125.7 (7)
C7—C6—H6	120.2	C22—C23—H23	120.1
C6—C7—C8	121.4 (8)	C22—C23—C24	119.9 (7)
C6—C7—C12	119.4 (7)	C24—C23—H23	120.1
C8—C7—C12	119.2 (8)	C19—C24—C23	121.3 (7)
C7—C8—H8	119.2	C19—C24—H24	119.3
C9—C8—C7	121.5 (8)	C23—C24—H24	119.3
C9—C8—H8	119.2	C21—O25—C26	117.1 (6)
C8—C9—H9	120.5	O25—C26—H26A	109.5
C8—C9—C10	118.9 (7)	O25—C26—H26B	109.5
C10—C9—H9	120.5	O25—C26—H26C	109.5
C9—C10—H10	119.3	H26A—C26—H26B	109.5
C11—C10—C9	121.3 (8)	H26A—C26—H26C	109.5
C11—C10—H10	119.3	H26B—C26—H26C	109.5
C10—C11—H11	119.9	C22—O27—C28	115.9 (5)
C10—C11—C12	120.1 (8)	O27—C28—H28A	110.0
C12—C11—H11	119.9	O27—C28—H28B	110.0
N3—C12—C7	119.6 (7)	O27—C28—C29	108.3 (6)
N3—C12—C11	121.5 (6)	H28A—C28—H28B	108.4
C11—C12—C7	118.8 (6)	C29—C28—H28A	110.0
O14—C13—C4	115.1 (6)	C29—C28—H28B	110.0
O15—C13—C4	120.6 (6)	O30—C29—C28	125.3 (7)
O15—C13—O14	124.3 (6)	O30—C29—O31	125.7 (6)
C13—O14—Pt1A	115.8 (4)	O31—C29—C28	109.0 (6)
C13—O14—Pt1B	112.0 (5)	C29—O31—C32	115.7 (6)
C17—C16—Pt1A	73.4 (4)	O31—C32—H32A	109.8
O14—PT1Aa—Cl2A	175.13 (14)	O31—C32—H32B	109.8
O14—PT1Aa—N3	80.8 (2)	O31—C32—C33	109.2 (6)
O14—PT1Bb—N3	74.4 (2)	H32A—C32—H32B	108.3
O14—PT1Aa—C16	90.4 (2)	C33—C32—H32A	109.8
O14—PT1Bb—C16	78.5 (3)	C33—C32—H32B	109.8
O14—PT1Aa—C17	89.8 (3)	C32—C33—H33A	109.9
C16—PT1Aa—Cl2A	87.0 (2)	C32—C33—H33B	109.9
C16—PT1Aa—C17	37.8 (3)	C32—C33—C34	108.8 (7)

C17—C16—Pt1B	57.4 (4)	H33A—C33—H33B	108.3
C17—C16—H16A	120.0	C34—C33—H33A	109.9
C17—C16—H16B	120.0	C34—C33—H33B	109.9
C16—C17—Pt1A	68.8 (4)	C33—C34—H34A	109.5
C16—C17—Pt1B	88.0 (5)	C33—C34—H34B	109.5
C16—C17—H17	114.7	C33—C34—H34C	109.5
C16—C17—H17A	112.8	H34A—C34—H34B	109.5
C16—C17—C18	121.3 (7)	H34A—C34—H34C	109.5
C17—PT1Aa—C12A	85.7 (2)	H34B—C34—H34C	109.5
C17—PT1Bb—C12B	83.1 (9)		
PT1Aa—N3—C4—C5	179.0 (6)	O15—C13—O14—PT1Bb	−150.9 (7)
PT1Bb—N3—C4—C5	159.5 (6)	O15—C13—O14—PT1Aa	−171.7 (6)
PT1Aa—N3—C4—C13	−2.3 (7)	PT1Aa—C16—C17—C18	106.5 (7)
PT1Bb—N3—C4—C13	−21.8 (7)	PT1Bb—C16—C17—C18	107.7 (7)
PT1Bb—N3—C12—C7	−155.0 (6)	PT1Aa—C17—C18—C19	177.7 (5)
PT1Aa—N3—C12—C7	−180.0 (5)	PT1Bb—C17—C18—C19	−163.8 (6)
PT1Bb—N3—C12—C11	26.1 (10)	C16—C17—C18—C19	98.5 (8)
PT1Aa—N3—C12—C11	1.2 (10)	C17—C18—C19—C20	−91.5 (9)
N3—C4—C5—C6	1.8 (11)	C17—C18—C19—C24	88.3 (9)
N3—C4—C13—O14	−4.9 (9)	C18—C19—C20—C21	179.6 (6)
N3—C4—C13—O15	176.6 (6)	C18—C19—C24—C23	−179.3 (7)
C4—N3—C12—C7	3.8 (9)	C19—C20—C21—C22	1.0 (10)
C4—N3—C12—C11	−175.0 (6)	C19—C20—C21—O25	179.7 (7)
C4—C5—C6—C7	0.6 (11)	C20—C19—C24—C23	0.5 (11)
C4—C13—O14—PT1Bb	30.8 (8)	C20—C21—C22—C23	−2.1 (10)
C4—C13—O14—PT1Aa	10.0 (8)	C20—C21—C22—O27	178.1 (6)
C5—C4—C13—O14	173.9 (6)	C20—C21—O25—C26	−4.3 (10)
C5—C4—C13—O15	−4.6 (10)	C21—C22—C23—C24	2.3 (11)
C5—C6—C7—C8	177.5 (7)	C21—C22—O27—C28	179.7 (6)
C5—C6—C7—C12	−0.6 (11)	C22—C21—O25—C26	174.5 (6)
C6—C7—C8—C9	−177.4 (8)	C22—C23—C24—C19	−1.6 (11)
C6—C7—C12—N3	−1.7 (10)	C22—O27—C28—C29	175.6 (6)
C6—C7—C12—C11	177.3 (7)	C23—C22—O27—C28	−0.1 (10)
C7—C8—C9—C10	−0.5 (12)	C24—C19—C20—C21	−0.2 (11)
C8—C7—C12—N3	−179.8 (6)	O25—C21—C22—C23	179.1 (6)
C8—C7—C12—C11	−0.9 (10)	O25—C21—C22—O27	−0.7 (9)
C8—C9—C10—C11	0.4 (12)	O27—C22—C23—C24	−177.9 (6)
C9—C10—C11—C12	−0.6 (12)	O27—C28—C29—O30	−28.6 (10)
C10—C11—C12—N3	179.7 (7)	O27—C28—C29—O31	153.3 (6)
C10—C11—C12—C7	0.8 (11)	C28—C29—O31—C32	177.5 (6)
C12—N3—C4—C5	−4.0 (10)	C29—O31—C32—C33	164.9 (7)
C12—N3—C4—C13	174.7 (6)	O30—C29—O31—C32	−0.5 (10)
C12—C7—C8—C9	0.7 (12)	O31—C32—C33—C34	174.8 (7)
C13—C4—C5—C6	−176.9 (7)		

Hydrogen-bond geometry (Å, °)

<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>
C11—H11 $\cdots$ Cl2 <i>A</i>	0.95	2.34	3.211 (8)	153
C11—H11 $\cdots$ Cl2 <i>B</i>	0.95	2.81	3.59 (3)	140
C16—H16 <i>A</i> $\cdots$ O30 ⁱ	0.95	2.55	3.452 (9)	159
C20—H20 $\cdots$ O30 ⁱ	0.95	2.59	3.524 (9)	167
C28—H28 <i>B</i> $\cdots$ Cl2 <i>A</i> ⁱⁱ	0.99	2.64	3.473 (7)	142
C32—H32 <i>A</i> $\cdots$ O30 ⁱⁱⁱ	0.99	2.52	3.459 (10)	158

Symmetry codes: (i) $x, -y+3/2, z-1/2$; (ii) $x, -y+5/2, z+1/2$; (iii) $-x+2, -y+2, -z+3$.