Acta Cryst C STRUCTURAL CHEMISTRY
ISSN 2053-2296

Synthesis, structure and *in vitro* cytotoxicity of platinum(II) complexes containing eugenol and a quinolin-8-ol-derived chelator[1]

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Received 11 October 2017
Accepted 18 October 2017

Edited by A. L. Spek, Utrecht University, The Netherlands

[1] Dedicated to Professor Harry Reynaers on the occasion of his 79th birthday.

Keywords: platinum(II) complexes; crystal structure; eugenol; quinolin-8-ol derivatives; cytotoxicity.

CCDC references: 1566223; 1566222

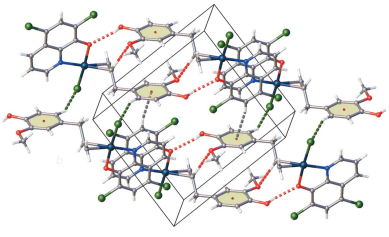
Supporting information: this article has supporting information at journals.iucr.org/c

The synthesis of potassium (η^2-4-allyl-2-methoxyphenol)trichloridoplatinate(II), K[$PtCl_3(C_{10}H_{12}O_2)$], (**1**), starting from Zeise's salt and *Ocimum sanctum* L. oil has been optimized. Starting from (**1**), three new platinum(II) complexes, namely (η^2-4-allyl-2-methoxyphenol)chlorido(2-methylquinolin-8-olato-κ^2N,O)-platinum(II), (**2**), (η^2-4-allyl-2-methoxyphenol)chlorido(5-nitroquinolin-8-olato-κ^2N,O)platinum(II), (**3**), and (η^2-4-allyl-2-methoxyphenol)chlorido(5,7-dichloroquinolin-8-olato-κ^2N,O)platinum(II), [$Pt(C_9H_4Cl_2NO)Cl(C_{10}H_{12}O_2)$], (**4**), containing eugenol and a quinolin-8-ol derivative (R-OQ), have been synthesized and characterized by elemental analyses, MS, IR, ^{1}H NMR and NOESY spectra. For (**1**) and (**4**), single-crystal X-ray diffraction studies were also carried out. Complexes (**2**)–(**4**) show good inhibiting abilities on three human cancer cell lines, *i.e.* KB, Hep-G2 and LU, with IC_{50} values of 1.42–17.8 μ*M*. Complex (**3**) gives an impressively high activity against KB, Hep-G2, LU and MCF-7, with IC_{50} values of 1.42–4.91 μ*M*, which are much lower than those of cisplatin and some other platinum(II) complexes.

1. Introduction

It is known that platinum-based drugs, including cisplatin, carboplatin and oxaliplatin, are globally approved in cancer treatment and half of all patients undergoing chemotherapy are treated with platinum drugs (Johnstone *et al.*, 2014). Despite the widespread use and significant outcomes, unwanted side effects due to high toxicity, increasing varieties of cancer and resistance of tumours have limited the clinical applications of these drugs (Shah & Dizon, 2009; Johnstone *et al.*, 2016). With the need to overcome these difficulties, thousands of other platinum complexes have been synthesized and tested for antitumour activity (Johnstone *et al.*, 2016; Galanski *et al.*, 2005; Da *et al.*, 2012, 2015*a*,*b*; Romerosa *et al.*, 2004). Studies over many years have shown that a potential anticancer complex is definitely not limited to the structural concept of cisplatin and the strategy of using a natural compound as ligand in platinum complexes has attracted much attention (Da *et al.*, 2012, 2015*a*,*b*; Romerosa *et al.*, 2004).

Eugenol (4-allyl-2-methoxyphenol), (I) (Scheme 1), can be extracted from certain essential oils of plants, for example, tulsi (*Ocimum sanctum* L.) or clove (*Syzygium aromaticum*). They are widespread plants in many places around the world, hence, these essential oils are certainly abundant and accessible (Padalia & Verma, 2011; Kumar *et al.*, 2010). In our previous work, eugenol and its derivatives, (I) (Scheme 1),



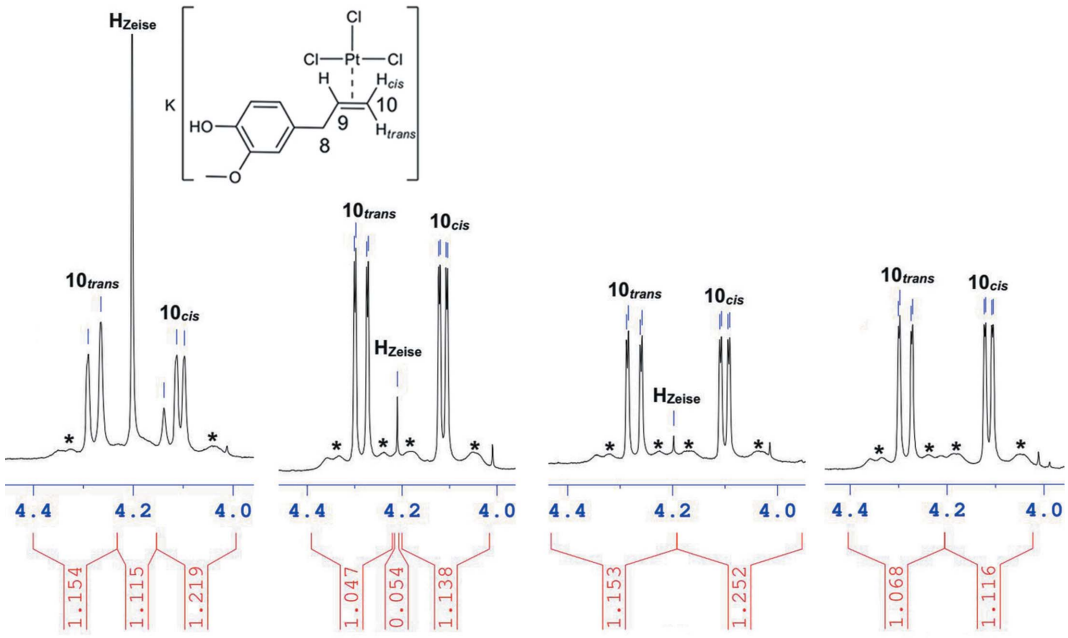
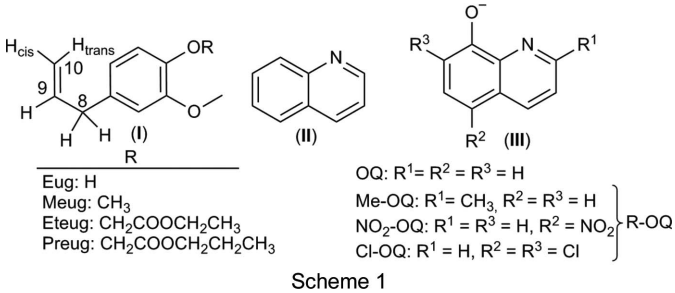


Figure 1
Partial ^{1}H NMR spectra of the reaction products from the reaction that yield compound (I) recorded after (*a*) 20, (*b*) 40, (*c*) 50 and (*d*) 60 min; ^{195}Pt satellites are indicated by asterisks (*).

have been used as ligands in some series of platinum(II) complexes containing amines, most of which were assayed for antitumour activity. Notably, complexes bearing quinoline, (II), or chelating 8-oxyquinolinate (OQ), (III) (Scheme 1), as a ligand have demonstrated potential inhibiting abilities on several tested cancer cell lines (Chi & Da, 2014; Chi *et al.*, 2017; Da *et al.*, 2015*a*,*b*).

In continuation of our encouraging results on complexes with derivatives of eugenol and quinoline, we report herein the synthesis and characterization of three platinum(II) complexes bearing eugenol (Eug) and a chelator derived from 8-hydoxyquinoline (R-OQ) (III), as well as their *in vitro* cytotoxicity on four human cancer cell lines.



Scheme 1

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.

Elemental analyses were performed 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 from KBr discs on an IMPACK-410 Nicolet spectrometer in the range 400–4000 cm^{-1}. ^{1}H NMR and NOESY 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).

2.1. Synthesis and crystallization

2.1.1. Synthesis of K[PtCl$_3$(Eug)], (1). *Ocimum sanctum* L. oil (2.5 ml, containing about 12.0 mmol eugenol) was mixed with Zeise's salt {K[PtCl$_3$(C$_2$H$_4$)]·H$_2$O; 3.86 g, 10.0 mmol}. The reaction mixture was stirred thoroughly for 1 h at ambient temperature until it began to transform to a viscous state and it was then washed with diethyl ether (5 × 5 ml). The product is obtained as a bright-yellow powder (yield: 95%, 4.80 g, 9.5 mmol). IR (KBr, cm^{-1}): 3325 (*s*), 3010 (*w*), 2943 (*m*), 2832 (*w*), 1601 (*m*), 1520 (*m*), 1458 (*m*), 1354 (*m*), 1277 (*m*), 1246 (*m*), 1196 (*m*), 1119 (*m*), 1030 (*m*), 937 (*w*), 799 (*m*), 629 (*w*), 567 (*w*). ^{1}H NMR (500 Hz, CD$_3$COCD$_3$, ppm): δ 7.33 (*d*, ^{4}J = 1.5 Hz, 1H, Ar-*H*), 6.79 (*dd*, ^{3}J = 8.0, ^{4}J = 1.5 Hz, 1H, Ar-*H*), 6.74 (*d*, ^{3}J = 8.0 Hz, 1H, Ar-*H*), 5.06 (*m*, $^{2}J_{PtH}$ = 70 Hz, 1H, C*H*═CH$_2$), 4.29 (*dd*, ^{3}J = 13.5, ^{4}J = 1.5, $^{2}J_{PtH}$ = 70 Hz, 1H, CH═C*H*$_2$), 4.12 (*dd*, ^{3}J = 7.5, ^{4}J = 1.5, $^{2}J_{PtH}$ = 70 Hz, 1H, CH═C*H*$_2$), 3.87 (*s*, 3H, OCH$_3$), 3.43 (*dd*, ^{2}J = 15.0, ^{3}J = 7.0 Hz, 1H, C*H*$_2$—CH), 2.90 (*dd*, ^{2}J = 15.0, ^{3}J = 7.5, $^{2}J_{PtH}$ = 50 Hz, 1H, C*H*$_2$—CH). Single crystals suitable for XRD measurements

Table 1
Experimental details.

	(**1**)	(**4**)
Crystal data		
Chemical formula	$K[PtCl_3(C_{10}H_{12}O_2)]$	$[Pt(C_9H_4Cl_2NO)Cl(C_{10}H_{12}O_2)]$
M_r	504.74	607.77
Crystal system, space group	Monoclinic, $P2_1/c$	Triclinic, $P\overline{1}$
Temperature (K)	100	100
a, b, c (Å)	12.0312 (6), 16.1528 (8), 8.1007 (4)	8.1313 (3), 11.2960 (5), 11.4294 (7)
α, β, γ (°)	90, 107.295 (6), 90	88.793 (4), 76.567 (4), 70.219 (4)
V (Å^3)	1503.09 (14)	958.93 (8)
Z	4	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	10.13	7.75
Crystal size (mm)	0.4 × 0.4 × 0.3	0.4 × 0.4 × 0.3
Data collection		
Diffractometer	Agilent SuperNova Single Source diffractometer with an Eos detector	Agilent SuperNova Single Source diffractometer with an Eos detector
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.548, 1.000	0.427, 1.000
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	15723, 3068, 2937	19518, 3916, 3594
R_{int}	0.040	0.075
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.625
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.023, 0.042, 1.20	0.036, 0.088, 1.11
No. of reflections	3068	3916
No. of parameters	223	301
No. of restraints	86	133
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.84, −0.92	2.51, −1.82

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

were obtained by slow evaporation over a period of 8 h from a concentrated acetone solution at ambient temperature.

2.1.2. Synthesis of [PtCl(Me-OQ)(Eug)], (2). A solution of 2-methylquinolin-8-ol (159 mg, 1.0 mmol) in aqueous acetone was added gradually to a mixture of (**1**) (505 mg, 1.0 mmol) in water (5 ml). The mixture was stirred at 298–303 K for 3 h. After cooling in an ice bath at about 278 K for 30 min, the yellow precipitated powder was filtered off, washed consecutively with a 0.1 *M* HCl solution (2 × 2 ml), water (3 × 2 ml) and cold ethanol (2 × 2 ml), and then dried in vacuum at 318 K for 3 h. Recrystallization from water/acetone gave a yellow powder (yield: 91%, 502.0 mg, 0.91 mmol). $C_{20}H_{20}ClNO_3Pt$: C 43.29 (calculated 43.47), H 3.64 (3.62), N 2.67 (2.54)%. ESI–MS (*m*/*z*): 517, 100%, $[M - Cl]^+$; 553, 10%, $[M + H]^+$. IR (KBr, cm^{-1}): 3445 (*s*), 3000 (*w*), 2932 (*m*), 1605 (*m*), 1566 (*m*), 1512 (*m*), 1462 (*m*), 1381 (*m*), 1327 (*m*), 1265 (*m*), 1195 (*m*), 1119 (*m*), 1030 (*m*), 907 (*w*), 829 (*m*), 752 (*m*), 660 (*w*). ^{1}H NMR (500 Hz, CD_3COCD_3, ppm): δ 8.22 (*d*, ^3J = 8.0 Hz, 1H, Ar-*H*), 7.32 (*t*, ^3J = 8.0 Hz, 1H, Ar-*H*), 7.30 (*d*, ^3J = 8.0 Hz, 1H, Ar-*H*), 6.99 (*br*, 1H, Ar-*H*), 6.96 (*d*, ^3J = 8.0 Hz, 1H, Ar-*H*), 6.86 (*ov*, 2H, Ar-*H*), 6.83 (*s*, 1H, Ar-*H*), 5.70 (*m*, $^2J_{PtH}$ = 70 Hz, 1H, C*H*═CH$_2$), 5.45 (*s*, 1H, OH), 4.75–4.78 (*ov*, 2H, CH═C*H*$_2$), 3.58 (*ov*, 4H, OCH$_3$, C*H*$_2$—CH), 3.16 (*ov*, 4H, C*H*$_2$—CH, CH$_3$).

2.1.3. Synthesis of [PtCl(NO$_2$-OQ)(Eug)], (3). Complex (**3**) was prepared starting from (**1**) (505 mg, 1.0 mmol) and 5-nitroquinolin-8-ol (190 mg, 1.0 mmol), according to the procedure for the preparation of (**2**). Recrystallization from ethanol/acetone gave a brown powder (yield: 90%, 525.0 mg, 0.90 mmol). $C_{19}H_{17}ClN_2O_5Pt$: C 39.22 (calculated 39.11), H 3.15 (2.92), N 4.69 (4.80)%. ESI–MS (*m*/*z*): 548, 100%, $[M - Cl]^+$; 584, 80%, $[M + H]^+$. IR (KBr, cm^{-1}): 3460 (*s*), 3080 (*w*), 2931 (*m*), 1601 (*m*), 1570 (*m*), 1504 (*m*), 1458 (*m*), 1377 (*m*), 1300 (*s*), 1230 (*m*), 1192 (*m*), 1146 (*m*), 1103 (*m*), 1030 (*m*), 814 (*m*), 756 (*m*), 671 (*w*), 637 (*w*). ^{1}H NMR (500 Hz, CD_3COCD_3, ppm): δ 9.76 (*dd*, ^3J = 9.0, ^4J = 1.0 Hz, 1H, Ar-*H*), 9.22 (*dd*, ^3J = 5.0, ^4J = 1.0, $^3J_{PtH}$ = 34 Hz, 1H, Ar-*H*), 8.67 (*d*, ^3J = 9.0 Hz, 1H, Ar-*H*), 8.20 (*dd*, ^3J = 5.0, ^3J = 9.0 Hz, 1H, Ar-*H*), 7.39 (*s*, 1H, O*H*), 7.10 (*d*, ^3J = 9.0 Hz, 1H, Ar-*H*), 7.08 (*d*, ^4J = 2.0 Hz, 1H, Ar-*H*), 6.88 (*dd*, ^3J = 8.0, ^4J = 2.0 Hz, 1H, Ar-*H*), 6.75 (*d*, ^3J = 8.0 Hz, 1H, Ar-*H*), 5.78 (*m*, $^2J_{PtH}$ = 70 Hz, 1H, C*H*═CH$_2$), 4.89 (*d*, ^3J = 12.0, $^2J_{PtH}$ = 70 Hz, 1H, CH═C*H*$_2$), 4.87 (*d*, ^3J = 6.5, $^2J_{PtH}$ = 70 Hz, 1H, CH═C*H*$_2$), 3.65 (*s*, 3H, OCH$_3$), 3.58 (*dd*, ^2J = 15.0, ^3J = 7.5 Hz, 1H, C*H*$_2$—CH), 3.32 (*dd*, ^2J = 15.0, ^3J = 7.5, $^2J_{PtH}$ = 50 Hz, 1H, C*H*$_2$—CH).

2.1.4. Synthesis of [PtCl(Cl-OQ)(Eug)], (4). Complex (**4**) was prepared starting from (**1**) (505 mg, 1.0 mmol) and 5,7-dichloroquinolin-8-ol (214 mg, 1.0 mmol), according to the procedure for the preparation of (**2**). Recrystallization from ethanol/acetone gave a yellow powder (yield: 90%, 545.0 mg, 0.90 mmol). Single crystals suitable for XRD determination were obtained by slow evaporation over 10 h from a concentrated chloroform/propan-2-ol solution at ambient temperature. $C_{19}H_{16}Cl_3NO_3Pt$: C 37.82 (calculated 37.62): H 2.78

(2.64), N 2.43 (2.31)%. ESI–MS (*m*/*z*): 571, 100% $[M - Cl]^+$; 607, 20%, $[M + H]^+$. IR (KBr, cm^{-1}): 3472 (*s*), 3059 (*w*), 2990 (*w*), 2955 (*m*), 2835 (*w*), 1605 (*m*), 1566 (*m*), 1497 (*m*), 1450 (*m*), 1369 (*m*), 1273 (*m*), 1234 (*m*), 1200 (*m*), 1146 (*m*), 1119 (*m*), 1034 (*m*), 980 (*m*), 891 (*m*), 802 (*m*), 756 (*m*), 683 (*w*), 648 (*m*). ^{1}H NMR (500 Hz, CD_3COCD_3, ppm): δ 9.17 (*dd*, ^3J = 5.5, ^4J = 1.0, $^3J_{PtH}$ = 35 Hz, 1H, Ar-*H*), 8.95 (*dd*, ^3J = 9.0, ^4J = 1.0 Hz, 1H, Ar-*H*), 8.03 (*dd*, ^3J = 9.0 Hz, 1H, Ar-*H*), 7.78 (*s*, 1H, Ar-*H*), 7.40 (*s*, 1H, O*H*), 7.05 (*d*, ^4J = 1.5 Hz, 1H, Ar-*H*), 6.88 (*dd*, ^3J = 8.0, ^4J = 1.5 Hz, 1H, Ar-*H*), 6.75 (*d*, ^3J = 8.0 Hz, 1H, Ar-*H*), 5.75 (*m*, $^2J_{PtH}$ = 70 Hz, 1H, C*H*═CH_2), 4.87 (*d*, ^3J = 14.0, $^2J_{PtH}$ = 70 Hz, 1H, CH═CH_2), 4.85 (*d*, ^3J = 7.0, $^2J_{PtH}$ = 70 Hz, 1H, CH═CH_2), 3.57–3.61 (*ov*, 4H, OCH_3, CH_2—CH), 3.33 (*dd*, ^2J = 15.0 Hz, ^3J = 6.0 Hz, $^2J_{PtH}$ = 50 Hz, 1H, CH_2—CH).

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms were placed in calculated positions and refined using a riding model, with C—H distances of 0.95 (aromatic), 1.00 (CH), 0.99 (CH_2) and 0.98 Å (CH_3), and with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) otherwise. In complex (**1**), atoms C6, C7, C8, C9, C10 and C13 of the eugenol ligand are disordered, with population parameters of 0.660 (7) and 0.340 (7) for the two positions (*A* and *B*). In complex (**4**), atoms C17, C18, C19, C20, C23 and C24 of the eugenol ligand are disordered, with population parameters of 0.642 (14) and 0.358 (14) for the two positions (*A* and *B*). For the disordered parts, bond lengths were restrained and enhanced rigid-bond restraints were applied to the displacement parameters.

2.3. *In vitro* cell tests

MTT assay was used to determine the cytotoxic activity of the compounds with human cancer cell lines (KB, LU-1, Hep-G2 and MCF-7) acquired from 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% CO_2 at 310 K. The testing substances were initially dissolved in dimethyl sulfoxide (DMSO) and diluted to the desired concentration, which was less than 0.5% in all the experiments, by adding cell culture medium. The samples (100 µl) of the complexes with different concentrations were added to the wells on 96-well plates. Cells were separated with trypsin and ethylenediaminetetraacetic acid (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 Na_2HPO_4 and 0.24 g KH_2PO_4 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.

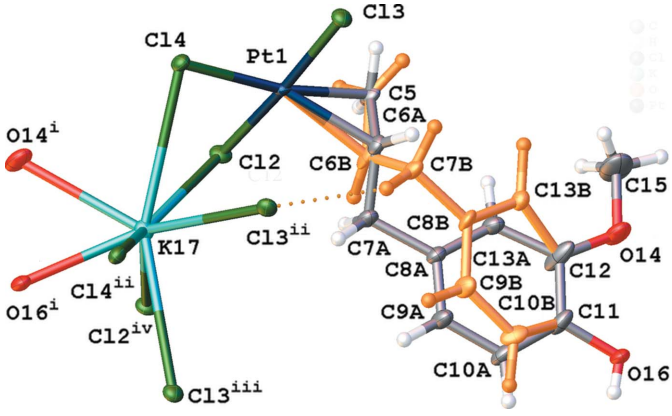


Figure 2
The molecular structure of complex (**1**), showing the atom-labelling scheme and the coordination of the K^+ ion. Displacement ellipsoids are drawn at the 50% probability level. The eugenol fragment with a population parameter of 0.340 (7) is shown in orange. [Symmetry codes: (i) $x - 1, y, z$; (ii) $x, -y + \frac{3}{2}, z + \frac{1}{2}$; (iii) $x, y, z + 1$; (iv) $-x, -y + 1, -z + 2$.]

3. Results and discussion

3.1. Synthesis and structure of K[$PtCl_3$(Eug)]

Recently, one of the authors reported a methodology to prepare K[$PtCl_3$(Eug)], (**1**), using Zeise's salt and eugenol. This protocol proceeds under mild conditions with a high yield. However, the main drawback of this procedure is the need for pure eugenol, which is extracted from *Ocimum sanctum* L. oil *via* elaborate steps, including obtaining an eugenolate solution, acidifying and distilling under reduced pressure and high temperature (Chi *et al.*, 2017). It is interesting to note that eugenol accounts for approximately 70% of the oil, the remaining components including α-caryophyllene and β-terpineol (Padalia & Verma, 2011), which do not coordinate with Pt^{II} as easily as eugenol. Thus, direct reaction using the oil instead of purified eugenol was carried out. To our pleasure, this more effective procedure furnished (**1**) as a bright-yellow powder in a high yield of 95%. Remarkably, to increase the contact between reactants, Zeise's salt must be completely crushed and the reaction mixture must be stirred thoroughly. These steps also facilitate emission of the formed ethylene prompting the reaction to continue. In addition, the number of washing times of the reaction mixture to separate (**1**) by diethyl ether and the reaction time greatly influenced the purification of (**1**). Specifically, the optimized washing protocol was 5 × 5 ml and in order to optimize the reaction time, ^{1}H NMR spectroscopy was used. The partial ^{1}H NMR spectra of the reaction products recorded after different reaction times are shown in Fig. 1 (the numbering scheme is used for NMR analysis only; see the supporting information for the full spectra).

As shown in Fig. 1, the product obtained after 20 min contains about 24% of Zeise's salt, as calculated from the integration. This percentage decreases as the reaction pro-

Table 2
Chemical shift (ppm), multiplicity and coupling constant (Hz) of the allyl protons of Eug in free Eug and in complexes (**1**)–(**4**).

Compound	H8a	H8b	H9	H10-*trans*	H10-*cis*
Free[a]	3.25 *d*		5.92 *m*	5.05 *dd*	4.99 *dd*
(**1**)[a]	2.90 *dd* $^3J_{PtH}$ 50	3.43 *dd*	5.06 *m* $^2J_{PtH}$ 70	4.29 *dd* $^2J_{PtH}$ 70	4.12 *dd* $^2J_{PtH}$ 70
(**2**)[b]	3.16 *ov*	3.58 *ov*	5.72 *m* $^2J_{PtH}$ 70	4.75–4.78 *ov*	4.75–4.78 *ov*
(**3**)[a]	3.32 *dd* $^3J_{PtH}$ 50	3.58 *dd*	5.78 *m* $^2J_{PtH}$ 70	4.89 *d* $^2J_{PtH}$ 70	4.87 *d* $^2J_{PtH}$ 70
(**4**)[a]	3.33 *dd* $^3J_{PtH}$ 50	3.57–3.61 *ov*	5.75 *m* $^2J_{PtH}$ 70	4.87 *d* $^2J_{PtH}$ 70	4.85 *d* $^2J_{PtH}$ 70

Notes: (*a*) acetone-d_6; (*b*) chloroform-d_1.

ceeds and reaches 0% after 60 min. In other words, the reaction between Zeise's salt and *Ocimum sanctum* L. oil to produce (**1**) has reached the endpoint after 60 min of stirring under ambient conditions.

The structure of K[$PtCl_3$(Eug)] has been determined previously by elemental analysis, IR, ^{1}H NMR, ^{13}C NMR and MS spectra (Chi *et al.*, 2017). In the present study, only the IR and ^{1}H NMR spectra of (**1**) were recorded. The assigned results (see *Experimental*, §2) are in good agreement with those in the previous work. However, as (**1**) is the key complex for the synthesis of complexes bearing eugenol and amine, which are potential candidates for anticancer activity, its structure was further studied by single-crystal X-ray diffraction.

The orange crystals of (**1**), obtained from a concentrated acetone solution by slow evaporation, belong to the monoclinic space group $P2_1/c$ (Table 1). The central Pt^{II} metal atom displays a distorted square-planar coordination (Fig. 2). Part of the eugenol ligand is disordered, with population parameters of 0.660 (7) and 0.340 (7) for the two positions. The K^+ ion acts as glue in the crystal packing and is coordinated by six Cl atoms [K···Cl = 3.0940 (14)–3.3878 (14) Å] and two O atoms [K···O = 2.645 (3) and 2.906 (3) Å]. The region close to the (100) plane is occupied by a two-dimensional array of Pt, K and Cl atoms (Fig. 3). Eugenol is suspended between these layers, which explains the observed disorder of the ligand. The shortest Pt···K distance is 3.9734 (9) Å and the shortest K···K distance is 5.2558 (13) Å.

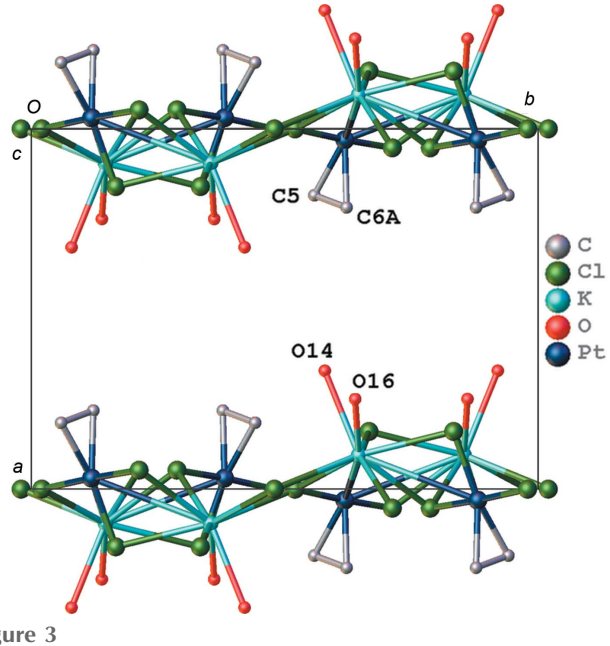
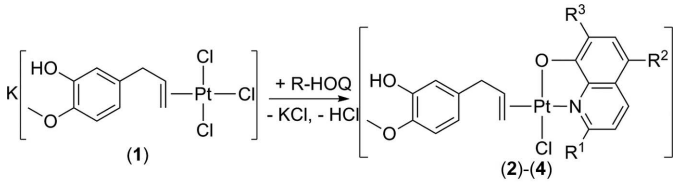


Figure 3
A partial packing diagram for complex (**1**), showing the atoms in the region close to the (100) plane. Eugenol is suspended between the layers.

3.2. Syntheses and structures of [PtCl(R-OQ)(Eug)], (2)–(4)

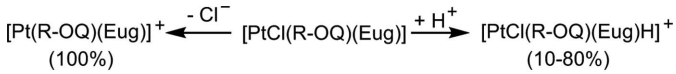
The interaction between K[$PtCl_3$(Eug)], (**1**), and the three quinolin-8-ol derivatives (R-HOQ) 2-methylquinolin-8-ol (Me-HOQ), 5-nitroquinolin-8-ol (NO_2-HOQ) and 5,7-dichloroquinolin-8-ol (Cl-HOQ) affords three new complexes [PtCl(R-OQ)(Eug)], (**2**)–(**4**), in good yields (see Scheme 2). The deprotonated quinolin-8-ol derivatives (R-OQ) replace two of the three Cl atoms present in (**1**) to form chelate complexes. The reactions were carried out at 298–303 K in a water–acetone mixture with a (**1**):R-HOQ molar ratio of 1:1. The neutral complexes (**2**)–(**4**) precipitated out and were easily isolated; they were further purified by recrystallization from a water–acetone mixture or an ethanol–acetone mixture. The complexes are well soluble in $CHCl_3$, $(CH_3)_2CO$ and DMSO, but insoluble in EtOH and Et_2O. Complexes (**2**) and (**4**) are orange–yellow solids, while (**3**) is brown.



(2) $R^1 = CH_3$, $R^2 = R^3 = H$
(3) $R^1 = R^3 = H$, $R^2 = NO_2$
(4) $R^1 = H$, $R^2 = R^3 = Cl$

Scheme 2

Base peaks with relative intensity 100% observed in the positive mode ESI mass spectra of all complexes are consistent with the pseudomolecular ion $[M - Cl]^+$, *i.e.* [Pt(R-OQ)(Eug)]$^+$. This provides evidence for the proposed R-OQ coordination. In addition, correct isotopic patterns for $[M + H]^+$ cations are also detected with different intensities (10–80%), as presented in Scheme 3.



Scheme 3

The IR spectra of (**2**)–(**4**) show bands for the presence of eugenol and R-OQ in the complexes (see *Experimental*, §2). Moreover, the band of ν(C=C allyl) is shifted to 1605–1497 cm^{-1} but not 1640 cm^{-1}, as in noncoordinated eugenol. This indicates that the allyl group has coordinated with Pt^{II} in an η^2 manner. The presence of only a strong sharp absorption at 3472–3445 cm^{-1} for the stretching vibration of the OH function in Eug agrees with deprotonation of the OH group of R-HOQ.

Table 3
Cytotoxic effects of the examined compounds (IC_{50}[a]) in μM).

Compound	KB	LU	Hep-G2	MCF-7
(**2**)	5.36 ± 0.27	3.79 ± 0.15	6.45 ± 0.13	19.5 ± 0.8
(**3**)	1.42 ± 0.11	4.9 ± 0.80	1.72 ± 0.12	2.45 ± 0.15
(**4**)	2.39 ± 0.12	17.8 ± 0.7	6.01 ± 0.18	26.5 ± 0.5
NO_2-HOQ	18.4 ± 0.9	26.8 ± 1.1	10.0 ± 0.5	12.1 ± 0.5
Cl-HOQ	24.4 ± 1.5	126.0 ± 6.3	125.2 ± 2.5	339.7 ± 6.0
Cisplatin	15.2 ± 0.8	42.9 ± 0.9	13.3 ± 1.1	45.7 ± 1.2
Ellipcitine	2.28 ± 0.09	1.95 ± 0.12	1.14 ± 0.06	1.26 ± 0.10
Other Pt^{II} complexes	5.98–22.54[b]	–	3.4–80.9[c]	3.1–76[d]

Note: (*a*) IC_{50} is the concentration of the compound required to inhibit cell growth by 50%. Mean values of IC_{50} (in μM) ± standard uncertainty from three experiments are presented. References: (*b*) Li *et al.* (2013); (*c*) Fang *et al.* (2016), Liu *et al.* (2014) and Rubino *et al.* (2017); (*d*) Liu *et al.* (2014), Rubino *et al.* (2017) and Wilson & Lippard (2012).

The ^{1}H NMR spectra of (**2**)–(**4**) demonstrate fully the proton signals of eugenol and R-OQ in these complexes (see *Experimental*, §2). To clarify the coordination of Eug with Pt^{II}, as well as the influence of the coordinated amines on the protons near the coordinating centres of Eug, the chemical shifts and coupling constants of the allyl protons of Eug in the free ligand and in (**1**)–(**4**) are reported in Table 2.

Upon coordination to Pt^{II}, the resonances of the olefinic protons (H9, H10-*cis* and H10-*trans*) are shifted upfield in comparison to those of noncoordinated Eug. The ^{195}Pt satellites from these protons are clear, with the distance between them, *i.e.* $^2J_{PtH}$ = 70 Hz, indicating that the allyl group of Eug is an η^2-coordinated olefin. Moreover, the two free Eug H8 protons give rise to a doublet at 3.25 ppm, with ^3J = 7.0 Hz, but in the spectra of (**2**)–(**4**), we observed one doublet of doublets centred at 3.16–3.33 ppm, with $^3J_{PtH}$ = 50 Hz for H8a, and another doublet of doublets centred at 3.57–3.61 ppm for H8b. This is expected since, upon coordination to Pt^{II}, atom C9 becomes a chiral centre, and atoms H8a and H8b become diastereotopic. The differentiation between H8a and H8b is tentative. In addition, the presence of a sharp singlet at 5.45 ppm for (**2**) (recorded in $CDCl_3$) and at ∼7.40 ppm for (**3**) and (**4**) (measured in acetone-d_6) indicates that the OH group of Eug is not deprotonated.

Convincing evidence for the coordination of R-OQ with Pt^{II} is as follows: (i) all the resonances of the allyl protons (H8, H9 and H10) of Eug in (**2**)–(**4**) shift significantly downfield compared to the parent complex (**1**) (Table 2); (ii) the ^{195}Pt satellites in the signals at 9.17 and 9.22 ppm of Hα of R-OQ in (**3**) and (**4**) are clearly visible, with the distance between the two satellites being $^3J_{PtH}$ = 34 Hz; (iii) IR bands of the OH group of R-HOQ are absent. In order to confirm the configuration of the complexes and to determine unambiguously the position of the donor atoms N and O of the quinolin-8-olate derivatives in the coordination sphere of Pt, single-crystal X-ray diffraction is still the most effective method. After numerous efforts, we obtained single crystals of (**4**) suitable for XRD measurements. The NOESY spectra were studied for (**2**) and (**3**).

In the NOESY spectra, there is no appearance of a cross peak between the protons of eugenol and the protons of R-OQ. This suggests that the nitrogen heteroatom of the amine and the allyl group of eugenol are not *cis* but *trans* to one another in the Pt^{II} coordination sphere. The NOESY results reinforce the assignment of the ^{1}H NMR spectra.

Complex (**4**) crystallizes in the triclinic space group $P\overline{1}$. The central Pt^{II} atom displays a distorted square-planar coordination (Fig. 4). One Cl atom, the C═C double bond of the eugenol ligand and the N and O atoms of the quinolin-8-ol ligand coordinate to the Pt^{II} atom, with the N atom and C═C group *trans* with respect to each other. Part of the eugenol ligand is again disordered, with population parameters of 0.642 (14) and 0.358 (14) for positions *A* and *B*. The dihedral angles between the best planes through the quinoline and phenyl rings are 77.5 (5) and 82.4 (8)° for *A* and *B*, respectively. The crystal packing is built up by O—H···O, C—H···O, C—H···Cl and C—H···π interactions (Fig. 5).

3.3. *In vitro* cytotoxicity of [PtCl(R-OQ)(Eug)], (2)–(4)

Complexes (**2**)–(**4**) were assayed for *in vitro* cytotoxicity against human cancer cells KB (human epidermal carcinoma),

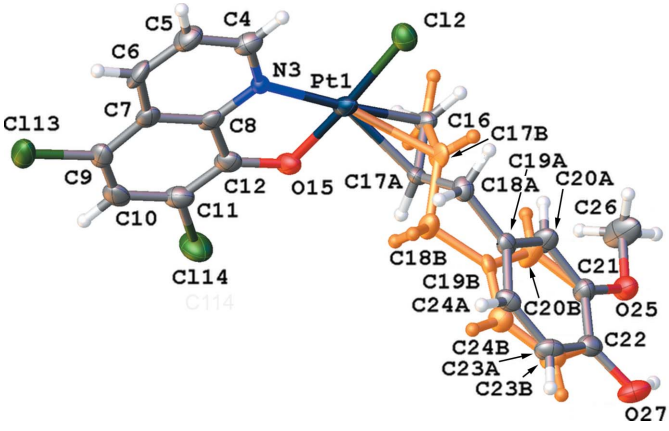


Figure 4
The molecular structure of complex (**4**), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. The eugenol fragment with a population parameter of 0.358 (14) is shown in orange.

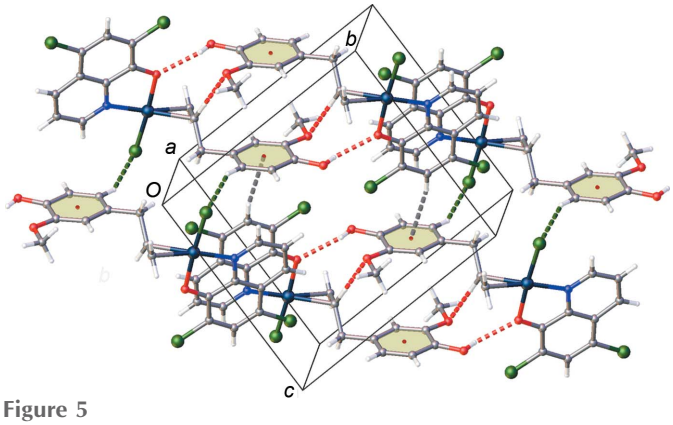


Figure 5
Packing diagram for complex (**4**), showing the O—H···O (red), C—H···O (red), C—H···Cl (green) and C—H···π (grey) interactions.

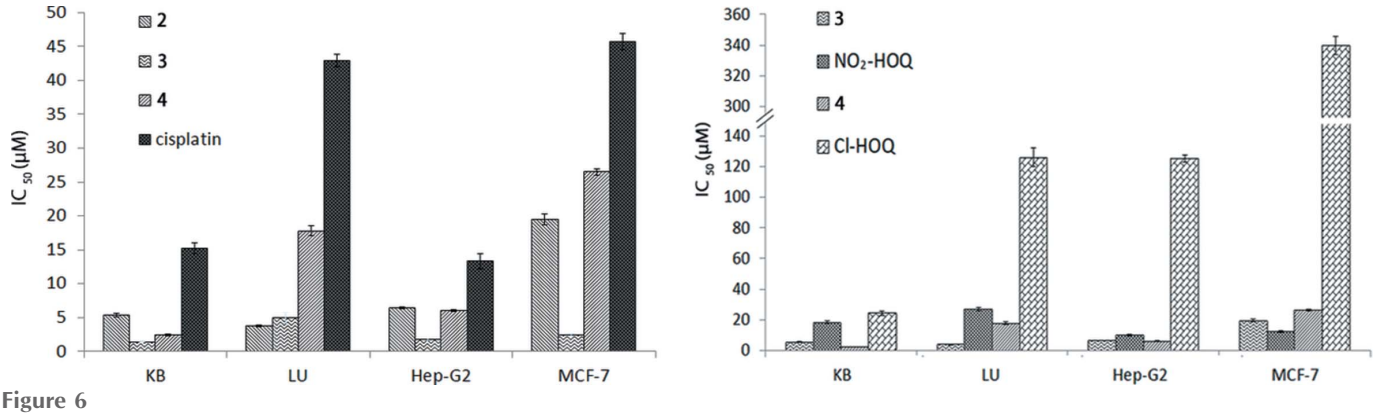


Figure 6
The cytotoxic effects (IC_{50} values) of NO_2-HOQ and Cl-HOQ, complexes (**2**)–(**4**) and cisplatin against the KB, LU, Hep-G2 and MCF-7 cell lines.

Hep-G2 (hepatocellular carcinoma), LU (human lung carcinoma) and MCF-7 (human breast carcinoma). The cytotoxicity of cisplatin and two ligands, *i.e.* NO_2-HOQ and Cl-HOQ, was also tested as the basis for an assessment of the anticancer ability of the synthesized complexes. The IC_{50} values are listed in Table 3, together with literature data for some other platinum(II) complexes.

The data in Table 3 indicate that complexes (**2**)–(**4**) have high activities against three cancer cell lines (KB, LU and Hep-G2), with IC_{50} values of 1.42–17.8 μ*M*. In particular, (**3**) exhibits impressively high activities, with IC_{50} values of 1.42–4.9 μ*M* for all four tested cell lines. These values show a better antitumour activity of (**3**) than some other platinum(II) complexes (Li *et al.*, 2013; Fang *et al.*, 2016; Liu *et al.*, 2014; Rubino *et al.*, 2017; Wilson & Lippard, 2012).

In comparison, complexes (**2**)–(**4**), as well as cisplatin, tend to display a higher cytotoxicity against the KB and Hep-G2 cell lines than against LU and MCF-7. Moreover, the IC_{50} values of the complexes are markedly lower than those of cisplatin. For instance, the IC_{50} value of (**3**) for the MCF-7 cell line is approximately 19 times lower than that of cisplatin (Fig. 6). Free NO_2-HOQ and Cl-HOQ cause only a weak inhibition of the growth of the four cancer cell lines, particularly Cl-HOQ. Nevertheless, their complexation with Pt^{II} results in a significant increase of the cytotoxicity of the formed complexes (**3**) and (**4**), respectively (Fig. 6). We are currently investigating further the anticancer mechanism of these promising compounds.

4. Conclusions

In this study, we have synthesized K[$PtCl_3$(Eug)], (**1**), in a high yield of 95% starting from Zeise's salt, *i.e.* K[$PtCl_3$-(C_2H_4)]·H_2O, and *Ocimum sanctum* L. oil, which contains up to 70% eugenol. The reaction between (**1**) and three quinolin-8-ol derivatives (R-HOQ) afforded the new complexes [PtCl(R-OQ)(Eug)], (**2**)–(**4**), in good yields (90%). The compounds were characterized spectroscopically and by single-crystal X-ray diffraction for (**1**) and (**4**). The *in vitro* cytotoxicities of complexes (**2**)–(**4**) against the four human cancer cell lines KB, Hep-G2, LU and MCF-7 was determined and showed higher activities than cisplatin. Complex (**3**) gives a very high activity on the four cell lines, with IC_{50} values of 1.42-4.91 μ*M*, which are lower than those of some other platinum(II) complexes and around 8–19 times lower than those of cisplatin.

Funding information

Funding for this research was provided by: Vietnam Ministry of Education and Training (grant No. B2017-DQN-04); Hercules Foundation (Belgium) (contract No. AKUL/09/0035; support for purchase of diffractometer); Vlaamse Interuniversitaire Raad (grant No. ZEIN2014Z182; travel support).

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supporting information

Acta Cryst. (2017). C**73**, 1030-1037 [https://doi.org/10.1107/S2053229617015200]

Synthesis, structure and *in vitro* cytotoxicity of platinum(II) complexes containing eugenol and a quinolin-8-ol-derived chelator

Chi Nguyen Thi Thanh, Mai Truong Thi Cam, Thong Pham Van, Long Nguyen, My Nguyen Ha and Luc Van Meervelt

Computing details

For both structures, data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); 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).

Potassium [2-methoxy-4-(prop-2-en-1-yl)phenol]trichloridoplatinate (chi46-bis)

Crystal data

$K[PtCl_3(C_{10}H_{12}O_2)]$
M_r = 504.74
Monoclinic, $P2_1/c$
a = 12.0312 (6) Å
b = 16.1528 (8) Å
c = 8.1007 (4) Å
β = 107.295 (6)°
V = 1503.09 (14) Å^3
Z = 4
$F(000)$ = 944
D_x = 2.230 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7771 reflections
θ = 2.9–28.9°
μ = 10.13 mm^{-1}
T = 100 K
Block, orange
0.4 × 0.4 × 0.3 mm

Data collection

Agilent SuperNova Single Source diffractometer with an Eos detector
Radiation source: micro-focus sealed X-ray tube, SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 15.9631 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.548, T_{max} = 1.000
15723 measured reflections
3068 independent reflections
2937 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 26.4°, θ_{min} = 2.5°
h = −15→15
k = −20→20
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.042
S = 1.20
3068 reflections
223 parameters
86 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0018P)^2 + 2.9267P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.84 e Å^{-3} $\Delta\rho_{min}$ = −0.92 e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Pt1	0.03063 (2)	0.61876 (2)	0.61000 (2)	0.01116 (5)	
Cl2	0.00007 (9)	0.52042 (7)	0.79589 (13)	0.0170 (2)	
Cl3	0.05273 (9)	0.71258 (7)	0.40833 (13)	0.0170 (2)	
Cl4	−0.16013 (8)	0.66642 (7)	0.57359 (13)	0.0157 (2)	
C5	0.1855 (3)	0.5583 (3)	0.5979 (6)	0.0182 (10)	
H5AA	0.190091	0.502123	0.634271	0.022*	0.660 (7)
H5AB	0.159096	0.571387	0.478275	0.022*	0.660 (7)
H5BC	0.208644	0.576818	0.501798	0.022*	0.340 (7)
H5BD	0.143483	0.507948	0.590767	0.022*	0.340 (7)
C6A	0.2179 (7)	0.6218 (7)	0.7211 (12)	0.019 (2)	0.660 (7)
H6A	0.255879	0.670123	0.682536	0.022*	0.660 (7)
C6B	0.2138 (13)	0.6057 (12)	0.752 (2)	0.024 (6)	0.340 (7)
H6B	0.229669	0.572319	0.860608	0.029*	0.340 (7)
C7A	0.2599 (5)	0.6066 (5)	0.9099 (8)	0.0218 (17)	0.660 (7)
H7AA	0.241063	0.549019	0.933938	0.026*	0.660 (7)
H7AB	0.219363	0.644363	0.969129	0.026*	0.660 (7)
C7B	0.2795 (9)	0.6850 (9)	0.7706 (17)	0.021 (3)	0.340 (7)
H7BA	0.241636	0.727150	0.824511	0.026*	0.340 (7)
H7BB	0.278844	0.705422	0.655138	0.026*	0.340 (7)
C8A	0.3914 (5)	0.6201 (5)	0.9814 (9)	0.0191 (17)	0.660 (7)
C8B	0.4047 (10)	0.6719 (9)	0.8824 (17)	0.022 (3)	0.340 (7)
C9A	0.4377 (6)	0.6569 (5)	1.1405 (10)	0.0260 (19)	0.660 (7)
H9A	0.388045	0.677607	1.202752	0.031*	0.660 (7)
C9B	0.4420 (10)	0.7014 (10)	1.0501 (19)	0.025 (4)	0.340 (7)
H9B	0.387507	0.729390	1.094352	0.030*	0.340 (7)
C10A	0.5587 (7)	0.6635 (7)	1.2095 (12)	0.027 (2)	0.660 (7)
H10A	0.594 (9)	0.693 (7)	1.326 (12)	0.032*	0.660 (7)
C10B	0.5561 (12)	0.6919 (10)	1.158 (2)	0.021 (4)	0.340 (7)
H10B	0.580 (17)	0.708 (13)	1.28 (3)	0.025*	0.340 (7)
C11	0.6324 (4)	0.6398 (3)	1.1107 (6)	0.0258 (11)	
C12	0.5895 (4)	0.6071 (4)	0.9453 (7)	0.0385 (15)	
C13A	0.4661 (6)	0.5932 (5)	0.8894 (10)	0.0225 (18)	0.660 (7)
H13A	0.433527	0.564059	0.784180	0.027*	0.660 (7)
C13B	0.4833 (11)	0.6285 (10)	0.816 (2)	0.019 (3)	0.340 (7)
H13B	0.451 (11)	0.620 (8)	0.676 (18)	0.023*	0.340 (7)
O14	0.6714 (3)	0.5793 (2)	0.8717 (4)	0.0346 (9)	
C15	0.6306 (5)	0.5409 (4)	0.7064 (7)	0.0557 (19)	
H15A	0.586848	0.490800	0.715270	0.084*	

H15B	0.697057	0.526185	0.665823	0.084*
H15C	0.579774	0.579406	0.624329	0.084*
O16	0.7498 (3)	0.6391 (2)	1.1804 (4)	0.0234 (8)
K17	−0.09497 (8)	0.64632 (6)	1.00825 (12)	0.0173 (2)
H16	0.763 (4)	0.653 (3)	1.271 (6)	0.019 (15)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.01111 (8)	0.01302 (10)	0.00792 (9)	0.00074 (7)	0.00064 (6)	−0.00023 (7)
Cl2	0.0220 (5)	0.0151 (6)	0.0135 (5)	0.0025 (4)	0.0048 (4)	0.0051 (4)
Cl3	0.0189 (5)	0.0183 (6)	0.0140 (5)	0.0008 (4)	0.0055 (4)	0.0046 (4)
Cl4	0.0118 (5)	0.0198 (6)	0.0140 (5)	0.0019 (4)	0.0015 (4)	−0.0004 (4)
C5	0.012 (2)	0.023 (3)	0.016 (2)	0.0063 (18)	−0.0003 (17)	0.0012 (19)
C6A	0.010 (5)	0.026 (5)	0.018 (4)	0.002 (4)	0.001 (3)	0.000 (3)
C6B	0.006 (8)	0.028 (9)	0.033 (10)	0.004 (6)	−0.001 (7)	−0.013 (8)
C7A	0.016 (3)	0.034 (5)	0.014 (3)	−0.003 (3)	0.002 (3)	−0.007 (3)
C7B	0.012 (5)	0.031 (7)	0.018 (7)	0.003 (5)	0.000 (5)	−0.006 (6)
C8A	0.013 (3)	0.027 (4)	0.014 (3)	−0.001 (3)	0.000 (2)	−0.001 (3)
C8B	0.008 (5)	0.032 (9)	0.021 (6)	−0.003 (5)	0.000 (4)	−0.005 (6)
C9A	0.015 (3)	0.042 (5)	0.018 (4)	0.003 (3)	0.001 (3)	−0.010 (4)
C9B	0.015 (5)	0.037 (10)	0.022 (6)	0.009 (6)	0.004 (5)	−0.007 (6)
C10A	0.016 (3)	0.033 (7)	0.024 (5)	0.001 (4)	−0.004 (3)	−0.007 (4)
C10B	0.023 (6)	0.014 (9)	0.019 (8)	0.005 (6)	−0.004 (5)	0.003 (6)
C11	0.013 (2)	0.029 (3)	0.030 (3)	−0.001 (2)	−0.0027 (19)	−0.008 (2)
C12	0.016 (2)	0.045 (4)	0.044 (3)	0.009 (2)	−0.006 (2)	−0.026 (3)
C13A	0.018 (4)	0.032 (5)	0.015 (4)	0.001 (3)	0.001 (3)	−0.005 (4)
C13B	0.013 (7)	0.026 (9)	0.019 (8)	0.001 (6)	0.004 (6)	0.000 (7)
O14	0.0207 (17)	0.052 (3)	0.026 (2)	−0.0032 (17)	−0.0019 (15)	−0.0183 (18)
C15	0.041 (3)	0.084 (5)	0.038 (4)	−0.015 (3)	0.005 (3)	−0.038 (4)
O16	0.0127 (16)	0.043 (2)	0.0118 (18)	−0.0013 (15)	−0.0005 (14)	−0.0029 (17)
K17	0.0186 (5)	0.0157 (5)	0.0187 (5)	0.0007 (4)	0.0071 (4)	0.0009 (4)

Geometric parameters (Å, º)

Pt1—Cl2	2.2924 (10)	Cl2—K17	3.0940 (14)
Pt1—Cl3	2.3010 (10)	Cl2—K17^{ii}	3.1619 (14)
Pt1—Cl4	2.3547 (10)	Cl3—K17^{i}	3.1405 (14)
Pt1—C5	2.132 (4)	Cl3—K17^{iii}	3.3738 (14)
Pt1—C6A	2.164 (8)	Cl4—K17^{i}	3.2078 (14)
C6A—H6A	1.0000	Cl4—K17	3.3878 (14)
Pt1—C6B	2.172 (14)	C5—H5AA	0.9500
C6B—H6B	1.0000	C5—H5AB	0.9500
C6A—C7A	1.482 (11)	C5—H5BC	0.9500
C7A—H7AA	0.9900	C5—H5BD	0.9500
C7A—H7AB	0.9900	C5—C6A	1.404 (9)
C6B—C7B	1.490 (17)	C5—C6B	1.417 (14)
C7B—H7BA	0.9900	C11—C12	1.389 (7)

C7B—H7BB	0.9900	C11—O16	1.356 (5)
C7A—C8A	1.529 (8)	C12—C13A	1.435 (8)
C7B—C8B	1.524 (13)	C12—C13B	1.433 (15)
C8A—C9A	1.378 (9)	C12—O14	1.371 (6)
C9A—H9A	0.9500	O14—C15	1.424 (6)
C8B—C9B	1.382 (18)	O14—K17^{iv}	2.906 (3)
C9B—H9B	0.9500	C15—H15A	0.9800
C9A—C10A	1.400 (9)	C15—H15B	0.9800
C10A—H10A	1.02 (12)	C15—H15C	0.9800
C9B—C10B	1.399 (13)	O16—K17^{iv}	2.645 (3)
C10B—H10B	1.0 (2)	O16—H16	0.74 (4)
C10A—C11	1.412 (8)	K17—Pt1^{v}	4.0769 (10)
C10B—C11	1.380 (12)	K17—Cl2^{ii}	3.1619 (14)
C8A—C13A	1.397 (9)	K17—Cl3^{vi}	3.3738 (14)
C13A—H13A	0.9500	K17—Cl3^{v}	3.1404 (14)
C8B—C13B	1.407 (18)	K17—Cl4^{v}	3.2078 (14)
C13B—H13B	1.09 (13)	K17—O14^{vii}	2.906 (3)
Pt1—K17^{i}	4.0769 (10)	K17—O16^{vii}	2.645 (3)
Pt1—K17	3.9734 (9)		

Cl2—Pt1—Cl3	176.11 (4)	C6B—C5—H5BC	120.0
Cl2—Pt1—Cl4	88.18 (4)	H5BC—C5—H5BD	120.0
Cl2—Pt1—K17^{i}	130.96 (3)	C6B—C5—H5BD	120.0
C7A—C6A—Pt1	114.8 (6)	C10B—C11—C12	114.3 (8)
C7B—C6B—Pt1	113.2 (12)	C12—C11—C10A	122.3 (5)
C6B—Pt1—Cl2	85.4 (6)	O16—C11—C10A	121.2 (5)
C6A—Pt1—Cl2	95.3 (3)	O16—C11—C10B	125.9 (8)
C6B—Pt1—Cl3	97.3 (6)	O16—C11—C12	116.1 (4)
C6A—Pt1—Cl3	87.4 (3)	C11—C12—C13A	114.7 (5)
C6A—Pt1—Cl4	154.2 (2)	C11—C12—C13B	127.5 (7)
C6B—Pt1—Cl4	153.6 (4)	O14—C12—C11	115.8 (4)
C7A—C6A—H6A	113.9	O14—C12—C13A	128.4 (5)
Pt1—C6A—H6A	113.9	O14—C12—C13B	111.1 (7)
Pt1—C6B—H6B	114.7	C12—O14—C15	117.4 (4)
C7B—C6B—H6B	114.7	C12—O14—K17^{iv}	116.8 (3)
C9A—C8A—C7A	120.1 (6)	C15—O14—K17^{iv}	123.0 (3)
Cl2—Pt1—K17	50.98 (3)	O14—C15—H15A	109.5
Cl3—Pt1—Cl4	90.56 (4)	O14—C15—H15B	109.5
Cl3—Pt1—K17	130.90 (3)	O14—C15—H15C	109.5
Cl3—Pt1—K17^{i}	50.03 (3)	H15A—C15—H15B	109.5
Cl4—Pt1—K17	58.22 (3)	H15A—C15—H15C	109.5
Cl4—Pt1—K17^{i}	51.79 (3)	H15B—C15—H15C	109.5
C5—Pt1—Cl2	91.46 (13)	C11—O16—K17^{iv}	126.3 (3)
C5—Pt1—Cl3	88.98 (13)	C11—O16—H16	107 (4)
C5—Pt1—Cl4	167.63 (12)	K17^{iv}—O16—H16	123 (4)
C5—Pt1—C6A	38.1 (3)	Pt1—K17—Pt1^{v}	93.488 (19)
C5—Pt1—C6B	38.4 (4)	Cl2—K17—Pt1	35.14 (2)
C5—Pt1—K17	129.58 (12)	Cl2—K17—Pt1^{v}	123.24 (3)

C13A—C8A—C7A	120.7 (6)	Cl2^{ii}—K17—Pt1	98.29 (3)
C6A—C7A—H7AA	109.4	Cl2^{ii}—K17—Pt1^{v}	129.38 (3)
C8A—C7A—H7AA	109.4	Cl2—K17—Cl2^{ii}	65.23 (4)
C6A—C7A—H7AB	109.4	Cl2—K17—Cl3^{v}	90.16 (3)
C8A—C7A—H7AB	109.4	Cl2^{ii}—K17—Cl3^{vi}	77.27 (3)
H7AA—C7A—H7AB	108.0	Cl2—K17—Cl3^{vi}	124.50 (4)
C13B—C8B—C7B	120.0 (12)	Cl2^{ii}—K17—Cl4^{v}	142.17 (4)
C9B—C8B—C7B	120.7 (11)	Cl2^{ii}—K17—Cl4	122.73 (4)
C8B—C7B—H7BA	109.7	Cl2—K17—Cl4^{v}	149.36 (4)
C5—Pt1—K17^{i}	133.93 (13)	Cl2—K17—Cl4	59.65 (3)
K17—Pt1—K17^{i}	81.506 (18)	Cl3^{vi}—K17—Pt1^{v}	56.83 (2)
Pt1—Cl2—K17	93.88 (4)	Cl3^{v}—K17—Pt1^{v}	34.16 (2)
Pt1—Cl2—K17^{ii}	144.62 (4)	Cl3^{vi}—K17—Pt1	126.63 (3)
K17—Cl2—K17^{ii}	114.77 (4)	Cl3^{v}—K17—Pt1	59.41 (2)
Pt1—Cl3—K17^{iii}	109.52 (4)	Cl3^{v}—K17—Cl2^{ii}	126.86 (4)
Pt1—Cl3—K17^{i}	95.81 (4)	Cl3^{v}—K17—Cl3^{vi}	80.83 (3)
K17^{i}—Cl3—K17^{iii}	107.52 (4)	Cl3^{v}—K17—Cl4^{v}	62.81 (3)
Pt1—Cl4—K17^{i}	92.98 (4)	Cl3^{v}—K17—Cl4	68.68 (3)
Pt1—Cl4—K17	85.57 (3)	Cl3^{vi}—K17—Cl4	149.44 (4)
K17^{i}—Cl4—K17	105.63 (4)	Cl4—K17—Pt1^{v}	94.49 (3)
Pt1—C5—H5AA	113.2	Cl4^{v}—K17—Pt1	114.22 (3)
Pt1—C5—H5AB	85.0	Cl4—K17—Pt1	36.216 (19)
Pt1—C5—H5BC	111.5	Cl4^{v}—K17—Pt1^{v}	35.23 (2)
Pt1—C5—H5BD	86.5	Cl4^{v}—K17—Cl3^{vi}	68.11 (3)
C6B—C7B—H7BA	109.7	Cl4^{v}—K17—Cl4	95.09 (3)
C6B—C7B—H7BB	109.7	C5—C6B—Pt1	69.3 (5)
H7BA—C7B—H7BB	108.2	C5—C6A—Pt1	69.7 (3)
C8B—C7B—H7BB	109.7	O14^{vii}—K17—Pt1	101.97 (7)
C6A—C7A—C8A	111.4 (6)	C5—C6A—H6A	113.9
C6B—C7B—C8B	110.0 (11)	O14^{vii}—K17—Pt1^{v}	133.01 (8)
C10A—C9A—H9A	120.3	O14^{vii}—K17—Cl2^{ii}	92.16 (8)
C8A—C9A—H9A	120.3	O14^{vii}—K17—Cl2	91.08 (7)
C8B—C9B—H9B	118.4	O14^{vii}—K17—Cl3^{v}	136.85 (8)
C10B—C9B—H9B	118.4	O14^{vii}—K17—Cl3^{vi}	131.10 (7)
C8A—C9A—C10A	119.4 (7)	O14^{vii}—K17—Cl4	75.01 (7)
C9A—C10A—H10A	120 (6)	C5—C6B—H6B	114.7
C8B—C9B—C10B	123.1 (12)	C5—C6A—C7A	123.3 (9)
C9B—C10B—H10B	122 (10)	C5—C6B—C7B	122.3 (17)
C9A—C10A—C11	120.4 (7)	C11—C10B—C9B	120.4 (13)
C8A—C13A—C12	123.5 (6)	C11—C10A—H10A	119 (6)
C8B—C13B—C12	113.2 (12)	C11—C10B—H10B	115 (10)
C9A—C8A—C13A	119.2 (6)	C12—C13A—H13A	118.2
C8A—C13A—H13A	118.2	C12—C13B—H13B	134 (7)
C9B—C8B—C13B	119.3 (11)	O14^{vii}—K17—Cl4^{v}	99.09 (8)
C8B—C13B—H13B	113 (7)	O16^{vii}—K17—Pt1	157.17 (8)
C6A—Pt1—K17	105.1 (3)	O16^{vii}—K17—Pt1^{v}	102.25 (8)
C6B—Pt1—K17	98.7 (5)	O16^{vii}—K17—Cl2	134.40 (9)
C6B—Pt1—K17^{i}	117.0 (5)	O16^{vii}—K17—Cl2^{ii}	84.49 (8)

C6A—Pt1—K17^{i}	109.9 (3)	O16^{vii}—K17—Cl3^{v}	135.28 (9)
C6B—C5—Pt1	72.3 (7)	O16^{vii}—K17—Cl3^{vi}	76.15 (8)
C6A—C5—Pt1	72.1 (4)	O16^{vii}—K17—Cl4	124.80 (8)
C6A—C5—H5AA	120.0	O16^{vii}—K17—Cl4^{v}	73.10 (9)
H5AA—C5—H5AB	120.0	O16^{vii}—K17—O14^{vii}	55.21 (10)
C6A—C5—H5AB	120.0		

Pt1—C6A—C7A—C8A	−173.1 (5)	C9B—C8B—C13B—C12	11 (2)
C10B—C11—C12—O14	158.7 (9)	C7A—C8A—C13A—C12	177.2 (7)
C7A—C8A—C9A—C10A	175.5 (8)	C9B—C10B—C11—C12	6.5 (18)
C10A—C11—C12—O14	−173.7 (7)	C9A—C10A—C11—C12	−2.0 (13)
C13A—C12—O14—C15	9.3 (10)	C9B—C10B—C11—O16	164.0 (11)
Pt1—C6B—C7B—C8B	175.9 (9)	C9A—C10A—C11—O16	−174.3 (7)
C13B—C12—O14—C15	−27.8 (10)	Pt1—C5—C6B—C7B	−105.0 (14)
C13A—C8A—C9A—C10A	−2.5 (12)	Pt1—C5—C6A—C7A	107.0 (8)
C13B—C8B—C9B—C10B	2 (2)	O16—C11—C12—C13A	167.8 (6)
C13A—C12—O14—K17^{iv}	171.0 (6)	O16—C11—C12—C13B	−152.2 (9)
C13B—C12—O14—K17^{iv}	133.9 (7)	C10B—C11—C12—C13B	7.6 (14)
C10A—C11—O16—K17^{iv}	−158.4 (6)	C10A—C11—C12—C13A	−4.8 (10)
C10B—C11—O16—K17^{iv}	−128.2 (10)	C5—C6A—C7A—C8A	105.7 (9)
C6A—C7A—C8A—C9A	141.5 (8)	C5—C6B—C7B—C8B	−104.7 (15)
C7B—C8B—C9B—C10B	−179.3 (14)	C11—C12—C13B—C8B	−16.3 (17)
C6B—C7B—C8B—C9B	−106.4 (17)	C11—C12—C13A—C8A	8.3 (11)
C6A—C7A—C8A—C13A	−40.6 (10)	C11—C12—O14—C15	176.4 (5)
C6B—C7B—C8B—C13B	72.7 (17)	C11—C12—O14—K17^{iv}	−21.9 (7)
C8B—C9B—C10B—C11	−11 (2)	C12—C11—O16—K17^{iv}	28.9 (6)
C8A—C9A—C10A—C11	5.9 (13)	O14—C12—C13B—C8B	−168.5 (10)
C9A—C8A—C13A—C12	−4.8 (13)	O14—C12—C13A—C8A	175.6 (7)
C7B—C8B—C13B—C12	−168.3 (11)	O16—C11—C12—O14	−1.1 (8)

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

Chlorido(5,7-dichloroquinolin-8-olato-κ^2N,O)[η^2-2-methoxy4-(prop-2-en-1-yl)phenol]platinum(II) (chi47)

Crystal data

[Pt($C_9H_4Cl_2NO$)Cl($C_{10}H_{12}O_2$)]	Z = 2
M_r = 607.77	F(000) = 580
Triclinic, $P\overline{1}$	D_x = 2.105 Mg m^{-3}
a = 8.1313 (3) Å	Mo $K\alpha$ radiation, λ = 0.71073 Å
b = 11.2960 (5) Å	Cell parameters from 8641 reflections
c = 11.4294 (7) Å	θ = 2.7–28.7°
α = 88.793 (4)°	μ = 7.75 mm^{-1}
β = 76.567 (4)°	T = 100 K
γ = 70.219 (4)°	Block, red
V = 958.93 (8) Å^3	0.4 × 0.4 × 0.3 mm

Data collection

Agilent SuperNova Single Source diffractometer with an Eos detector
Radiation source: micro-focus sealed X-ray tube, SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 15.9631 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)′
T_{min} = 0.427, T_{max} = 1.000
19518 measured reflections
3916 independent reflections
3594 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 26.4°, θ_{min} = 2.6°
h = −10→10
k = −14→14
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.088
S = 1.11
3916 reflections
301 parameters
133 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0357P)^2 + 3.4074P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 2.51 e Å^{-3}
$\Delta\rho_{min}$ = −1.82 e Å^{-3}

Special details

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

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Pt1	0.14705 (3)	0.96032 (2)	0.26050 (2)	0.02811 (10)	
Cl2	0.0222 (2)	1.11888 (15)	0.14588 (16)	0.0345 (3)	
N3	0.1551 (6)	1.0774 (5)	0.3907 (5)	0.0262 (11)	
C4	0.1051 (9)	1.2027 (6)	0.3969 (6)	0.0330 (14)	
H4	0.047134	1.248354	0.338451	0.040*	
C5	0.1352 (10)	1.2685 (6)	0.4864 (7)	0.0400 (17)	
H5	0.100651	1.357709	0.487104	0.048*	
C6	0.2139 (9)	1.2058 (6)	0.5728 (6)	0.0355 (15)	
H6	0.235347	1.251198	0.633300	0.043*	
C7	0.2646 (8)	1.0718 (6)	0.5730 (6)	0.0308 (14)	
C8	0.2319 (8)	1.0114 (6)	0.4770 (6)	0.0281 (13)	
C9	0.3429 (8)	0.9951 (6)	0.6578 (6)	0.0310 (14)	
C10	0.3859 (8)	0.8670 (7)	0.6481 (6)	0.0374 (16)	
H10	0.438456	0.816484	0.706339	0.045*	
C11	0.3528 (9)	0.8103 (6)	0.5528 (7)	0.0366 (15)	
C12	0.2794 (8)	0.8787 (6)	0.4643 (6)	0.0321 (14)	
Cl13	0.3868 (2)	1.06459 (19)	0.77586 (17)	0.0451 (4)	
Cl14	0.4066 (3)	0.64855 (16)	0.5444 (2)	0.0515 (5)	
O15	0.2484 (6)	0.8261 (4)	0.3718 (4)	0.0293 (10)	
C16	0.0992 (8)	0.8260 (5)	0.1543 (6)	0.0275 (13)	

H16A	0.028415	0.865219	0.099486	0.033*	0.642 (14)
H16B	0.044563	0.800448	0.228535	0.033*	0.642 (14)
H16C	0.119883	0.751658	0.197415	0.033*	0.358 (14)
H16D	−0.020384	0.880995	0.158895	0.033*	0.358 (14)
C17A	0.2824 (11)	0.8061 (9)	0.1258 (9)	0.023 (2)	0.642 (14)
H17A	0.359776	0.726697	0.153591	0.027*	0.642 (14)
C18A	0.3650 (13)	0.8478 (8)	0.0073 (8)	0.026 (2)	0.642 (14)
H18A	0.441328	0.895982	0.020389	0.031*	0.642 (14)
H18B	0.268854	0.903299	−0.028744	0.031*	0.642 (14)
C17B	0.248 (2)	0.8553 (18)	0.0823 (17)	0.032 (4)	0.358 (14)
H17B	0.221031	0.907729	0.012979	0.038*	0.358 (14)
C18B	0.443 (2)	0.7762 (17)	0.0675 (16)	0.033 (5)	0.358 (14)
H18C	0.456357	0.725518	0.138688	0.039*	0.358 (14)
H18D	0.514423	0.832591	0.064764	0.039*	0.358 (14)
C19A	0.4779 (13)	0.7327 (10)	−0.0775 (9)	0.022 (2)	0.642 (14)
C19B	0.520 (2)	0.6883 (18)	−0.0453 (15)	0.023 (4)	0.358 (14)
C20A	0.3996 (19)	0.6476 (11)	−0.1080 (11)	0.033 (3)	0.642 (14)
H20A	0.274710	0.664134	−0.075862	0.040*	0.642 (14)
C20B	0.419 (3)	0.6252 (17)	−0.0844 (17)	0.050 (9)	0.358 (14)
H20B	0.297018	0.640626	−0.043390	0.060*	0.358 (14)
C21	0.4993 (8)	0.5401 (6)	−0.1837 (6)	0.0299 (13)	
C22	0.6812 (8)	0.5156 (6)	−0.2377 (6)	0.0293 (13)	
C23A	0.762 (4)	0.600 (2)	−0.203 (2)	0.033 (4)	0.642 (14)
H23A	0.886790	0.583737	−0.234774	0.040*	0.642 (14)
C23B	0.775 (8)	0.576 (4)	−0.208 (4)	0.033 (8)	0.358 (14)
H23B	0.894799	0.561564	−0.252360	0.039*	0.358 (14)
C24A	0.6623 (15)	0.7057 (13)	−0.1242 (14)	0.026 (3)	0.642 (14)
H24A	0.719814	0.759358	−0.102246	0.031*	0.642 (14)
C24B	0.698 (3)	0.664 (2)	−0.110 (3)	0.031 (6)	0.358 (14)
H24B	0.767578	0.707108	−0.085722	0.037*	0.358 (14)
O25	0.4277 (6)	0.4582 (4)	−0.2227 (4)	0.0329 (10)	
C26	0.2421 (10)	0.4809 (8)	−0.1717 (9)	0.058 (3)	
H26A	0.203159	0.421892	−0.210399	0.087*	
H26B	0.171820	0.567540	−0.184504	0.087*	
H26C	0.223374	0.468880	−0.085070	0.087*	
O27	0.7760 (6)	0.4213 (4)	−0.3243 (5)	0.0380 (11)	
H27	0.711748	0.379066	−0.332794	0.057*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.01719 (13)	0.03008 (14)	0.03482 (17)	−0.00513 (9)	−0.00551 (10)	−0.00864 (10)
Cl2	0.0328 (8)	0.0408 (8)	0.0348 (9)	−0.0167 (7)	−0.0116 (7)	0.0031 (7)
N3	0.016 (2)	0.034 (3)	0.024 (3)	−0.002 (2)	−0.002 (2)	−0.006 (2)
C4	0.027 (3)	0.030 (3)	0.037 (4)	−0.007 (3)	0.000 (3)	−0.004 (3)
C5	0.036 (4)	0.035 (3)	0.043 (4)	−0.007 (3)	−0.003 (3)	−0.014 (3)
C6	0.035 (4)	0.041 (4)	0.027 (4)	−0.014 (3)	0.005 (3)	−0.018 (3)
C7	0.016 (3)	0.042 (3)	0.028 (3)	−0.006 (3)	0.002 (2)	−0.008 (3)

C8	0.014 (3)	0.034 (3)	0.030 (3)	−0.006 (2)	0.004 (2)	−0.008 (3)
C9	0.019 (3)	0.046 (4)	0.030 (4)	−0.013 (3)	−0.006 (3)	−0.005 (3)
C10	0.016 (3)	0.057 (4)	0.037 (4)	−0.008 (3)	−0.007 (3)	0.002 (3)
C11	0.024 (3)	0.034 (3)	0.047 (4)	−0.005 (3)	−0.007 (3)	−0.002 (3)
C12	0.016 (3)	0.038 (3)	0.040 (4)	−0.007 (2)	−0.004 (3)	−0.006 (3)
Cl13	0.0286 (8)	0.0715 (12)	0.0349 (10)	−0.0157 (8)	−0.0075 (7)	−0.0130 (8)
Cl14	0.0568 (12)	0.0340 (9)	0.0632 (13)	−0.0055 (8)	−0.0288 (10)	0.0048 (8)
O15	0.022 (2)	0.028 (2)	0.039 (3)	−0.0065 (17)	−0.0110 (19)	−0.0055 (18)
C16	0.020 (3)	0.027 (3)	0.033 (3)	−0.003 (2)	−0.009 (2)	−0.009 (2)
C17A	0.017 (4)	0.026 (5)	0.021 (5)	−0.001 (3)	−0.008 (3)	0.001 (4)
C18A	0.031 (5)	0.025 (4)	0.025 (5)	−0.012 (4)	−0.010 (4)	0.003 (3)
C17B	0.025 (7)	0.043 (11)	0.033 (11)	−0.014 (6)	−0.011 (6)	−0.016 (8)
C18B	0.023 (7)	0.049 (10)	0.027 (9)	−0.014 (7)	−0.003 (6)	−0.012 (7)
C19A	0.021 (5)	0.030 (5)	0.017 (5)	−0.011 (4)	−0.004 (4)	0.004 (4)
C19B	0.024 (8)	0.030 (9)	0.014 (8)	−0.008 (6)	−0.010 (6)	0.004 (6)
C20A	0.019 (5)	0.043 (5)	0.038 (7)	−0.015 (4)	−0.001 (5)	−0.009 (4)
C20B	0.033 (11)	0.077 (17)	0.041 (12)	−0.030 (11)	0.007 (9)	−0.030 (12)
C21	0.024 (3)	0.038 (3)	0.027 (3)	−0.010 (2)	−0.006 (2)	−0.005 (2)
C22	0.024 (3)	0.032 (3)	0.028 (3)	−0.004 (2)	−0.007 (2)	0.005 (2)
C23A	0.020 (6)	0.037 (8)	0.038 (9)	−0.008 (6)	−0.001 (5)	0.003 (6)
C23B	0.025 (10)	0.034 (15)	0.032 (13)	−0.005 (10)	−0.003 (8)	−0.004 (10)
C24A	0.019 (5)	0.030 (7)	0.032 (6)	−0.012 (5)	−0.009 (4)	0.008 (5)
C24B	0.027 (9)	0.035 (14)	0.033 (11)	−0.013 (9)	−0.007 (8)	−0.001 (9)
O25	0.026 (2)	0.036 (2)	0.037 (3)	−0.0098 (19)	−0.008 (2)	−0.0086 (19)
C26	0.030 (4)	0.065 (5)	0.082 (7)	−0.025 (4)	−0.003 (4)	−0.032 (5)
O27	0.027 (2)	0.030 (2)	0.047 (3)	−0.0040 (19)	0.003 (2)	−0.004 (2)

Geometric parameters (Å, º)

Pt1—Cl2	2.2898 (17)	C4—H4	0.9500
Pt1—N3	2.038 (5)	C4—C5	1.389 (9)
Pt1—O15	2.039 (5)	C5—H5	0.9500
Pt1—C16	2.150 (5)	C5—C6	1.358 (10)
Pt1—C17A	2.155 (10)	C6—H6	0.9500
C17A—H17A	1.0000	C6—C7	1.428 (9)
C17A—C18A	1.507 (12)	C7—C8	1.425 (9)
C18A—H18A	0.9900	C7—C9	1.405 (10)
C18A—H18B	0.9900	C8—C12	1.417 (9)
Pt1—C17B	2.213 (18)	C9—C10	1.370 (10)
C17B—H17B	1.0000	C9—Cl13	1.737 (6)
C17B—C18B	1.506 (17)	C10—H10	0.9500
C18B—H18C	0.9900	C10—C11	1.397 (10)
C18B—H18D	0.9900	C11—C12	1.383 (10)
C18A—C19A	1.518 (11)	C11—Cl14	1.728 (7)
C18B—C19B	1.516 (16)	C12—O15	1.336 (8)
C19A—C20A	1.408 (11)	C16—H16A	0.9500
C20A—H20A	0.9500	C16—H16B	0.9500
C19B—C20B	1.402 (15)	C16—H16C	0.9500

C20B—H20B	0.9500	C16—H16D	0.9500
C20B—C21	1.384 (15)	C16—C17A	1.388 (10)
C20A—C21	1.390 (11)	C16—C17B	1.432 (16)
C23A—H23A	0.9500	C21—C22	1.397 (9)
C23B—H23B	0.9500	C21—O25	1.377 (7)
C19A—C24A	1.397 (11)	C22—C23A	1.44 (3)
C23A—C24A	1.393 (13)	C22—C23B	1.28 (5)
C24A—H24A	0.9500	C22—O27	1.357 (7)
C19B—C24B	1.398 (15)	O25—C26	1.420 (8)
C23B—C24B	1.388 (16)	C26—H26A	0.9800
C24B—H24B	0.9500	C26—H26B	0.9800
N3—C4	1.331 (8)	C26—H26C	0.9800
N3—C8	1.364 (8)	O27—H27	0.8400

C18A—C17A—Pt1	112.3 (6)	N3—C8—C12	115.8 (6)
C18B—C17B—Pt1	109.0 (12)	C12—C8—C7	122.1 (6)
C17A—Pt1—Cl2	100.9 (3)	C7—C9—Cl13	119.2 (5)
N3—Pt1—Cl2	95.07 (15)	C10—C9—C7	120.9 (6)
C17B—Pt1—Cl2	80.9 (6)	C10—C9—Cl13	119.9 (5)
N3—Pt1—O15	82.14 (19)	C9—C10—H10	119.9
C18A—C17A—H17A	115.7	C9—C10—C11	120.2 (7)
N3—Pt1—C16	167.6 (2)	C11—C10—H10	119.9
N3—Pt1—C17A	150.1 (3)	C10—C11—Cl14	118.9 (6)
Pt1—C17A—H17A	115.7	C12—C11—C10	122.5 (6)
C24A—C19A—C18A	121.5 (10)	C12—C11—Cl14	118.6 (5)
N3—Pt1—C17B	153.8 (4)	C11—C12—C8	116.6 (6)
C20A—C19A—C18A	120.4 (8)	O15—C12—C8	120.0 (6)
O15—Pt1—Cl2	176.45 (12)	O15—C12—C11	123.4 (6)
C19A—C18A—H18A	109.8	C12—O15—Pt1	110.4 (4)
O15—Pt1—C16	91.8 (2)	Pt1—C16—H16A	112.4
O15—Pt1—C17A	82.5 (3)	Pt1—C16—H16B	86.5
O15—Pt1—C17B	102.6 (6)	Pt1—C16—H16C	105.6
C17A—C18A—H18A	109.8	C23A—C24A—H24A	120.0
H18A—C18A—H18B	108.3	C19B—C24B—H24B	119.5
C19A—C18A—H18B	109.8	C23B—C24B—H24B	119.5
C16—Pt1—Cl2	90.53 (18)	C17A—C16—Pt1	71.4 (5)
C16—Pt1—C17A	37.6 (3)	C17B—C16—Pt1	73.2 (7)
C16—Pt1—C17B	38.3 (4)	C17A—C16—H16A	120.0
C4—N3—Pt1	129.0 (5)	C17A—C16—H16B	120.0
C17A—C18A—H18B	109.8	H16A—C16—H16B	120.0
C18B—C17B—H17B	114.8	C17B—C16—H16C	120.0
Pt1—C17B—H17B	114.8	C17B—C16—H16D	120.0
C24B—C19B—C18B	120.1 (18)	H16C—C16—H16D	120.0
C4—N3—C8	119.4 (5)	Pt1—C16—H16D	91.2
C8—N3—Pt1	111.5 (4)	C20B—C21—C22	118.7 (12)
C20B—C19B—C18B	121.4 (14)	O25—C21—C20A	124.5 (7)
C17B—C18B—H18C	108.9	O25—C21—C20B	125.8 (12)
N3—C4—H4	119.0	O25—C21—C22	114.4 (5)

N3—C4—C5	122.0 (7)	C20A—C21—C22	120.8 (8)
C5—C4—H4	119.0	C21—C22—C23A	116.8 (11)
C19B—C18B—H18C	108.9	C23B—C22—C21	123.7 (19)
H18C—C18B—H18D	107.8	C23B—C22—O27	114.1 (19)
C17B—C18B—H18D	108.9	C16—C17A—Pt1	71.0 (4)
C4—C5—H5	119.9	C16—C17B—Pt1	68.5 (7)
C6—C5—C4	120.3 (6)	C16—C17A—H17A	115.7
C6—C5—H5	119.9	C16—C17A—C18A	118.7 (8)
C5—C6—H6	119.9	C16—C17B—H17B	114.8
C5—C6—C7	120.2 (6)	C16—C17B—C18B	125.2 (17)
C7—C6—H6	119.9	C21—C20A—C19A	122.1 (11)
C8—C7—C6	116.0 (6)	C21—C20B—C19B	118.9 (18)
C9—C7—C6	126.4 (6)	C21—C20A—H20A	119.0
C9—C7—C8	117.6 (6)	C21—C20B—H20B	120.5
C19B—C18B—H18D	108.9	O27—C22—C21	122.2 (6)
C17A—C18A—C19A	109.3 (7)	O27—C22—C23A	120.8 (10)
C23A—C24A—C19A	120.1 (17)	C21—O25—C26	116.3 (5)
C23B—C24B—C19B	121 (3)	C22—C23A—H23A	119.0
C17B—C18B—C19B	113.2 (14)	C22—C23B—H23B	120.5
C24A—C19A—C20A	118.1 (11)	C22—C23B—C24B	119 (4)
C19A—C20A—H20A	119.0	O25—C26—H26A	109.5
C24B—C19B—C20B	118.4 (19)	O25—C26—H26B	109.5
C19B—C20B—H20B	120.5	O25—C26—H26C	109.5
C24A—C23A—C22	122 (2)	H26A—C26—H26B	109.5
C24A—C23A—H23A	119.0	H26A—C26—H26C	109.5
C24B—C23B—H23B	120.5	H26B—C26—H26C	109.5
C19A—C24A—H24A	120.0	C22—O27—H27	109.5
N3—C8—C7	122.1 (6)		

Pt1—C17A—C18A—C19A	172.6 (6)	C6—C7—C9—C10	−179.9 (6)
Pt1—C17B—C18B—C19B	173.0 (13)	C6—C7—C9—Cl13	−0.3 (9)
C18A—C19A—C24A—C23A	−179.1 (18)	C7—C8—C12—C11	2.7 (9)
C20B—C19B—C24B—C23B	−2 (4)	C7—C8—C12—O15	−179.0 (5)
C17A—C18A—C19A—C24A	−119.8 (11)	C7—C9—C10—C11	0.2 (10)
C20A—C19A—C24A—C23A	3 (2)	C8—N3—C4—C5	2.6 (9)
C17A—C18A—C19A—C20A	58.2 (12)	C8—C7—C9—C10	0.0 (9)
C18B—C19B—C24B—C23B	175 (3)	C8—C7—C9—Cl13	179.6 (4)
C17B—C18B—C19B—C20B	−39 (2)	C8—C12—O15—Pt1	3.6 (7)
C17B—C18B—C19B—C24B	144.0 (19)	C9—C7—C8—N3	179.5 (5)
C18A—C19A—C20A—C21	−178.9 (11)	C9—C7—C8—C12	−1.5 (9)
C24B—C19B—C20B—C21	0.8 (18)	C9—C10—C11—C12	1.1 (10)
C18B—C19B—C20B—C21	−176.0 (19)	C9—C10—C11—Cl14	−179.3 (5)
C24A—C19A—C20A—C21	−0.9 (15)	C10—C11—C12—C8	−2.5 (10)
C19B—C20B—C21—C22	3.1 (17)	C10—C11—C12—O15	179.3 (6)
C19A—C20A—C21—C22	−3.3 (14)	C11—C12—O15—Pt1	−178.2 (5)
C19B—C20B—C21—O25	170.2 (11)	Cl13—C9—C10—C11	−179.4 (5)
C19A—C20A—C21—O25	−175.6 (9)	Cl14—C11—C12—C8	178.0 (5)
Pt1—N3—C4—C5	−173.6 (5)	Cl14—C11—C12—O15	−0.3 (9)

Pt1—N3—C8—C7	175.4 (4)	C20A—C21—C22—O27	−170.9 (8)
Pt1—N3—C8—C12	−3.7 (6)	C20B—C21—C22—O27	170.7 (11)
Pt1—C16—C17A—C18A	−105.6 (8)	O25—C21—C22—C23A	178.3 (16)
Pt1—C16—C17B—C18B	98.6 (16)	O25—C21—C22—C23B	−175 (3)
C20B—C21—C22—C23B	−7 (4)	C20B—C21—O25—C26	13.5 (14)
C20A—C21—C22—C23A	5 (2)	C20A—C21—O25—C26	−6.1 (11)
N3—C4—C5—C6	−1.6 (11)	C16—C17A—C18A—C19A	−107.5 (9)
N3—C8—C12—C11	−178.2 (6)	C16—C17B—C18B—C19B	96 (2)
N3—C8—C12—O15	0.1 (8)	C21—C22—C23A—C24A	−3 (3)
C4—N3—C8—C7	−1.5 (9)	C21—C22—C23B—C24B	6 (6)
C4—N3—C8—C12	179.4 (6)	C22—C23B—C24B—C19B	−2 (6)
C4—C5—C6—C7	−0.6 (10)	C22—C23A—C24A—C19A	−1 (3)
C5—C6—C7—C8	1.6 (9)	C22—C21—O25—C26	−178.9 (7)
C5—C6—C7—C9	−178.4 (6)	O25—C21—C22—O27	2.2 (9)
C6—C7—C8—N3	−0.6 (9)	O27—C22—C23A—C24A	172.9 (18)
C6—C7—C8—C12	178.4 (6)	O27—C22—C23B—C24B	−172 (3)