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trans-Dichlorido{3,4-dimethoxy-2-[(2,3-η)-prop-2-en-1-yl]benzene}(pyridine-κN)platinum(II)

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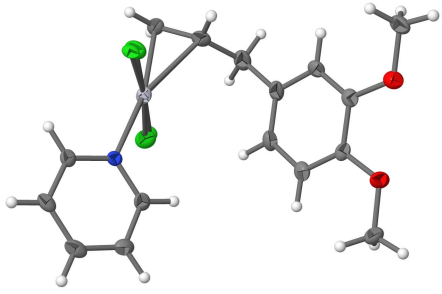
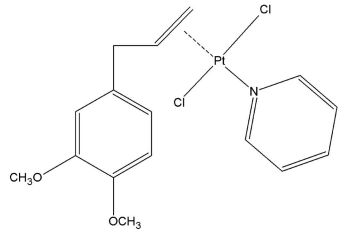
Structural data: full structural data are available from iucrdata.iucr.org

In the title organoplatinum(II) complex, $[PtCl_2(C_5H_5N)(C_{11}H_{14}O_2)]$, the methyleugenol ligand only coordinates to the Pt^{II} atom through the ethylenic double bond. The coordination is completed by the N atom of the pyridine ligand and two Cl atoms positioned *trans* with respect to each other. The pyridine and benzene rings are inclined to one another by 68.6 (2)°. In the crystal, molecules are linked *via* a number of C—H···Cl and C—H···O hydrogen bonds, forming sheets parallel to the *bc* plane.

3D view



Chemical scheme



Structure description

The crystal structure of the title complex was determined in order to clarify the Pt^{II} coordination to the ligand methyleugenol. It was found that it only coordinates to Pt^{II} through the ethylenic double bond (Fig. 1). The coordination is completed by the N atom of the pyridine ligand and two Cl atoms positioned *trans* with respect to each other. The pyridine and benzene rings are inclined to one another by 68.6 (2)°. In the crystal, molecules are linked *via* a number of C—H···Cl and C—H···O hydrogen bonds (Table 1), forming sheets parallel to the *bc* plane.

The activities of the title compound on HepG2 and Lu cell lines show IC50 values of 9.7 and 7.8 µg/ml, respectively. The synthesis and antitumor activity on the human cancer cell lines KB and MCF7 of the title compound and other organoplatinum(II) complexes containing methyleugenol and amines have been reported (Da, Chi *et al.*, 2015; Da, Hai *et al.*, 2015), as have the structures of organoplatinum(II) complexes containing eugenol (Da *et al.*, 2008; Da, Chi *et al.*, 2015; Mangwala Kimpende *et al.*, 2014).

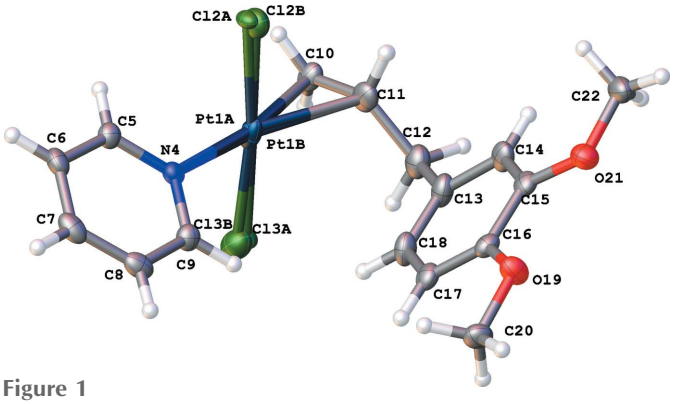


Figure 1
A view of the molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level. Both the major and minor components (*A*/*B*) of the disordered Pt and Cl atoms are shown.

Synthesis and crystallization

The synthesis of the title complex has been reported elsewhere (Da, Chi *et al.*, 2015).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Atoms Pt1, Cl2 and Cl3 are disordered over two sets of sites (*A*/*B*) with final occupancies of 0.59 (4) and 0.41 (4).

Acknowledgements

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References

Agilent (2012). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Da, T. T., Chi, N. T. T., Meervelt, L. V., Kimpende, P. M. & Dinh, N. H. (2015). *Polyhedron*, **85**, 104–109.
Da, T. T., Hong Hai, L. T., Meervelt, L. V. & Dinh, N. H. (2015). *J. Coord. Chem.* **68**, 3525–3536.
Da, T. T., Kim, Y.-M., Chi, N. T. T., Chien, L. X., Minh, N. V. & Dinh, N. H. (2008). *Organometallics*, **27**, 3611–3613.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···Cl3*B*^{i}	0.95	2.76	3.54 (2)	140
C12—H12*A*···O21^{ii}	0.99	2.57	3.397 (6)	141
C12—H12*B*···Cl3*A*	0.99	2.68	3.371 (13)	127
C17—H17···Cl2*A*^{iii}	0.95	2.78	3.671 (14)	156
C17—H17···Cl2*B*^{iii}	0.95	2.70	3.59 (2)	156

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[PtCl_2(C_5H_5N)(C_{11}H_{14}O_2)]$
M_r	523.31
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	95
a, *b*, *c* (Å)	15.1282 (5), 7.25666 (17), 16.3038 (5)
β (°)	108.013 (3)
V (Å^3)	1702.11 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	8.56
Crystal size (mm)	0.24 × 0.19 × 0.14
Data collection	
Diffractometer	Agilent SuperNova (single source at offset, Eos CCD detector) diffractometer
Absorption correction	Gaussian (*CrysAlis PRO*; Agilent, 2012)
T_{min}, T_{max}	0.771, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6822, 3459, 3165
R_{int}	0.023
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.024, 0.051, 1.11
No. of reflections	3459
No. of parameters	229
No. of restraints	219
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.13, −1.01

Computer programs: *CrysAlis PRO* (Agilent, 2012), *SHELXS2014* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009).

Mangwala Kimpende, P., Thi Da, T., Nguyen Huu, D. & Van Meervelt, L. (2014). *Acta Cryst.* E**70**, 435–437.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2016). **1**, x152176 [https://doi.org/10.1107/S2414314615021768]

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***trans*-Dichlorido{3,4-dimethoxy-2-[(2,3-η)-prop-2-en-1-yl]benzene}(pyridine-κN)platinum(II)**

Crystal data

$[PtCl_2(C_5H_5N)(C_{11}H_{14}O_2)]$
M_r = 523.31
Monoclinic, $P2_1/n$
a = 15.1282 (5) Å
b = 7.25666 (17) Å
c = 16.3038 (5) Å
β = 108.013 (3)°
V = 1702.11 (9) Å^3
Z = 4
$F(000)$ = 1000
D_x = 2.042 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4267 reflections
θ = 3.1–29.0°
μ = 8.56 mm^{-1}
T = 95 K
Block, yellow
0.24 × 0.19 × 0.14 mm

Data collection

Agilent SuperNova (single source at offset, Eos CCD detector) diffractometer
Radiation source: SuperNova (Mo) X-ray Source
Graphite monochromator
ω scans
Absorption correction: gaussian (CrysAlisPro; Agilent, 2012)
T_{min} = 0.771, T_{max} = 1.000
6822 measured reflections
3459 independent reflections
3165 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 26.4°, θ_{min} = 2.6°
h = −18→14
k = −8→9
l = −13→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.051
S = 1.11
3459 reflections
229 parameters
219 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0139P)^2 + 1.1858P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.13 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Pt1A	0.23303 (17)	0.9480 (4)	0.06520 (17)	0.0122 (5)	0.59 (4)
Cl2A	0.3517 (9)	1.1609 (16)	0.0976 (9)	0.0165 (12)	0.59 (4)
Cl3A	0.1127 (6)	0.7382 (17)	0.0436 (8)	0.0171 (12)	0.59 (4)
Pt1B	0.2283 (4)	0.9392 (8)	0.0651 (3)	0.0269 (9)	0.41 (4)
Cl2B	0.3413 (14)	1.155 (3)	0.0861 (15)	0.031 (3)	0.41 (4)
Cl3B	0.1121 (11)	0.724 (3)	0.0542 (15)	0.036 (3)	0.41 (4)
N4	0.3057 (2)	0.8103 (4)	0.1768 (2)	0.0176 (7)	
C5	0.3352 (3)	0.9011 (6)	0.2524 (3)	0.0208 (9)	
H5	0.3197	1.0276	0.2543	0.025*	
C6	0.3873 (3)	0.8148 (6)	0.3270 (3)	0.0241 (10)	
H6	0.4063	0.8804	0.3800	0.029*	
C7	0.4116 (3)	0.6320 (6)	0.3240 (3)	0.0265 (10)	
H7	0.4475	0.5703	0.3748	0.032*	
C8	0.3832 (3)	0.5414 (6)	0.2467 (3)	0.0248 (10)	
H8	0.4002	0.4163	0.2432	0.030*	
C9	0.3296 (3)	0.6326 (6)	0.1737 (3)	0.0216 (9)	
H9	0.3093	0.5684	0.1204	0.026*	
C10	0.1398 (3)	1.1197 (6)	−0.0314 (3)	0.0246 (10)	
H10A	0.0771	1.0816	−0.0425	0.030*	0.59 (4)
H10B	0.1636	1.2196	0.0067	0.030*	0.59 (4)
H10C	0.0771	1.0816	−0.0425	0.030*	0.41 (4)
H10D	0.1636	1.2196	0.0067	0.030*	0.41 (4)
C11	0.1977 (3)	1.0276 (6)	−0.0715 (3)	0.0294 (10)	
H11	0.2450	1.1096	−0.0842	0.035*	0.59 (4)
H11A	0.2468	1.1075	−0.0824	0.035*	0.41 (4)
C12	0.1693 (3)	0.8703 (7)	−0.1320 (3)	0.0314 (11)	
H12A	0.1402	0.9177	−0.1912	0.038*	
H12B	0.1224	0.7956	−0.1160	0.038*	
C13	0.2522 (3)	0.7484 (6)	−0.1306 (3)	0.0287 (10)	
C14	0.3107 (3)	0.7908 (6)	−0.1809 (3)	0.0262 (10)	
H14	0.2992	0.8986	−0.2156	0.031*	
C15	0.3841 (3)	0.6785 (6)	−0.1803 (3)	0.0212 (9)	
C16	0.4019 (3)	0.5190 (6)	−0.1278 (3)	0.0198 (9)	
C17	0.3454 (3)	0.4820 (6)	−0.0781 (3)	0.0236 (9)	
H17	0.3572	0.3760	−0.0422	0.028*	
C18	0.2717 (3)	0.5960 (6)	−0.0793 (3)	0.0271 (10)	
H18	0.2341	0.5676	−0.0439	0.033*	
O19	0.4741 (2)	0.4120 (4)	−0.1327 (2)	0.0257 (7)	
C20	0.4890 (3)	0.2442 (6)	−0.0832 (3)	0.0275 (10)	

H20A	0.4332	0.1672	−0.1023	0.041*
H20B	0.5022	0.2738	−0.0219	0.041*
H20C	0.5418	0.1774	−0.0916	0.041*
O21	0.4432 (2)	0.7041 (4)	−0.22853 (19)	0.0261 (7)
C22	0.4344 (3)	0.8716 (6)	−0.2759 (3)	0.0307 (11)
H22A	0.3715	0.8804	−0.3167	0.046*
H22B	0.4799	0.8733	−0.3075	0.046*
H22C	0.4457	0.9762	−0.2359	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1A	0.0117 (9)	0.0113 (7)	0.0146 (6)	−0.0012 (5)	0.0055 (4)	0.0006 (4)
Cl2A	0.0166 (19)	0.015 (2)	0.015 (3)	−0.0052 (15)	0.001 (2)	0.0019 (16)
Cl3A	0.014 (2)	0.019 (2)	0.019 (2)	−0.0040 (15)	0.0064 (14)	0.0013 (16)
Pt1B	0.0369 (17)	0.0252 (13)	0.0143 (9)	0.0112 (10)	0.0015 (9)	−0.0011 (7)
Cl2B	0.036 (6)	0.032 (4)	0.021 (5)	0.002 (3)	0.002 (4)	0.005 (3)
Cl3B	0.043 (4)	0.030 (4)	0.030 (6)	0.003 (3)	0.003 (3)	−0.001 (3)
N4	0.0177 (17)	0.0185 (16)	0.0178 (17)	0.0009 (14)	0.0071 (13)	0.0022 (13)
C5	0.019 (2)	0.024 (2)	0.019 (2)	0.0004 (18)	0.0072 (16)	0.0001 (17)
C6	0.023 (2)	0.031 (2)	0.019 (2)	−0.0027 (19)	0.0084 (17)	0.0051 (18)
C7	0.018 (2)	0.035 (2)	0.027 (2)	0.0013 (19)	0.0075 (18)	0.0119 (19)
C8	0.021 (2)	0.024 (2)	0.033 (2)	0.0042 (18)	0.0142 (19)	0.0074 (18)
C9	0.020 (2)	0.025 (2)	0.021 (2)	0.0021 (18)	0.0071 (17)	−0.0002 (17)
C10	0.026 (2)	0.026 (2)	0.018 (2)	0.0064 (19)	−0.0004 (17)	−0.0005 (18)
C11	0.038 (3)	0.028 (2)	0.018 (2)	0.007 (2)	0.0011 (18)	0.0062 (18)
C12	0.033 (3)	0.039 (3)	0.021 (2)	0.005 (2)	0.0056 (19)	0.000 (2)
C13	0.032 (2)	0.035 (2)	0.017 (2)	0.007 (2)	0.0061 (18)	−0.0026 (19)
C14	0.032 (2)	0.029 (2)	0.014 (2)	0.0071 (19)	0.0021 (17)	0.0033 (18)
C15	0.020 (2)	0.024 (2)	0.017 (2)	−0.0048 (17)	0.0016 (16)	−0.0041 (17)
C16	0.017 (2)	0.0201 (19)	0.021 (2)	−0.0011 (16)	0.0038 (16)	−0.0059 (17)
C17	0.024 (2)	0.028 (2)	0.017 (2)	−0.0036 (18)	0.0027 (17)	−0.0058 (18)
C18	0.026 (2)	0.037 (2)	0.019 (2)	0.0065 (19)	0.0082 (18)	−0.0017 (19)
O19	0.0245 (16)	0.0247 (15)	0.0306 (18)	0.0074 (13)	0.0122 (14)	0.0065 (14)
C20	0.032 (3)	0.019 (2)	0.033 (3)	0.0033 (19)	0.012 (2)	0.0002 (19)
O21	0.0265 (16)	0.0245 (16)	0.0274 (17)	−0.0024 (13)	0.0083 (13)	0.0021 (13)
C22	0.043 (3)	0.028 (2)	0.019 (2)	−0.007 (2)	0.006 (2)	0.0016 (19)

Geometric parameters (Å, º)

Pt1A—Cl2A	2.303 (10)	C11—H11	1.0000
Pt1A—Cl3A	2.315 (9)	C11—H11A	1.0000
Pt1A—N4	2.069 (4)	C11—C12	1.483 (6)
Pt1A—C10	2.156 (5)	C12—H12A	0.9900
Pt1A—C11	2.203 (5)	C12—H12B	0.9900
Pt1B—Cl2B	2.265 (17)	C12—C13	1.530 (6)
Pt1B—Cl3B	2.316 (16)	C13—C14	1.414 (6)
Pt1B—N4	2.061 (5)	C13—C18	1.363 (6)

Pt1B—C10	2.163 (6)	C14—H14	0.9500
Pt1B—C11	2.225 (6)	C14—C15	1.375 (6)
N4—C5	1.346 (5)	C15—C16	1.415 (6)
N4—C9	1.344 (5)	C15—O21	1.375 (5)
C5—H5	0.9500	C16—C17	1.373 (6)
C5—C6	1.379 (6)	C16—O19	1.362 (5)
C6—H6	0.9500	C17—H17	0.9500
C6—C7	1.381 (6)	C17—C18	1.384 (6)
C7—H7	0.9500	C18—H18	0.9500
C7—C8	1.367 (6)	O19—C20	1.440 (5)
C8—H8	0.9500	C20—H20A	0.9800
C8—C9	1.384 (6)	C20—H20B	0.9800
C9—H9	0.9500	C20—H20C	0.9800
C10—H10A	0.9500	O21—C22	1.423 (5)
C10—H10B	0.9500	C22—H22A	0.9800
C10—H10C	0.9500	C22—H22B	0.9800
C10—H10D	0.9500	C22—H22C	0.9800
C10—C11	1.413 (6)		

Cl2A—Pt1A—Cl3A	175.4 (5)	C11—C10—H10D	120.0
N4—Pt1A—Cl2A	87.6 (4)	Pt1A—C11—H11	113.6
N4—Pt1A—Cl3A	89.7 (3)	Pt1B—C11—H11A	114.1
N4—Pt1A—C10	166.24 (19)	C10—C11—Pt1A	69.3 (3)
N4—Pt1A—C11	156.0 (2)	C10—C11—Pt1B	68.9 (3)
C10—Pt1A—Cl2A	93.9 (4)	C10—C11—H11	113.6
C10—Pt1A—Cl3A	87.9 (4)	C10—C11—H11A	114.1
C10—Pt1A—C11	37.81 (17)	C10—C11—C12	125.3 (4)
C11—Pt1A—Cl2A	89.1 (4)	C12—C11—Pt1A	113.6 (3)
C11—Pt1A—Cl3A	94.9 (4)	C12—C11—Pt1B	111.8 (3)
Cl2B—Pt1B—Cl3B	175.5 (8)	C12—C11—H11	113.6
N4—Pt1B—Cl2B	89.1 (6)	C12—C11—H11A	114.1
N4—Pt1B—Cl3B	88.4 (5)	C11—C12—H12A	109.3
N4—Pt1B—C10	166.5 (3)	C11—C12—H12B	109.3
N4—Pt1B—C11	154.4 (3)	C11—C12—C13	111.6 (4)
C10—Pt1B—Cl2B	87.7 (7)	H12A—C12—H12B	108.0
C10—Pt1B—Cl3B	93.9 (6)	C13—C12—H12A	109.3
C10—Pt1B—C11	37.53 (17)	C13—C12—H12B	109.3
C11—Pt1B—Cl2B	82.3 (7)	C14—C13—C12	121.6 (4)
C11—Pt1B—Cl3B	101.5 (7)	C18—C13—C12	119.9 (4)
C5—N4—Pt1A	120.2 (3)	C18—C13—C14	118.5 (4)
C5—N4—Pt1B	121.6 (3)	C13—C14—H14	119.5
C9—N4—Pt1A	120.4 (3)	C15—C14—C13	121.0 (4)
C9—N4—Pt1B	119.2 (3)	C15—C14—H14	119.5
C9—N4—C5	119.2 (4)	C14—C15—C16	119.4 (4)
N4—C5—H5	119.3	O21—C15—C14	125.6 (4)
N4—C5—C6	121.5 (4)	O21—C15—C16	114.9 (4)
C6—C5—H5	119.3	C17—C16—C15	118.7 (4)
C5—C6—H6	120.3	O19—C16—C15	115.9 (4)

C5—C6—C7	119.4 (4)	O19—C16—C17	125.4 (4)
C7—C6—H6	120.3	C16—C17—H17	119.3
C6—C7—H7	120.6	C16—C17—C18	121.4 (4)
C8—C7—C6	118.9 (4)	C18—C17—H17	119.3
C8—C7—H7	120.6	C13—C18—C17	120.9 (4)
C7—C8—H8	120.1	C13—C18—H18	119.5
C7—C8—C9	119.8 (4)	C17—C18—H18	119.5
C9—C8—H8	120.1	C16—O19—C20	116.0 (3)
N4—C9—C8	121.3 (4)	O19—C20—H20A	109.5
N4—C9—H9	119.4	O19—C20—H20B	109.5
C8—C9—H9	119.4	O19—C20—H20C	109.5
Pt1A—C10—H10A	111.1	H20A—C20—H20B	109.5
Pt1A—C10—H10B	86.2	H20A—C20—H20C	109.5
Pt1B—C10—H10C	108.6	H20B—C20—H20C	109.5
Pt1B—C10—H10D	87.9	C15—O21—C22	117.2 (3)
H10A—C10—H10B	120.0	O21—C22—H22A	109.5
H10C—C10—H10D	120.0	O21—C22—H22B	109.5
C11—C10—Pt1A	72.9 (2)	O21—C22—H22C	109.5
C11—C10—Pt1B	73.6 (3)	H22A—C22—H22B	109.5
C11—C10—H10A	120.0	H22A—C22—H22C	109.5
C11—C10—H10B	120.0	H22B—C22—H22C	109.5
C11—C10—H10C	120.0		

Pt1A—N4—C5—C6	−177.1 (3)	C12—C13—C14—C15	−178.9 (4)
Pt1A—N4—C9—C8	175.9 (3)	C12—C13—C18—C17	178.9 (4)
Pt1A—C10—C11—C12	104.9 (4)	C13—C14—C15—C16	−0.7 (6)
Pt1A—C11—C12—C13	−72.6 (5)	C13—C14—C15—O21	177.9 (4)
Pt1B—N4—C5—C6	−179.7 (3)	C14—C13—C18—C17	−1.8 (7)
Pt1B—N4—C9—C8	178.6 (4)	C14—C15—C16—C17	−0.6 (6)
Pt1B—C10—C11—C12	102.4 (5)	C14—C15—C16—O19	178.1 (4)
Pt1B—C11—C12—C13	−74.3 (5)	C14—C15—O21—C22	7.4 (6)
N4—C5—C6—C7	1.4 (6)	C15—C16—C17—C18	0.7 (6)
C5—N4—C9—C8	0.4 (6)	C15—C16—O19—C20	−176.6 (3)
C5—C6—C7—C8	0.0 (6)	C16—C15—O21—C22	−173.9 (3)
C6—C7—C8—C9	−1.2 (6)	C16—C17—C18—C13	0.6 (7)
C7—C8—C9—N4	1.0 (6)	C17—C16—O19—C20	2.1 (6)
C9—N4—C5—C6	−1.6 (6)	C18—C13—C14—C15	1.9 (7)
C10—C11—C12—C13	−153.2 (4)	O19—C16—C17—C18	−177.9 (4)
C11—C12—C13—C14	−84.2 (5)	O21—C15—C16—C17	−179.3 (4)
C11—C12—C13—C18	95.0 (5)	O21—C15—C16—O19	−0.6 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···Cl3*B*^{i}	0.95	2.76	3.54 (2)	140
C12—H12*A*···O21^{ii}	0.99	2.57	3.397 (6)	141
C12—H12*B*···Cl3*A*	0.99	2.68	3.371 (13)	127

C17—H17···Cl2*A*^{iii}	0.95	2.78	3.671 (14)	156
C17—H17···Cl2*B*^{iii}	0.95	2.70	3.59 (2)	156

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