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{4,5-Dimethoxy-2-[(2,3-η)-2-prop-2-en-1-yl]phenyl-κC^1}(8-hydroxyquinolinato-$\kappa N,O$)platinum(II)

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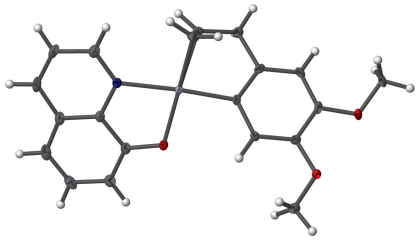
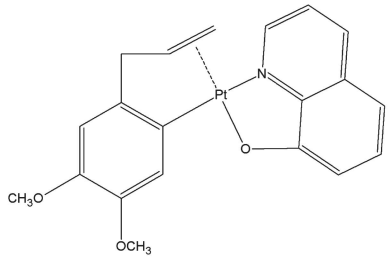
Structural data: full structural data are available from iucrdata.iucr.org

The crystal structure of the organoplatinum(II) title complex, $[Pt(C_9H_6NO)(C_{11}H_{13}O_2)]$ or [Pt(methyleugenol)(8-hydroxyquinolinato)], has been determined in order to verify the coordination environment of the Pt^{II} cation, which was found to be square-planar with the N and O atoms of the quinolinate ligand *cis* and *trans*, respectively, with respect to the ethylenic double bond. The least-squares planes through the two aromatic ring systems make an angle of 39.87 (10)°. In the crystal, chains are formed parallel to [100] sustained by C—H···O hydrogen bonds. Parallel chains further interact *via* C—H···O and C—H···π contacts. The complex shows interesting activity on four human cancer cell lines with IC_{50} values between 1.92 and 4.86 μ*M*.

3D view



Chemical scheme



Structure description

The title compound is shown in Fig. 1. Numerical details of the hydrogen-bonding interactions are given in Table 1 and the packing is shown in Fig. 2. For the synthesis and antitumor activity of organoplatinum(II) complexes containing aryl olefins and quinolines, see: Da *et al.* (2015*b*). For similar structures of organoplatinum(II) complexes containing eugenol, see: Da *et al.* (2008, 2015*a*); Mangwala Kimpende *et al.* (2014).

Synthesis and crystallization

The title compound was synthesized according to Da *et al.* (2015*b*) and recrystallized in acetone/water (5/1 *v*/*v*) to obtain brown crystals.

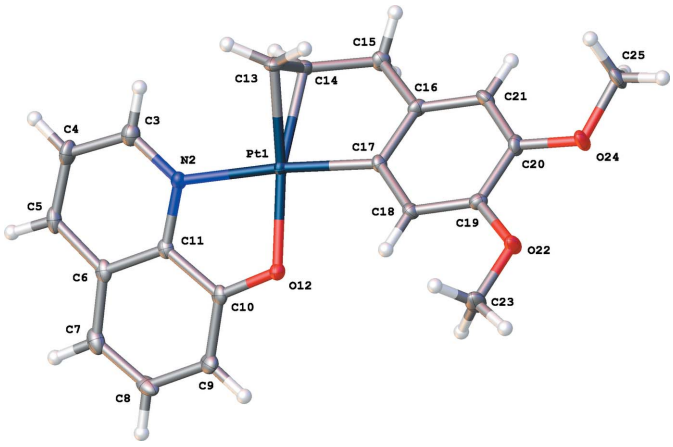


Figure 1
Molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

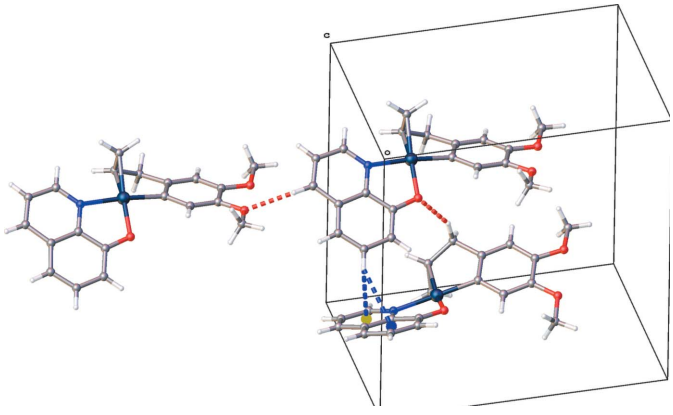


Figure 2
Partial packing diagram showing C—H···O interactions (red dotted lines) and C—H···π interactions (blue dotted lines).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors thank VLIR–UOS for financial support through project ZEIN2014Z182 and the Hercules Foundation for supporting the purchase of the diffractometer through project AKUL/09/0035.

References

Agilent (2012). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.

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

*Cg*5 and *Cg*6 are the centroids of the N2–C11 and C6–C11 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O22^{i}	0.95	2.39	3.330 (3)	169
C15—H15B···O12^{ii}	0.99	2.51	3.425 (3)	153
C8—H8···Cg5^{iii}	0.95	2.82	3.389 (3)	119
C8—H8···Cg6^{iii}	0.95	2.89	3.745 (3)	150

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Pt(C_9H_6NO)(C_{11}H_{13}O_2)]$
M_r	516.45
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	13.2250 (5), 15.0844 (6), 8.4294 (3)
β (°)	93.951 (3)
V (Å^3)	1677.59 (11)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	8.38
Crystal size (mm)	0.2 × 0.1 × 0.1
Data collection	
Diffractometer	Agilent SuperNova (single source at offset, Eos detector) diffractometer
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min}, T_{max}	0.715, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17650, 3429, 3106
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.015, 0.034, 1.05
No. of reflections	3429
No. of parameters	228
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.44

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

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full crystallographic data

IUCrData (2016). **1**, x152428 [doi:10.1107/S2414314615024281]

{4,5-Dimethoxy-2-[(2,3-η)-2-prop-2-en-1-yl]phenyl-κC^1}(8-hydroxyquinolinato-$\kappa N,O$)platinum(II)

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Crystal data

$[Pt(C_9H_6NO)(C_{11}H_{13}O_2)]$
M_r = 516.45
Monoclinic, $P2_1/c$
a = 13.2250 (5) Å
b = 15.0844 (6) Å
c = 8.4294 (3) Å
β = 93.951 (3)°
V = 1677.59 (11) Å^3
Z = 4
$F(000)$ = 992
D_x = 2.045 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9136 reflections
θ = 3.1–29.1°
μ = 8.38 mm^{-1}
T = 100 K
Block, brown
0.2 × 0.1 × 0.1 mm

Data collection

Agilent SuperNova (single source at offset, Eos detector) diffractometer
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 15.9631 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.715, T_{max} = 1.000
17650 measured reflections
3429 independent reflections
3106 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 26.4°, θ_{min} = 2.7°
h = −16→16
k = −18→18
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.015
$wR(F^2)$ = 0.034
S = 1.05
3429 reflections
228 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0116P)^2 + 1.0756P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Special details

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

Refinement. All H atoms were placed in idealized positions and refined in riding mode, with U_{iso}(H) values assigned as $1.2U_{eq}$ of the parent atoms (1.5 times for methyl groups) and with C—H distances of 0.95 (aromatic), 0.99 (CH_2), 1.00 (CH) or 0.98 Å (CH_3).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pt1	0.12790 (2)	0.09931 (2)	0.17780 (2)	0.01039 (4)
O12	0.11032 (14)	0.14501 (12)	−0.0478 (2)	0.0135 (4)
O24	0.58770 (14)	0.16254 (13)	0.2776 (2)	0.0196 (4)
C25	0.6319 (2)	0.1692 (2)	0.4370 (3)	0.0202 (6)
H25A	0.7059	0.1712	0.4355	0.030*
H25B	0.6122	0.1176	0.4984	0.030*
H25C	0.6078	0.2234	0.4863	0.030*
C10	0.0132 (2)	0.15209 (17)	−0.0999 (3)	0.0132 (6)
N2	−0.02987 (17)	0.08111 (14)	0.1373 (3)	0.0127 (5)
C5	−0.2370 (2)	0.08998 (17)	0.0501 (3)	0.0176 (6)
H5	−0.3079	0.0932	0.0231	0.021*
C17	0.2759 (2)	0.12436 (17)	0.2018 (3)	0.0116 (5)
C14	0.1447 (2)	0.10721 (18)	0.4297 (3)	0.0155 (6)
H14	0.0826	0.1244	0.4836	0.019*
C21	0.4200 (2)	0.16086 (17)	0.3832 (3)	0.0147 (6)
H21	0.4465	0.1767	0.4869	0.018*
O22	0.51395 (14)	0.12214 (13)	−0.0056 (2)	0.0175 (4)
C15	0.2403 (2)	0.15860 (18)	0.4792 (3)	0.0156 (6)
H15A	0.2697	0.1365	0.5829	0.019*
H15B	0.2240	0.2222	0.4908	0.019*
C16	0.3160 (2)	0.14691 (17)	0.3533 (3)	0.0135 (6)
C23	0.4760 (2)	0.0986 (2)	−0.1624 (3)	0.0223 (7)
H23A	0.5325	0.0939	−0.2313	0.033*
H23B	0.4286	0.1442	−0.2041	0.033*
H23C	0.4409	0.0414	−0.1595	0.033*
C13	0.1492 (2)	0.01869 (18)	0.3798 (3)	0.0164 (6)
H13A	0.0915	−0.0197	0.4042	0.020*
H13B	0.2159	−0.0110	0.3963	0.020*
C6	−0.1675 (2)	0.12442 (17)	−0.0548 (3)	0.0146 (6)
C18	0.3412 (2)	0.11678 (17)	0.0781 (3)	0.0125 (6)
H18	0.3145	0.1026	−0.0263	0.015*
C20	0.4843 (2)	0.15159 (18)	0.2610 (3)	0.0154 (6)
C11	−0.0634 (2)	0.11804 (16)	−0.0059 (3)	0.0120 (6)
C8	−0.1220 (2)	0.19969 (18)	−0.2892 (3)	0.0200 (6)
H8	−0.1416	0.2278	−0.3874	0.024*
C7	−0.1953 (2)	0.16732 (18)	−0.1991 (3)	0.0197 (6)

H7	−0.2648	0.1737	−0.2337	0.024*
C3	−0.0977 (2)	0.04905 (18)	0.2309 (3)	0.0177 (6)
H3	−0.0747	0.0229	0.3294	0.021*
C19	0.4443 (2)	0.12990 (17)	0.1077 (3)	0.0129 (6)
C9	−0.0180 (2)	0.19275 (17)	−0.2414 (3)	0.0164 (6)
H9	0.0310	0.2163	−0.3072	0.020*
C4	−0.2018 (2)	0.05227 (18)	0.1900 (3)	0.0190 (6)
H4	−0.2480	0.0281	0.2597	0.023*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.00723 (6)	0.01203 (6)	0.01194 (6)	0.00009 (4)	0.00097 (4)	0.00022 (4)
O12	0.0096 (9)	0.0165 (10)	0.0144 (10)	−0.0013 (8)	0.0002 (7)	0.0027 (8)
O24	0.0080 (10)	0.0366 (12)	0.0139 (10)	−0.0025 (9)	−0.0016 (8)	−0.0010 (9)
C25	0.0111 (14)	0.0314 (17)	0.0171 (15)	−0.0003 (12)	−0.0057 (11)	−0.0027 (13)
C10	0.0133 (14)	0.0099 (13)	0.0164 (14)	−0.0022 (11)	0.0003 (11)	−0.0037 (11)
N2	0.0110 (12)	0.0150 (12)	0.0121 (11)	−0.0016 (9)	0.0009 (9)	−0.0015 (9)
C5	0.0094 (14)	0.0155 (14)	0.0278 (16)	−0.0006 (11)	0.0004 (12)	−0.0071 (12)
C17	0.0085 (13)	0.0128 (13)	0.0132 (14)	0.0011 (11)	−0.0004 (10)	−0.0003 (11)
C14	0.0143 (14)	0.0225 (15)	0.0097 (14)	−0.0016 (12)	0.0016 (11)	0.0017 (11)
C21	0.0143 (14)	0.0183 (14)	0.0108 (14)	0.0006 (12)	−0.0035 (11)	−0.0021 (11)
O22	0.0099 (10)	0.0315 (11)	0.0113 (10)	−0.0018 (9)	0.0009 (8)	−0.0013 (8)
C15	0.0137 (14)	0.0183 (14)	0.0149 (14)	0.0015 (12)	0.0028 (11)	−0.0028 (12)
C16	0.0124 (14)	0.0149 (14)	0.0137 (14)	0.0020 (11)	0.0048 (11)	0.0005 (11)
C23	0.0178 (16)	0.0365 (18)	0.0129 (15)	−0.0030 (13)	0.0035 (12)	−0.0037 (13)
C13	0.0175 (15)	0.0193 (15)	0.0121 (14)	0.0004 (12)	−0.0002 (11)	0.0058 (11)
C6	0.0128 (14)	0.0093 (13)	0.0215 (15)	−0.0004 (11)	−0.0001 (11)	−0.0049 (11)
C18	0.0111 (14)	0.0145 (13)	0.0117 (14)	0.0005 (11)	−0.0009 (11)	0.0009 (11)
C20	0.0079 (14)	0.0184 (14)	0.0198 (15)	0.0001 (11)	0.0001 (11)	0.0006 (12)
C11	0.0115 (14)	0.0092 (13)	0.0151 (14)	0.0008 (10)	0.0001 (11)	−0.0035 (10)
C8	0.0258 (16)	0.0117 (13)	0.0210 (15)	0.0002 (12)	−0.0091 (12)	0.0034 (12)
C7	0.0154 (15)	0.0140 (14)	0.0289 (17)	0.0003 (12)	−0.0042 (12)	−0.0046 (12)
C3	0.0154 (15)	0.0178 (15)	0.0201 (15)	−0.0009 (12)	0.0025 (12)	−0.0028 (12)
C19	0.0130 (14)	0.0139 (13)	0.0121 (14)	0.0013 (11)	0.0023 (11)	0.0014 (11)
C9	0.0185 (15)	0.0118 (13)	0.0184 (14)	−0.0035 (12)	−0.0013 (11)	0.0002 (11)
C4	0.0111 (14)	0.0206 (15)	0.0260 (16)	−0.0017 (12)	0.0067 (12)	−0.0045 (13)

Geometric parameters (Å, º)

Pt1—O12	2.0214 (17)	C21—C20	1.388 (4)
Pt1—N2	2.109 (2)	O22—C23	1.425 (3)
Pt1—C17	1.990 (3)	O22—C19	1.377 (3)
Pt1—C14	2.123 (3)	C15—H15A	0.9900
Pt1—C13	2.096 (3)	C15—H15B	0.9900
O12—C10	1.333 (3)	C15—C16	1.519 (3)
O24—C25	1.431 (3)	C23—H23A	0.9800
O24—C20	1.375 (3)	C23—H23B	0.9800

C25—H25A	0.9800	C23—H23C	0.9800
C25—H25B	0.9800	C13—H13A	0.9900
C25—H25C	0.9800	C13—H13B	0.9900
C10—C11	1.424 (4)	C6—C11	1.413 (4)
C10—C9	1.379 (4)	C6—C7	1.404 (4)
N2—C11	1.375 (3)	C18—H18	0.9500
N2—C3	1.327 (3)	C18—C19	1.383 (4)
C5—H5	0.9500	C20—C19	1.401 (4)
C5—C6	1.418 (4)	C8—H8	0.9500
C5—C4	1.362 (4)	C8—C7	1.362 (4)
C17—C16	1.391 (4)	C8—C9	1.411 (4)
C17—C18	1.403 (4)	C7—H7	0.9500
C14—H14	1.0000	C3—H3	0.9500
C14—C15	1.516 (4)	C3—C4	1.396 (4)
C14—C13	1.402 (4)	C9—H9	0.9500
C21—H21	0.9500	C4—H4	0.9500
C21—C16	1.396 (4)		

O12—Pt1—N2	81.01 (8)	C17—C16—C21	120.7 (2)
O12—Pt1—C14	156.82 (9)	C17—C16—C15	116.2 (2)
O12—Pt1—C13	164.32 (9)	C21—C16—C15	123.0 (2)
N2—Pt1—C14	101.75 (9)	O22—C23—H23A	109.5
C17—Pt1—O12	94.56 (9)	O22—C23—H23B	109.5
C17—Pt1—N2	175.14 (9)	O22—C23—H23C	109.5
C17—Pt1—C14	81.55 (11)	H23A—C23—H23B	109.5
C17—Pt1—C13	87.21 (11)	H23A—C23—H23C	109.5
C13—Pt1—N2	97.60 (10)	H23B—C23—H23C	109.5
C13—Pt1—C14	38.82 (10)	Pt1—C13—H13A	116.4
C10—O12—Pt1	112.50 (15)	Pt1—C13—H13B	116.4
C20—O24—C25	116.3 (2)	C14—C13—Pt1	71.63 (15)
O24—C25—H25A	109.5	C14—C13—H13A	116.4
O24—C25—H25B	109.5	C14—C13—H13B	116.4
O24—C25—H25C	109.5	H13A—C13—H13B	113.4
H25A—C25—H25B	109.5	C11—C6—C5	117.0 (3)
H25A—C25—H25C	109.5	C7—C6—C5	124.6 (3)
H25B—C25—H25C	109.5	C7—C6—C11	118.4 (2)
O12—C10—C11	119.6 (2)	C17—C18—H18	119.9
O12—C10—C9	122.9 (2)	C19—C18—C17	120.2 (2)
C9—C10—C11	117.4 (3)	C19—C18—H18	119.9
C11—N2—Pt1	110.18 (16)	O24—C20—C21	124.7 (2)
C3—N2—Pt1	130.82 (19)	O24—C20—C19	115.6 (2)
C3—N2—C11	118.6 (2)	C21—C20—C19	119.7 (2)
C6—C5—H5	120.2	N2—C11—C10	115.9 (2)
C4—C5—H5	120.2	N2—C11—C6	122.2 (2)
C4—C5—C6	119.7 (3)	C6—C11—C10	122.0 (2)
C16—C17—Pt1	116.74 (19)	C7—C8—H8	118.9
C16—C17—C18	119.1 (2)	C7—C8—C9	122.1 (3)
C18—C17—Pt1	124.07 (19)	C9—C8—H8	118.9

Pt1—C14—H14	115.9	C6—C7—H7	120.2
C15—C14—Pt1	109.38 (17)	C8—C7—C6	119.6 (3)
C15—C14—H14	115.9	C8—C7—H7	120.2
C13—C14—Pt1	69.55 (15)	N2—C3—H3	118.8
C13—C14—H14	115.9	N2—C3—C4	122.4 (3)
C13—C14—C15	121.2 (2)	C4—C3—H3	118.8
C16—C21—H21	120.1	O22—C19—C18	124.1 (2)
C20—C21—H21	120.1	O22—C19—C20	115.5 (2)
C20—C21—C16	119.8 (2)	C18—C19—C20	120.3 (2)
C19—O22—C23	117.0 (2)	C10—C9—C8	120.5 (3)
C14—C15—H15A	109.9	C10—C9—H9	119.8
C14—C15—H15B	109.9	C8—C9—H9	119.8
C14—C15—C16	109.0 (2)	C5—C4—C3	120.1 (3)
H15A—C15—H15B	108.3	C5—C4—H4	120.0
C16—C15—H15A	109.9	C3—C4—H4	120.0
C16—C15—H15B	109.9		

Pt1—O12—C10—C11	−7.8 (3)	C15—C14—C13—Pt1	−100.9 (2)
Pt1—O12—C10—C9	171.0 (2)	C16—C17—C18—C19	1.3 (4)
Pt1—N2—C11—C10	5.4 (3)	C16—C21—C20—O24	−179.1 (2)
Pt1—N2—C11—C6	−172.66 (19)	C16—C21—C20—C19	1.2 (4)
Pt1—N2—C3—C4	171.8 (2)	C23—O22—C19—C18	−0.4 (4)
Pt1—C17—C16—C21	176.5 (2)	C23—O22—C19—C20	178.9 (2)
Pt1—C17—C16—C15	−5.8 (3)	C13—C14—C15—C16	48.9 (3)
Pt1—C17—C18—C19	−175.8 (2)	C6—C5—C4—C3	1.2 (4)
Pt1—C14—C15—C16	−28.4 (3)	C18—C17—C16—C21	−0.8 (4)
O12—C10—C11—N2	1.4 (4)	C18—C17—C16—C15	176.9 (2)
O12—C10—C11—C6	179.5 (2)	C20—C21—C16—C17	−0.5 (4)
O12—C10—C9—C8	−178.9 (2)	C20—C21—C16—C15	−178.0 (2)
O24—C20—C19—O22	0.2 (3)	C11—C10—C9—C8	0.0 (4)
O24—C20—C19—C18	179.5 (2)	C11—N2—C3—C4	−0.7 (4)
C25—O24—C20—C21	10.9 (4)	C11—C6—C7—C8	1.4 (4)
C25—O24—C20—C19	−169.4 (2)	C7—C6—C11—C10	−1.3 (4)
N2—C3—C4—C5	−0.6 (4)	C7—C6—C11—N2	176.7 (2)
C5—C6—C11—C10	−178.6 (2)	C7—C8—C9—C10	0.2 (4)
C5—C6—C11—N2	−0.7 (4)	C3—N2—C11—C10	179.3 (2)
C5—C6—C7—C8	178.5 (3)	C3—N2—C11—C6	1.3 (4)
C17—C18—C19—O22	178.7 (2)	C9—C10—C11—N2	−177.5 (2)
C17—C18—C19—C20	−0.5 (4)	C9—C10—C11—C6	0.6 (4)
C14—C15—C16—C17	23.3 (3)	C9—C8—C7—C6	−0.9 (4)
C14—C15—C16—C21	−159.1 (3)	C4—C5—C6—C11	−0.6 (4)
C21—C20—C19—O22	180.0 (2)	C4—C5—C6—C7	−177.7 (3)
C21—C20—C19—C18	−0.7 (4)		

Hydrogen-bond geometry (Å, º)

*Cg*5 and *Cg*6 are the centroids of the N2–C11 and C6–C11 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O22^{i}	0.95	2.39	3.330 (3)	169
C15—H15*B*···O12^{ii}	0.99	2.51	3.425 (3)	153
C8—H8···*Cg*5^{iii}	0.95	2.82	3.389 (3)	119
C8—H8···*Cg*6^{iii}	0.95	2.89	3.745 (3)	150

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