



IUCrData

ISSN 2414-3146

Received 19 April 2016

Accepted 23 April 2016

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

Keywords: crystal structure; azo; 1-phenylazo-2-naphthol; palladium(II); C—H...Cl hydrogen bonds;  $\pi$ – $\pi$  interactions.

CCDC reference: 1476177

Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

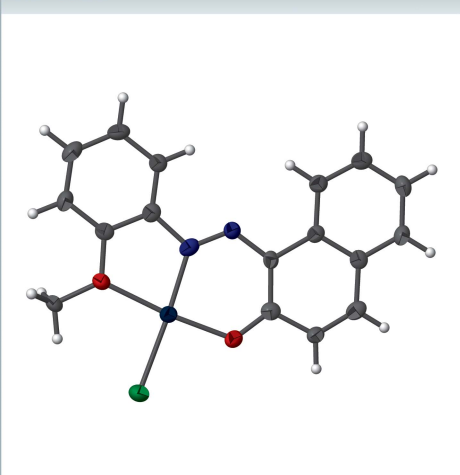
# Chlorido{(E)-1-[(2-methoxyphenyl)diazenyl]naphthalen-2-olato}palladium(II)

Assia Mili,<sup>a</sup> Souheyla Chetioui,<sup>a\*</sup> Djamil-Azeddine Rouag,<sup>a</sup> Jean-Pierre Djukic<sup>b</sup> and Corinne Bailly<sup>c</sup>

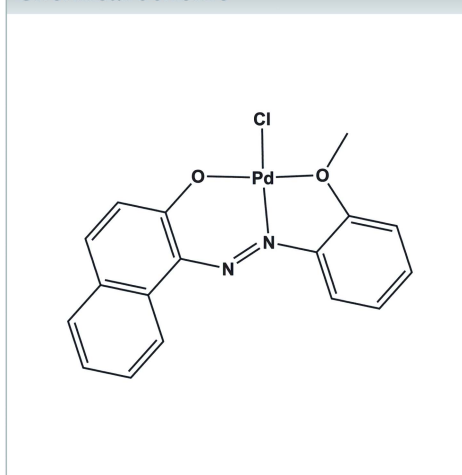
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In the title complex, [Pd(C<sub>17</sub>H<sub>13</sub>N<sub>2</sub>O<sub>2</sub>)Cl], the Pd<sup>II</sup> atom is tetracoordinated by an N and two O atoms of an (E)-1-[(2-methoxyphenyl)diazenyl]naphthalen-2-olate ligand and by a Cl atom, and has a square-planar coordination. In the crystal, molecules are linked by pairs of C—H...Cl hydrogen bonds, forming inversion dimers. The dimers are linked *via* offset  $\pi$ – $\pi$  interactions [inter-centroid distance = 3.546 (3) Å], forming chains running parallel to [100].

3D view

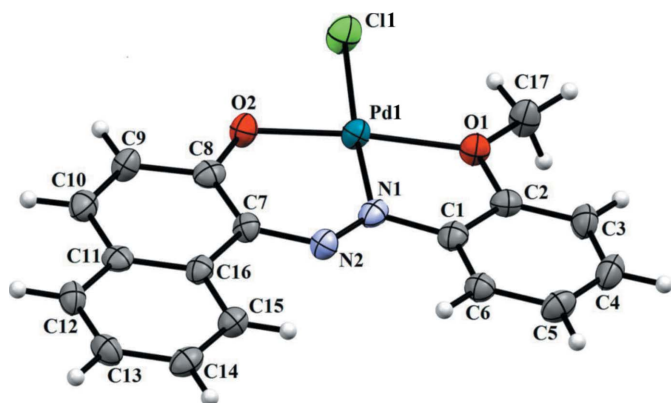


Chemical scheme



## Structure description

Azo compounds are highly coloured and have long been used as dyes and pigments. They have any practical applications such as colouring fibers, photo-electronic applications, printing systems, optical storage technology (Wang *et al.*, 2000), textile dyes as well as being used in many biological reactions and in analytical chemistry. We are interested in the colour generation mechanism of azo pigments typically characterized by the chromophore of the azo group (–N=N–) (Chetioui *et al.*, 2013a,b). Recently, 1-phenylazo-2-naphthol derivatives have attracted our attention because the phenylazo-naphtholate group can provide *N,O*-bidentate chelation to form transition metal or main-group metal complexes. Having successfully synthesized and structurally characterized two Cu<sup>II</sup> complexes with the ligand (E)-1-[(2-methoxyphenyl)diazenyl]naphthalen-2-ol (Chetioui *et al.*, 2015c,d), we describe herein the synthesis and crystal structure of the title palladium(II) complex, obtained by the reaction of (E)-1-[(2-methoxyphenyl)diazenyl]naphthalen-2-ol with Pd(OAc)<sub>2</sub>.



**Figure 1**  
The molecular structure of the title complex, with atom labelling and 50% probability displacement ellipsoids.

The molecular structure of the title complex is illustrated in Fig. 1. It contains a six- and a five-membered chelate ring by coordination of the Pd<sup>II</sup> atom to the *N,O*-bidentate phenylazophthalate ligand. The tetrahedral coordination sphere is completed by a Cl atom. The geometry around atom Pd1 is almost perfectly square-planar; the  $\tau(4)$  parameter = 0.07 (extreme Forms: 0.00 for SQP and 1.00 for TET; 0.85 for TRP; Yang *et al.*, 2007; Spek, 2009).

The N and Cl atoms and the two O atoms coordinated to the Pd<sup>II</sup> atom are *trans* to each other, with bond angles O1–Pd1–O2 = 174.19 (16) and N1–Pd1–Cl1 = 175.38 (15)°. The

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

<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>
C10–H10···Cl <sup>i</sup>	0.95	2.79	3.575 (6)	141

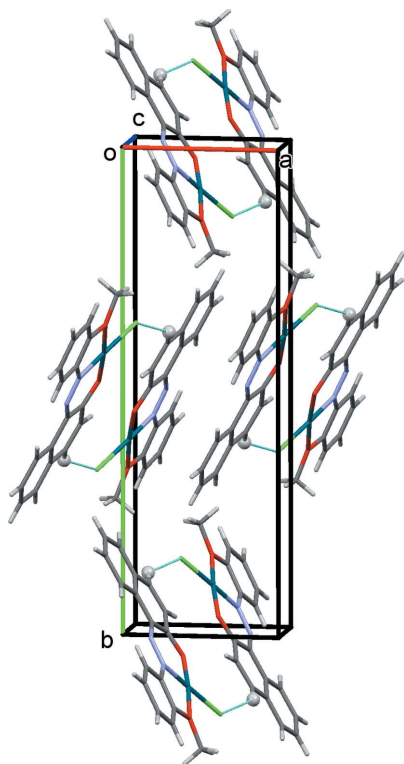
Symmetry code: (i)  $-x + 1, -y, -z + 2$ .

distances between atom Pd1 and atoms O1, O2, N1 and Cl1 are 2.070 (4), 1.945 (4), 1.945 (4) and 2.3184 (15) Å, respectively. These bond lengths are similar to those found in the crystal structure of bis{[(*E*)-*o*-tolylidiazanyl]naphthalen-2-yloxy}palladium(II) (Lin *et al.*, 2010).

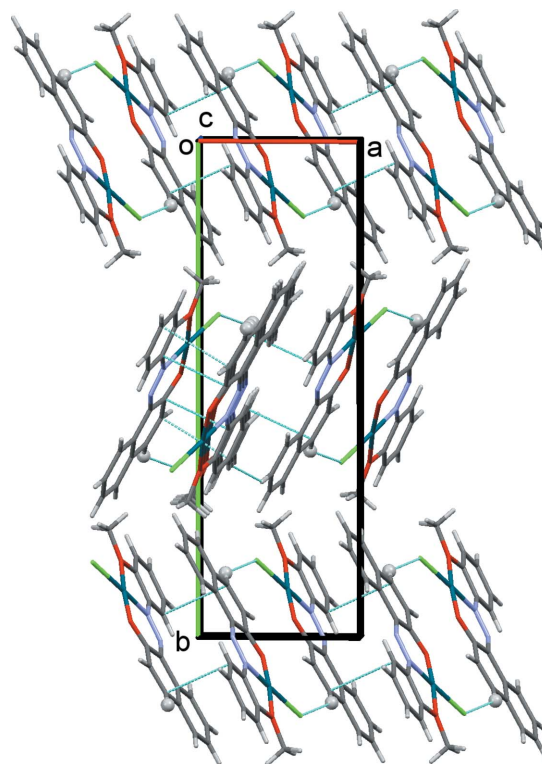
In the crystal, molecules are linked by pairs of C–H···Cl hydrogen bonds, forming inversion dimers (Table 1 and Fig. 2). The dimers are linked by slipped parallel  $\pi$ – $\pi$  interactions [ $Cg3 \cdots Cg4^i = 3.546$  (3) Å, *Cg3* and *Cg4* are the centroids of rings C1–C6 and C7–C11/C16), respectively, interplanar distance = 3.323 (3) Å, slippage 1.11 Å, symmetry code (i):  $-x + 1, -y, -z + 1$ ], forming chains running parallel to the *a* axis (Fig. 3).

### Synthesis and crystallization

A methanolic solution (15 ml) of (*E*)-1-[(2-methoxyphenyl)diazanyl]naphthalen-2-ol (0.19 g, 0.77 mmol) was slowly added to a methanolic solution of Pd(OAc)<sub>2</sub> (0.17 g) at 303 K with constant stirring for 1 h. The mixture was stirred for a further 4 h and the reddish brown compound that slowly



**Figure 2**  
A partial view along the *c* axis of the crystal packing of the title complex, showing the C–H···Cl hydrogen-bonded inversion dimers (dashed lines; see Table 1).



**Figure 3**  
The crystal packing of the title compound viewed along the *c* axis. The C–H···Cl hydrogen bonds (see Table 1) and  $\pi$ – $\pi$  interactions are shown as dashed lines.

separated out was filtered and washed several times with hexane and finally dried under vacuum. The vacuum dried compound, was then stirred in dry DMF for 6 h. Slow evaporation of DMF led to the formation of deep-red plate-like crystals of the title complex.

## Refinement

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

## Acknowledgements

The authors acknowledge the Algerian Ministry of Higher Education and Scientific Research, the Algerian Directorate General for Scientific Research and Technological Development and University of Constantine for financial support.

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**Table 2**

Experimental details.

Crystal data	
Chemical formula	[Pd(C <sub>17</sub> H <sub>13</sub> N <sub>2</sub> O <sub>2</sub> )Cl]
<i>M<sub>r</sub></i>	419.14
Crystal system, space group	Monoclinic, <i>P2<sub>1</sub>/n</i>
Temperature (K)	173
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.5429 (4), 21.4003 (16), 9.7773 (6)
$\beta$ (°)	112.325 (3)
<i>V</i> (Å <sup>3</sup> )	1459.95 (16)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	1.47
Crystal size (mm)	0.35 × 0.08 × 0.04
Data collection	
Diffractometer	Nonius KappaCCD
Absorption correction	Multi-scan ( <i>MULABS</i> ; Spek, 2009)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.660, 0.746
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	9359, 3327, 2045
<i>R<sub>int</sub></i>	0.106
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.649
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.054, 0.127, 1.03
No. of reflections	3327
No. of parameters	208
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	1.68, -1.73

Computer programs: *COLLECT* (Nonius, 1998), *DENZO* (Nonius, 1998), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae et al., 2008) and *PLATON* (Spek, 2009).

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## full crystallographic data

*IUCrData* (2016). **1**, x160691 [doi:10.1107/S241431461600691X]

## Chlorido{(E)-1-[(2-methoxyphenyl)diazenyl]naphthalen-2-olato}palladium(II)

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## Chlorido{(E)-1-[(2-methoxyphenyl)diazenyl]naphthalen-2-olato}palladium(II)

*Crystal data*

[Pd(C<sub>17</sub>H<sub>13</sub>N<sub>2</sub>O<sub>2</sub>)Cl]  
*M<sub>r</sub>* = 419.14  
 Monoclinic, *P*2<sub>1</sub>/*n*  
 Hall symbol: -*P* 2<sub>1</sub>*n*  
*a* = 7.5429 (4) Å  
*b* = 21.4003 (16) Å  
*c* = 9.7773 (6) Å  
 $\beta$  = 112.325 (3)°  
*V* = 1459.95 (16) Å<sup>3</sup>  
*Z* = 4

*F*(000) = 832  
*D<sub>x</sub>* = 1.907 Mg m<sup>-3</sup>  
 Mo *K*α radiation,  $\lambda$  = 0.71073 Å  
 Cell parameters from 8954 reflections  
 $\theta$  = 1.0–27.5°  
 $\mu$  = 1.47 mm<sup>-1</sup>  
*T* = 173 K  
 Plate, red  
 0.35 × 0.08 × 0.04 mm

*Data collection*

Nonius KappaCCD  
 diffractometer  
 Radiation source: sealed tube  
 Graphite monochromator  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (*MULABS*; Spek, 2009)  
*T<sub>min</sub>* = 0.660, *T<sub>max</sub>* = 0.746

9359 measured reflections  
 3327 independent reflections  
 2045 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.106  
 $\theta_{\max}$  = 27.5°,  $\theta_{\min}$  = 3.0°  
*h* = -9→7  
*k* = -20→27  
*l* = -11→12

*Refinement*

Refinement on *F*<sup>2</sup>  
 Least-squares matrix: full  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.054  
*wR*(*F*<sup>2</sup>) = 0.127  
*S* = 1.03  
 3327 reflections  
 208 parameters  
 0 restraints  
 0 constraints  
 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0534P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 1.68 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -1.73 \text{ e \AA}^{-3}$

*Special details*

**Geometry.** Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted R-factor wR and goodness of fit S are based on  $F^2$ , conventional R-factors R are based on F, with F set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Pd	0.44934 (6)	0.09641 (2)	0.62765 (4)	0.0255 (2)
Cl	0.6396 (2)	0.15537 (7)	0.82879 (15)	0.0389 (5)
O1	0.4706 (5)	0.15712 (18)	0.4697 (4)	0.0285 (12)
O2	0.4059 (5)	0.03610 (18)	0.7605 (4)	0.0285 (12)
N1	0.3047 (6)	0.0483 (2)	0.4517 (5)	0.0257 (16)
N2	0.2247 (6)	−0.0052 (2)	0.4422 (5)	0.0250 (16)
C1	0.2981 (7)	0.0749 (3)	0.3161 (6)	0.0272 (17)
C2	0.3823 (7)	0.1340 (3)	0.3273 (6)	0.0264 (19)
C3	0.3824 (8)	0.1640 (3)	0.2026 (6)	0.0314 (19)
C4	0.3000 (8)	0.1355 (3)	0.0678 (6)	0.0351 (19)
C5	0.2139 (8)	0.0771 (3)	0.0532 (6)	0.0340 (19)
C6	0.2144 (7)	0.0471 (3)	0.1787 (6)	0.0267 (17)
C7	0.2209 (7)	−0.0353 (3)	0.5636 (6)	0.0231 (17)
C8	0.3053 (7)	−0.0144 (3)	0.7138 (6)	0.0266 (19)
C9	0.2845 (8)	−0.0534 (3)	0.8261 (6)	0.0272 (17)
C10	0.1868 (8)	−0.1074 (3)	0.7927 (6)	0.0303 (19)
C11	0.1035 (7)	−0.1314 (3)	0.6454 (6)	0.0252 (17)
C12	0.1204 (7)	−0.0950 (3)	0.5299 (6)	0.0245 (17)
C13	0.0366 (7)	−0.1183 (3)	0.3853 (6)	0.0277 (17)
C14	−0.0595 (7)	−0.1752 (3)	0.3578 (6)	0.0302 (19)
C15	−0.0733 (7)	−0.2104 (3)	0.4709 (6)	0.031 (2)
C16	0.0087 (7)	−0.1890 (3)	0.6144 (6)	0.0282 (19)
C17	0.5458 (9)	0.2202 (3)	0.4890 (6)	0.0331 (19)
H3	0.43910	0.20420	0.21010	0.0370*
H4	0.30170	0.15610	−0.01780	0.0420*
H5	0.15580	0.05820	−0.04130	0.0410*
H6	0.15680	0.00710	0.17040	0.0320*
H9	0.34130	−0.04070	0.92660	0.0330*
H10	0.17240	−0.13080	0.87050	0.0370*
H13	0.04560	−0.09500	0.30550	0.0330*
H14	−0.11670	−0.19000	0.25910	0.0360*
H15	−0.13890	−0.24930	0.45030	0.0370*
H16	0.00080	−0.21360	0.69280	0.0340*
H17A	0.60360	0.23010	0.59470	0.0500*
H17B	0.64310	0.22360	0.44570	0.0500*
H17C	0.44140	0.24960	0.43960	0.0500*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Pd	0.0295 (3)	0.0238 (3)	0.0233 (3)	0.0008 (2)	0.0102 (2)	-0.0012 (2)
Cl	0.0532 (9)	0.0320 (9)	0.0274 (8)	-0.0085 (7)	0.0107 (7)	-0.0059 (7)
O1	0.035 (2)	0.025 (2)	0.025 (2)	-0.0044 (18)	0.0107 (17)	-0.0040 (17)
O2	0.036 (2)	0.027 (2)	0.024 (2)	0.0006 (19)	0.0132 (17)	0.0004 (18)
N1	0.024 (2)	0.031 (3)	0.023 (3)	0.010 (2)	0.010 (2)	0.004 (2)
N2	0.028 (2)	0.022 (3)	0.025 (3)	0.001 (2)	0.010 (2)	0.000 (2)
C1	0.026 (3)	0.027 (3)	0.029 (3)	0.006 (3)	0.011 (2)	0.003 (3)
C2	0.023 (3)	0.028 (4)	0.027 (3)	0.001 (2)	0.008 (2)	-0.002 (3)
C3	0.037 (3)	0.028 (4)	0.031 (3)	0.001 (3)	0.015 (3)	0.008 (3)
C4	0.041 (3)	0.040 (4)	0.027 (3)	0.009 (3)	0.016 (3)	0.010 (3)
C5	0.038 (3)	0.039 (4)	0.022 (3)	0.002 (3)	0.008 (3)	-0.004 (3)
C6	0.026 (3)	0.026 (3)	0.028 (3)	0.001 (2)	0.010 (2)	0.000 (3)
C7	0.026 (3)	0.017 (3)	0.027 (3)	0.003 (2)	0.011 (2)	0.002 (2)
C8	0.024 (3)	0.028 (4)	0.028 (3)	0.006 (3)	0.010 (2)	-0.001 (3)
C9	0.035 (3)	0.024 (3)	0.022 (3)	0.002 (3)	0.010 (2)	0.001 (3)
C10	0.029 (3)	0.038 (4)	0.027 (3)	0.007 (3)	0.014 (3)	0.004 (3)
C11	0.020 (3)	0.024 (3)	0.031 (3)	0.006 (2)	0.009 (2)	0.002 (3)
C12	0.025 (3)	0.025 (3)	0.024 (3)	0.005 (3)	0.010 (2)	0.003 (3)
C13	0.028 (3)	0.028 (3)	0.026 (3)	0.002 (3)	0.009 (2)	0.001 (3)
C14	0.031 (3)	0.031 (4)	0.026 (3)	0.008 (3)	0.008 (2)	0.000 (3)
C15	0.029 (3)	0.025 (4)	0.040 (4)	-0.004 (3)	0.015 (3)	0.000 (3)
C16	0.033 (3)	0.025 (4)	0.031 (3)	0.003 (3)	0.017 (3)	0.006 (3)
C17	0.049 (4)	0.022 (3)	0.027 (3)	-0.009 (3)	0.013 (3)	-0.006 (3)

*Geometric parameters (Å, °)*

Pd—C1	2.3184 (15)	C10—C11	1.430 (8)
Pd—O1	2.070 (4)	C11—C12	1.417 (8)
Pd—O2	1.945 (4)	C11—C16	1.399 (9)
Pd—N1	1.945 (4)	C12—C13	1.403 (8)
O1—C2	1.387 (7)	C13—C14	1.390 (9)
O1—C17	1.449 (8)	C14—C15	1.374 (8)
O2—C8	1.300 (7)	C15—C16	1.379 (8)
N1—N2	1.281 (6)	C3—H3	0.9500
N1—C1	1.426 (7)	C4—H4	0.9500
N2—C7	1.360 (7)	C5—H5	0.9500
C1—C2	1.401 (9)	C6—H6	0.9500
C1—C6	1.383 (8)	C9—H9	0.9500
C2—C3	1.378 (8)	C10—H10	0.9500
C3—C4	1.369 (8)	C13—H13	0.9500
C4—C5	1.391 (9)	C14—H14	0.9500
C5—C6	1.384 (8)	C15—H15	0.9500
C7—C8	1.432 (8)	C16—H16	0.9500
C7—C12	1.458 (9)	C17—H17A	0.9800
C8—C9	1.435 (8)	C17—H17B	0.9800

C9—C10	1.343 (9)	C17—H17C	0.9800
Pd···N1 <sup>i</sup>	3.838 (5)	C8···C6 <sup>i</sup>	3.439 (8)
Pd···N2 <sup>i</sup>	3.406 (5)	C8···C1 <sup>i</sup>	3.373 (8)
Pd···C1 <sup>i</sup>	4.071 (6)	C9···C3 <sup>i</sup>	3.540 (9)
Pd···C6 <sup>i</sup>	3.975 (6)	C9···C5 <sup>i</sup>	3.546 (9)
Pd···C7 <sup>i</sup>	3.864 (6)	C9···C4 <sup>i</sup>	3.393 (9)
Pd···C11 <sup>ii</sup>	4.077 (6)	C10···C1 <sup>iv</sup>	3.575 (6)
Pd···C12 <sup>ii</sup>	3.977 (6)	C10···C6 <sup>ii</sup>	3.398 (9)
Pd···C12 <sup>i</sup>	4.087 (6)	C10···C3 <sup>i</sup>	3.452 (9)
Pd···C13 <sup>ii</sup>	3.649 (6)	C10···C1 <sup>ii</sup>	3.470 (9)
Pd···C13 <sup>i</sup>	3.955 (6)	C11···Pd <sup>ii</sup>	4.077 (6)
Pd···C14 <sup>ii</sup>	3.439 (6)	C11···C1 <sup>ii</sup>	3.413 (8)
Pd···C15 <sup>ii</sup>	3.584 (6)	C11···N1 <sup>ii</sup>	3.365 (8)
Pd···C16 <sup>ii</sup>	3.905 (6)	C12···O1 <sup>i</sup>	3.358 (7)
Pd···H6 <sup>i</sup>	3.6300	C12···C2 <sup>i</sup>	3.569 (8)
Pd···H13 <sup>i</sup>	3.6100	C12···Pd <sup>ii</sup>	3.977 (6)
Pd···H14 <sup>ii</sup>	3.6900	C12···Pd <sup>i</sup>	4.087 (6)
Cl···O1	3.249 (4)	C12···N1 <sup>ii</sup>	3.428 (8)
Cl···O2	3.029 (4)	C13···Pd <sup>ii</sup>	3.649 (6)
Cl···C17	3.417 (6)	C13···Pd <sup>i</sup>	3.955 (6)
Cl···C15 <sup>iii</sup>	3.617 (6)	C14···Pd <sup>ii</sup>	3.439 (6)
Cl···C16 <sup>iii</sup>	3.623 (6)	C15···Pd <sup>ii</sup>	3.584 (6)
Cl···C10 <sup>iv</sup>	3.575 (6)	C15···Cl <sup>vii</sup>	3.617 (6)
Cl···H17A	2.7200	C16···Cl <sup>vii</sup>	3.623 (6)
Cl···H15 <sup>iii</sup>	2.9700	C16···Pd <sup>ii</sup>	3.905 (6)
Cl···H16 <sup>iii</sup>	2.9800	C16···C2 <sup>ii</sup>	3.418 (8)
Cl···H10 <sup>iv</sup>	2.7900	C17···C3 <sup>v</sup>	3.595 (9)
Cl···H17C <sup>v</sup>	2.9400	C17···C4 <sup>v</sup>	3.561 (9)
O1···Cl	3.249 (4)	C3···H17A <sup>vi</sup>	3.0000
O1···N1	2.618 (6)	C3···H17C	2.8500
O1···C1	2.358 (7)	C3···H17B	2.7600
O1···C12 <sup>i</sup>	3.358 (7)	C9···H5 <sup>viii</sup>	3.0500
O2···Cl	3.029 (4)	C14···H3 <sup>ix</sup>	2.9000
O2···N1	2.831 (6)	C15···H3 <sup>ix</sup>	2.9800
O2···N2	3.017 (6)	C15···H17B <sup>i</sup>	3.0400
O2···C6 <sup>i</sup>	3.230 (7)	C16···H17B <sup>i</sup>	2.9900
N1···O1	2.618 (6)	C17···H3	2.5600
N1···O2	2.831 (6)	H3···C17	2.5600
N1···C2	2.393 (8)	H3···H17B	2.2700
N1···C8	2.891 (7)	H3···H17C	2.4400
N1···Pd <sup>i</sup>	3.838 (5)	H3···C14 <sup>x</sup>	2.9000
N1···C11 <sup>ii</sup>	3.365 (8)	H3···C15 <sup>x</sup>	2.9800
N1···C12 <sup>ii</sup>	3.428 (8)	H3···H14 <sup>x</sup>	2.5900
N2···O2	3.017 (6)	H4···H14 <sup>xi</sup>	2.3500
N2···Pd <sup>i</sup>	3.406 (5)	H5···C9 <sup>xii</sup>	3.0500
N2···H6	2.5200	H5···H13 <sup>xi</sup>	2.5700
N2···H13	2.4400	H6···N2	2.5200

C1...Pd <sup>i</sup>	4.071 (6)	H6...Pd <sup>i</sup>	3.6300
C1...C7 <sup>i</sup>	3.467 (8)	H10...H16	2.4700
C1...C8 <sup>i</sup>	3.373 (8)	H10...Cl <sup>iv</sup>	2.7900
C1...C10 <sup>ii</sup>	3.470 (9)	H13...N2	2.4400
C1...C11 <sup>ii</sup>	3.413 (8)	H13...Pd <sup>i</sup>	3.6100
C2...C7 <sup>i</sup>	3.483 (8)	H13...H5 <sup>xi</sup>	2.5700
C2...C12 <sup>i</sup>	3.569 (8)	H14...H3 <sup>ix</sup>	2.5900
C2...C16 <sup>ii</sup>	3.418 (8)	H14...Pd <sup>ii</sup>	3.6900
C3...C10 <sup>i</sup>	3.452 (9)	H14...H4 <sup>xi</sup>	2.3500
C3...C17 <sup>vi</sup>	3.595 (9)	H15...Cl <sup>vii</sup>	2.9700
C3...C9 <sup>i</sup>	3.540 (9)	H16...H10	2.4700
C4...C17 <sup>vi</sup>	3.561 (9)	H16...Cl <sup>vii</sup>	2.9800
C4...C9 <sup>i</sup>	3.393 (9)	H17A...C1	2.7200
C5...C9 <sup>i</sup>	3.546 (9)	H17A...C3 <sup>v</sup>	3.0000
C6...C10 <sup>ii</sup>	3.398 (9)	H17B...C3	2.7600
C6...O2 <sup>i</sup>	3.230 (7)	H17B...H3	2.2700
C6...C8 <sup>i</sup>	3.439 (8)	H17B...C15 <sup>i</sup>	3.0400
C6...Pd <sup>i</sup>	3.975 (6)	H17B...C16 <sup>i</sup>	2.9900
C7...C2 <sup>i</sup>	3.483 (8)	H17C...C3	2.8500
C7...C7 <sup>ii</sup>	3.433 (8)	H17C...H3	2.4400
C7...Pd <sup>i</sup>	3.864 (6)	H17C...Cl <sup>vi</sup>	2.9400
C7...C1 <sup>i</sup>	3.467 (8)		
Cl—Pd—O1	95.33 (11)	C12—C11—C16	120.3 (5)
Cl—Pd—O2	90.10 (12)	C7—C12—C11	119.9 (5)
Cl—Pd—N1	175.38 (15)	C7—C12—C13	122.4 (5)
O1—Pd—O2	174.19 (16)	C11—C12—C13	117.7 (6)
O1—Pd—N1	81.30 (17)	C12—C13—C14	120.6 (5)
O2—Pd—N1	93.40 (17)	C13—C14—C15	121.2 (5)
Pd—O1—C2	112.4 (3)	C14—C15—C16	119.7 (6)
Pd—O1—C17	128.7 (3)	C11—C16—C15	120.5 (5)
C2—O1—C17	118.6 (4)	C2—C3—H3	120.00
Pd—O2—C8	122.8 (3)	C4—C3—H3	120.00
Pd—N1—N2	128.9 (4)	C3—C4—H4	119.00
Pd—N1—C1	114.9 (4)	C5—C4—H4	119.00
N2—N1—C1	116.1 (5)	C4—C5—H5	121.00
N1—N2—C7	121.7 (5)	C6—C5—H5	121.00
N1—C1—C2	115.7 (5)	C1—C6—H6	120.00
N1—C1—C6	125.0 (6)	C5—C6—H6	120.00
C2—C1—C6	119.4 (5)	C8—C9—H9	119.00
O1—C2—C1	115.6 (5)	C10—C9—H9	119.00
O1—C2—C3	124.1 (5)	C9—C10—H10	119.00
C1—C2—C3	120.3 (5)	C11—C10—H10	118.00
C2—C3—C4	119.5 (6)	C12—C13—H13	120.00
C3—C4—C5	121.5 (5)	C14—C13—H13	120.00
C4—C5—C6	118.8 (5)	C13—C14—H14	119.00
C1—C6—C5	120.6 (6)	C15—C14—H14	119.00
N2—C7—C8	126.8 (6)	C14—C15—H15	120.00



N2—C7—C12	113.5 (5)	C16—C15—H15	120.00
C8—C7—C12	119.7 (5)	C11—C16—H16	120.00
O2—C8—C7	126.4 (5)	C15—C16—H16	120.00
O2—C8—C9	115.7 (5)	O1—C17—H17A	110.00
C7—C8—C9	117.9 (5)	O1—C17—H17B	109.00
C8—C9—C10	121.6 (5)	O1—C17—H17C	109.00
C9—C10—C11	123.0 (5)	H17A—C17—H17B	109.00
C10—C11—C12	117.8 (6)	H17A—C17—H17C	109.00
C10—C11—C16	121.8 (5)	H17B—C17—H17C	109.00
Cl—Pd—O1—C2	175.1 (3)	O1—C2—C3—C4	176.4 (6)
Cl—Pd—O1—C17	-11.6 (5)	C1—C2—C3—C4	-0.2 (9)
N1—Pd—O1—C2	-1.7 (4)	C2—C3—C4—C5	0.7 (10)
N1—Pd—O1—C17	171.6 (5)	C3—C4—C5—C6	-0.8 (10)
Cl—Pd—O2—C8	-177.9 (4)	C4—C5—C6—C1	0.4 (9)
N1—Pd—O2—C8	-0.9 (4)	N2—C7—C8—O2	-2.5 (10)
O1—Pd—N1—N2	179.3 (5)	N2—C7—C8—C9	179.9 (6)
O1—Pd—N1—C1	3.6 (4)	C12—C7—C8—O2	176.7 (6)
O2—Pd—N1—N2	-3.1 (5)	C12—C7—C8—C9	-0.9 (8)
O2—Pd—N1—C1	-178.8 (4)	N2—C7—C12—C11	-179.5 (5)
Pd—O1—C2—C1	-0.6 (6)	N2—C7—C12—C13	0.0 (8)
Pd—O1—C2—C3	-177.3 (5)	C8—C7—C12—C11	1.2 (9)
C17—O1—C2—C1	-174.6 (5)	C8—C7—C12—C13	-179.3 (6)
C17—O1—C2—C3	8.7 (8)	O2—C8—C9—C10	-178.9 (6)
Pd—O2—C8—C7	3.4 (8)	C7—C8—C9—C10	-1.0 (9)
Pd—O2—C8—C9	-179.0 (4)	C8—C9—C10—C11	2.6 (10)
Pd—N1—N2—C7	4.6 (8)	C9—C10—C11—C12	-2.2 (9)
C1—N1—N2—C7	-179.8 (5)	C9—C10—C11—C16	177.5 (6)
Pd—N1—C1—C2	-5.1 (6)	C10—C11—C12—C7	0.2 (8)
Pd—N1—C1—C6	175.7 (5)	C10—C11—C12—C13	-179.3 (6)
N2—N1—C1—C2	178.7 (5)	C16—C11—C12—C7	-179.5 (5)
N2—N1—C1—C6	-0.6 (8)	C16—C11—C12—C13	1.0 (9)
N1—N2—C7—C8	-1.8 (9)	C10—C11—C16—C15	178.8 (6)
N1—N2—C7—C12	178.9 (5)	C12—C11—C16—C15	-1.5 (9)
N1—C1—C2—O1	3.6 (8)	C7—C12—C13—C14	-179.4 (6)
N1—C1—C2—C3	-179.6 (5)	C11—C12—C13—C14	0.1 (9)
C6—C1—C2—O1	-177.1 (5)	C12—C13—C14—C15	-0.7 (9)
C6—C1—C2—C3	-0.3 (9)	C13—C14—C15—C16	0.3 (9)
N1—C1—C6—C5	179.4 (6)	C14—C15—C16—C11	0.9 (9)
C2—C1—C6—C5	0.2 (9)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
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C10—H10···Cl <sup>iv</sup>	0.95	2.79	3.575 (6)	141
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Symmetry code: (iv)  $-x+1, -y, -z+2$ .