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Crystal structures of (*S*)-(−)-1-(4-chlorophenyl)-*N*-[(pyridin-2-yl)methylidene]ethan-1-amine and its *cis*-dichlorido{(*S*)-(−)-1-(4-chlorophenyl)-*N*-[(pyridin-2-yl)methylidene]ethan-1-amine}-palladium(II) complex

Teresa Pacheco-Álvarez,[a] Alejandro Yañez-Cabrera,[b] C. Claudia P. Villamizar,[c] Pankaj Sharma,[c] Bertin Anzaldo,[b] Angel Mendoza[d] and Guadalupe Hernández Téllez[b]*

[a]Lab. Síntesis de Complejos, Fac. Cs. Quím. Benemérita Universidad, Autónoma de Puebla, Ciudad Universitaria, PO, Box, 72592 Puebla, Mexico, [b]Lab. Síntesis de Complejos, Fac. Cs. Quím., Benemérita Universidad Autónoma de Puebla, Ciudad Universitaria, PO Box 72592, Puebla, Mexico, [c]Instituto de Química Universidad Autónoma de México UNAM, Circuito Exterior Cd. Universitaria, PO Box 04510, Ciudad de México, Mexico, and [d]Centro de Química, ICUAP, Benemérita Universidad Autónoma de Puebla, 72570 Puebla, Mexico. *Correspondence e-mail: guadalupe.hernandez@correo.buap.mx

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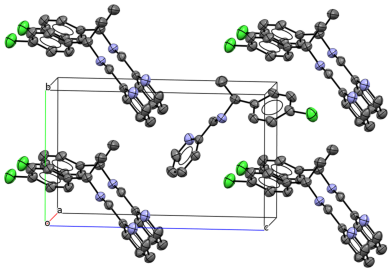
One of the title compounds, the chiral Schiff base (*S*)-(−)-1-(4-chlorophenyl)-*N*-[(pyridin-2-yl)methylidene]ethan-1-amine ($C_{14}H_{13}ClN_2$) crystallizes in the monoclinic Sohncke space group $P2_1$ with one molecule in the asymmetric unit. The ligand is obtained by condensation of (*S*)-(−)-1-(4-chlorophenyl)ethan-1-amine with 2-pyridinecarboxaldehyde. Its palladium(II) chloride complex, *cis*-dichlorido{(*S*)-(−)-1-(4-chlorophenyl)-*N*-[(pyridin-2-yl)methylidene]ethan-1-amine-κ^2N,N'}palladium(II), $[PdCl_2(C_{14}H_{13}ClN_2)]$, crystallizes in the orthorhombic Sohncke space group $P2_12_12_1$, with one molecule in the asymmetric unit. The central Pd^{II} atom adopts a slightly distorted square-planar coordination environment, defined by two nitrogen donors (pyridyl-N and imine-N) and two chlorido ligands in a *cis* arrangement.

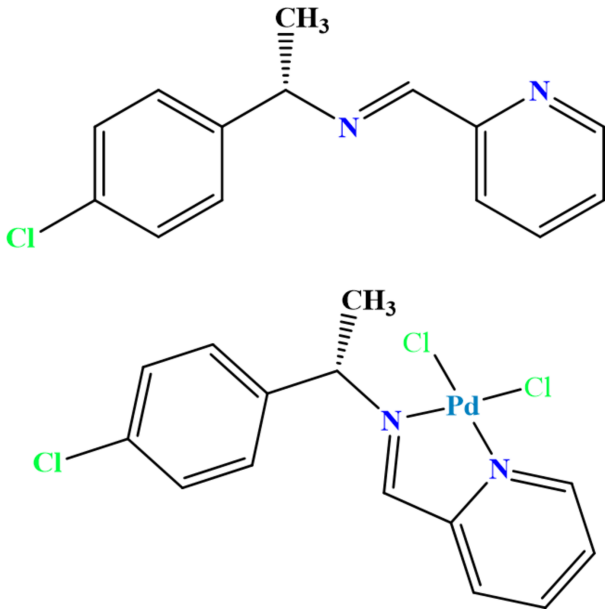
1. Chemical context

Molecules containing imine or azomethine C═N groups are widespread in chemical and biological systems. Schiff bases, formed readily by the condensation of aldehydes or ketones with primary amines, are synthetically accessible and structurally versatile (Anzaldo Olivares *et al.*, 2019; Hernández Téllez *et al.*, 2025). These features make them particularly valuable in coordination chemistry, enabling the rational design of various metal complexes (Dalia *et al.*, 2018). In *d*-block chemistry, Schiff-base ligands can stabilize metals in multiple oxidation states, while systematic modifications of the imine framework allows fine-tuning of electronic and steric properties (Takeda *et al.*, 2023).

Chelation governs many processes in organometallic and bioinorganic chemistry: steric factors strongly influence coordination, geometry and reactivity (Mandal & Pratihar, 2023; Fabbrizzi, 2020). In particular, Pd^{II} complexes are central in catalytic reactions; their kinetic reactivity often exceeds that of Pt^{II} analogues by 4-5 orders of magnitude (Bugarčić *et al.*, 2015).

Herein we report the synthesis and crystal structures of a chiral Schiff base, $C_{14}H_{13}ClN_2$, and its corresponding $PdCl_2$ complex, $[PdCl_2(C_{14}H_{13}ClN_2)]$.





2. Structural commentary

The molecular structure of the Schiff base ligand is shown in Fig. 1. The crystal belongs to the monoclinic Sohncke space group $P2_1$ and the molecule displays the *E* configuration about the C═N double bond and the *(S)* configuration at the stereogenic center. The free ligand exhibits an imine C9═N1 bond length of 1.253 (4) Å, within the expected range for >C═N bonds, and a C7—N1—C9 bond angle of 117.4 (3)°, consistent with sp^2 hybridization at C9 and N1. The ligand adopts a conformation governed by steric repulsion: the two aromatic rings are not coplanar, the angle between the plane defined by ring N2–C14–C13–C12–C11–C10 and the plane defined by ring C6–C1–C2–C3–C4–C5 is 32.08 (16)°.

The corresponding $PdCl_2$ complex crystallizes in the orthorhombic Sohncke space group $P2_12_12_1$, with one molecule in the asymmetric unit. The imine ligand bonds to the Pd^{II} atom via two nitrogen donors (imine N1 and pyridyl N2) within an N^N five-membered chelate ring. Together with the two chlorido ligands, a distorted square-planar coordination is realized (Fig. 2), with an N1—Pd—N2 bite angle of 80.8 (3)°. Observed bond lengths are Pd1—N1 = 2.045 (8) Å, Pd1—N2 = 2.036 (8) Å, Pd1—Cl1 = 2.291 (3) Å and Pd1—N2 = 2.282 (3) Å, values consistent with closely related Pd(II) complexes. The Cl1—Pd—Cl2 angle of 90.85 (9)° approximates the ideal 90° for ideal square-planar coordination. The imine bond in the complex, C9═N1 = 1.287 (10) Å, is slightly longer than in the free ligand and, together with a C7—N1—C9 angle of 122.0 (8)°, is consistent with sp^2 hybridization. The Pd(II) atom lies 0.012 Å out of the mean N_2Cl_2 coordination plane. Coordination to the metal increases steric effects in the ligand backbone, reflected by the change in torsion angle C1—C7—N1—C9 from −142.4 (3)° in the free ligand to 24.3 (12)° in the complex. Weak intramolecular C—H···Cl interactions stabilize the molecular conformation (Table 1; entries 3–5)

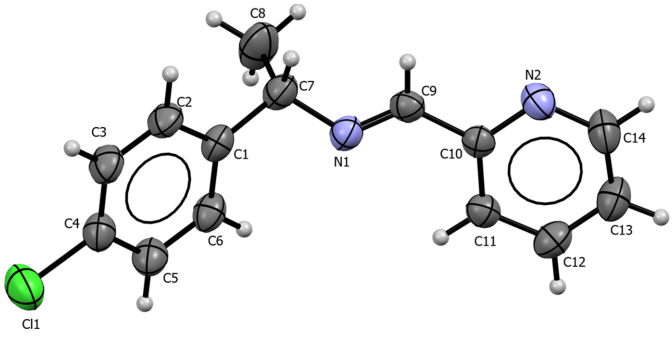


Figure 1
Molecular structure of (*S*)-(−)-1-(4-chlorophenyl)-*N*-[(pyridin-2-yl)-methylidene]ethan-1-amine. Displacement ellipsoids are drawn at the 30% probability level; H atoms are given as spheres of arbitrary radius.

Table 1
Hydrogen-bond geometry (Å, °) for the $PdCl_2$ complex.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Cl2^{i}	0.95	2.83	3.4765 (5)	126
C6—H6···Cl2^{ii}	0.95	2.73	3.5996 (5)	153
C7—H7···Cl1	1.00	2.80	3.318 (10)	113
C8—H8*A*···Cl1	0.98	2.78	3.464 (11)	127
C14—H14···Cl2	0.95	2.63	3.207 (11)	120

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

3. Supramolecular features

Packing analysis of the imine ligand reveals no significant hydrogen-bonding interactions, and π–π stacking is negligible: centroid-to-centroid separations exceed 4.50 Å, larger than the typical range of 3.30–3.80 Å for these interactions (Fig. 3).

In the crystal of the palladium complex, some short intermolecular contacts organize the packing into extended motifs.

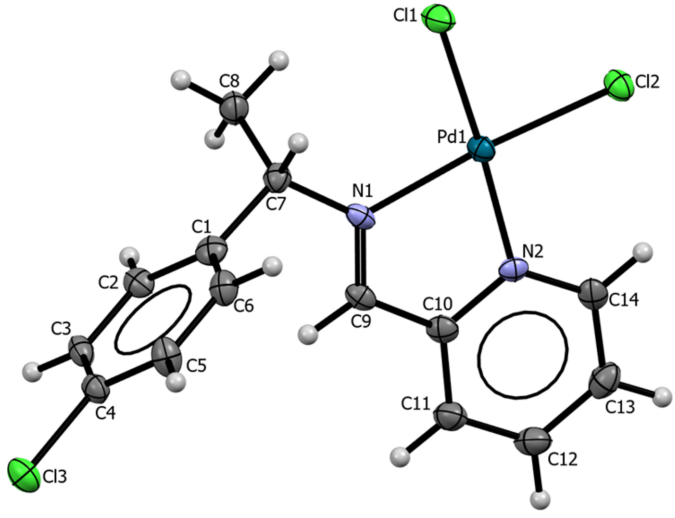


Figure 2
Molecular structure of the dichlorido{(*S*)-(−)-1-(4-chlorophenyl)-*N*-[(pyridin-2-yl)methylidene]ethan-1-amine}palladium(II) complex. Displacement ellipsoids are drawn at the 30% probability level; H atoms are given as spheres of arbitrary radius.

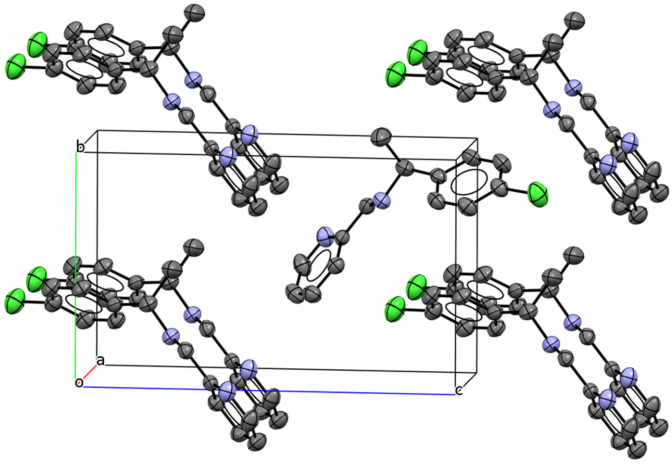


Figure 3
Crystal packing of the imine ligand. Displacement ellipsoids are as in Fig. 1; all H atoms have been omitted for clarity.

Numerical data of intermolecular C—H···Cl interactions are listed in Table 1 (entries 1–2), and additional interactions are observed [Pd1···Cl2($x - \frac{1}{2}$, $-y + \frac{3}{2}$, $-z + 1$) = 3.798 (3) Å; Pd1···Cl3($-x + 2$, $y - \frac{1}{2}$, $-z + \frac{3}{2}$) = 3.80 (1) Å]. Weak π–π stacking is present here with centroid-to-centroid separations falling within the typical range of 3.30–3.80 Å: the centroid of the C6–C1–C2–C3–C4–C5 ring is located 3.5915 (5) Å from the centroid of the N2–C14–C13–C12–C11–C10 ring with a slippage of 0.356 Å. A short intermolecular contact Pd1···H13 = 2.905 Å is also identified. All of these contacts contribute to the packing of the crystal (Fig. 4). The shortest Pd···Pd separations exceed 6.00 Å, indicating the absence of significant metal–metal interactions.

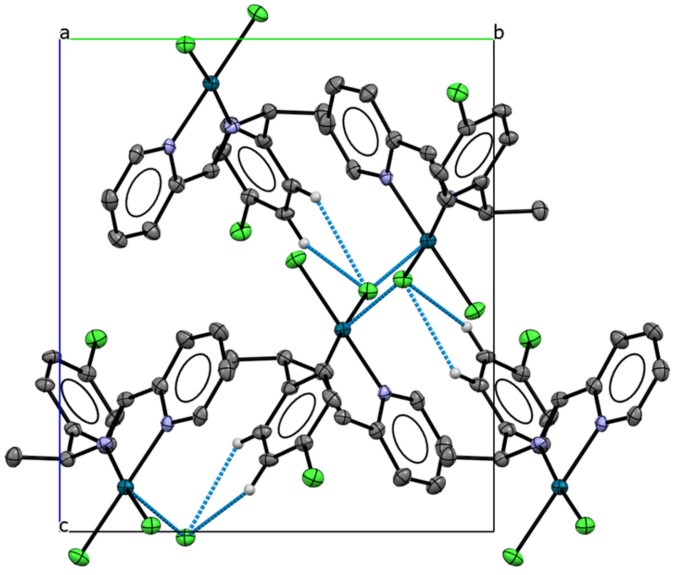


Figure 4
Crystal packing of the Pd^{II} complex; hydrogen bonds are shown as dashed lines. Displacement ellipsoids are drawn at the 30% probability level. All H atoms not involved in these interactions have been omitted for clarity

4. Database survey

A search in the Cambridge Structural Database (CSD, Version 5.42, April 2025; Groom *et al.*, 2016) revealed numerous Pd^{II} complexes featuring N^N bidentate ligands with a square-planar coordination environment. Representative examples include GUTRAS, a palladium complex where the metal is coordinated by pyridine–oxazoline (Pyox) moieties bearing binaftyl and biaryl bridges (Guo *et al.*, 2025); AJADOH, containing sterically hindered Pyox ligands bound to $PdCl_2$ in a *cis* configuration (Chen *et al.*, 2019); IBEKUY, which displays the typical square-planar environment expected for [$Pd^{II}Cl_2L$] complexes (Gutiérrez *et al.*, 2015). Complexes ITAJEV, ITAJIZ, and ITAJOF, derived from (imino)pyridine ligands, show an N^N bidentate coordination mode leading to slightly distorted square-planar environments (Ngcobo *et al.*, 2021). Similarly, IVIREM exhibits elongated Pd—N bond lengths attributed to steric and electron-donating effects (Tang *et al.*, 2016). KELRAV contains an *R*-configured Pyox ligand coordinating in a planar fashion (Dodd *et al.*, 2006). Other examples include MOBSED and MOBSUT, which incorporate hemilabile 2-(1*H*-imidazol-2-yl)pyridine and 2-(oxazol-2-yl)pyridine ligands forming five-membered chelate rings (Eseola *et al.*, 2014); ONACEO, ONACIS, and ONACOY, which feature moderately bulky Pyox ligands in a square-planar $PdCl_2$ array (Tian *et al.*, 2021); PAGJAJ and PAGJEN show that Pd—N(pyridine) bonds are typically longer than Pd—N(imine) bonds due to the *trans* influence of coordinating substituents (Bastero *et al.*, 2004). PIKJEA presents a distorted four-coordinate environment involving two chlorido ligands and two nitrogen donors of an *R*-enantiomeric ligand (De Crisci *et al.*, 2013); QASXIR and QASXOX display *cis* chelation and near-ideal square-planar geometry, with short Pd···Pd intermolecular contacts within the crystal structure (Mishnev *et al.*, 2000); QEJSAZ, where C—H···Cl and C—H···O interactions consolidate the packing of the Pd^{II} complex (Svensson *et al.*, 1999), RILLUW, corresponding to a $PdCl_2$ complex employed in a novel enantioselective Pd-catalyzed 6-endo aminoacetoxylation of unactivated alkenes (Qi *et al.*, 2018); RUCXOF01 and RUCXUL01, involve quinoline-oxazoline (Quox) ligands, which promote a *cis* square-planar coordination environment around Pd^{II}. This arrangement has been associated with enhanced enantioselective control in catalytic transformations; WUMLEV and WUMLIZ show a slightly tetrahedrally distorted square-planar environment, with donor atoms deviating from the coordination plane (Bastero *et al.*, 2002).

5. Synthesis and crystallization

Under solvent-free conditions, a 1:1 molar mixture of (*S*)-(−)-1-(4-chlorophenyl)ethan-1-amine (0.222 g, 1.42 mmol) and 2-pyridinecarboxaldehyde (0.152 g, 1.42 mmol) was stirred at room temperature, producing a white solid. The crude product was recrystallized twice from hexane/CH_2Cl_2 to give colorless crystals of the ligand.

Table 2
Experimental details.

	$C_{14}H_{13}ClN_2$	$[PdCl_2(C_{14}H_{13}ClN_2)]$
Crystal data		
M_r	244.71	422.01
Crystal system, space group	Monoclinic, $P2_1$	Orthorhombic, $P2_12_12_1$
Temperature (K)	293	150
a, b, c (Å)	5.6763 (2), 8.5159 (4), 13.7606 (6)	10.2429 (9), 11.4188 (14), 12.9466 (17)
α, β, γ (°)	90, 89.226 (4), 90	90, 90, 90
V (Å^3)	665.11 (5)	1514.3 (3)
Z	2	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.27	1.74
Crystal size (mm)	0.7 × 0.59 × 0.08	0.62 × 0.24 × 0.12
Data collection		
Diffractometer	Xcalibur, Atlas, Gemini	Xcalibur, Atlas, Gemini
Absorption correction	Gaussian [*CrysAlis PRO* (Rigaku OD, 2015) using a multifaceted crystal model based on expressions derived by Clark & Reid (1995)]	Analytical [*CrysAlis PRO* (Rigaku OD, 2015) using a multifaceted crystal model based on expressions derived by Clark & Reid (1995)]
T_{min}, T_{max}	0.923, 0.989	0.870, 0.966
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	41587, 3728, 2109	16724, 3328, 2665
R_{int}	0.050	0.064
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.694	0.641
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.123, 1.01	0.046, 0.092, 1.07
No. of reflections	3728	3328
No. of parameters	155	182
No. of restraints	1	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.15, −0.19	1.38, −0.67
Absolute structure	Flack x determined using 770 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)	Flack x determined using 1011 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.03 (3)	−0.06 (3)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS* (Sheldrick, 2008), *OLEX2.solve* (Bourhis *et al.*, 2015), *SHELXL* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

For complex formation, a solution of bis(benzonitrile)-palladium(II) chloride (0.100 g, 0.40 mmol) in CH_2Cl_2 (5 ml) was combined with a CH_2Cl_2 solution (10 ml) of (*S*)-(−)-*N*-[(2-pyridyl)methylidene]-1-(4-chlorophenyl)ethan-1-amine (0.157 g, 0.40 mmol). The mixture was stirred at room temperature for 24 h, during which a light-orange precipitate formed. The solid was collected by filtration and recrystallized from hexane/CH_2Cl_2 to afford light-orange crystals of the Pd^{II} complex.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. For H atoms, U_{iso}(H) was set to 1.2xU_{eq} of the parent carbon for CH and aromatic/amide hydrogen atoms, and to 1.5xU_{eq} for methyl (CH_3) groups. Hydrogen atoms were placed in geometrically idealized positions and refined using a riding model: the tertiary CH attached to C7 (H7) was refined as a ternary CH in riding mode, and the aromatic/amide hydrogen atoms attached to C2, C3, C5, C6, C9, C11, C12, C13 and C14 were refined with riding coordinates. The methyl group at C8 (H8*A*, H8*B*, H8*C*) was treated as an idealized methyl and refined as a rotating group.

Acknowledgements

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supporting information

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Crystal structures of (*S*)-(−)-1-(4-chlorophenyl)-*N*-[(pyridin-2-yl)methylidene]ethan-1-amine and its *cis*-dichlorido{(*S*)-(−)-1-(4-chlorophenyl)-*N*-[(pyridin-2-yl)methylidene]ethan-1-amine}palladium(II) complex

Teresa Pacheco-Álvarez, Alejandro Yañez-Cabrera, C. Claudia P. Villamizar, Pankaj Sharma, Bertin Anzaldo, Angel Mendoza and Guadalupe Hernández Téllez

Computing details

(*S*)-(-)-1-(4-Chlorophenyl)-*N*-[(pyridin-2-yl)methylidene]ethan-1-amine (im-i-l_mo)

Crystal data

$C_{14}H_{13}ClN_2$
M_r = 244.71
Monoclinic, $P2_1$
a = 5.6763 (2) Å
b = 8.5159 (4) Å
c = 13.7606 (6) Å
β = 89.226 (4)°
V = 665.11 (5) Å^3
Z = 2
$F(000)$ = 256
D_x = 1.222 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6050 reflections
θ = 3.6–21.3°
μ = 0.27 mm^{-1}
T = 293 K
Block, colourless
0.7 × 0.59 × 0.08 mm

Data collection

Xcalibur, Atlas, Gemini diffractometer
Detector resolution: 10.5564 pixels mm^{-1}
ω scans
Absorption correction: gaussian [CrysAlisPro (Rigaku OD, 2015) using a multifaceted crystal model based on expressions derived by Clark & Reid (1995)]
T_{min} = 0.923, T_{max} = 0.989
41587 measured reflections
3728 independent reflections
2109 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 29.6°, θ_{min} = 3.0°
h = −7→7
k = −11→11
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.123
S = 1.01
3728 reflections
155 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2 + 0.0411P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack x determined using 770 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.03 (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}
C1	0.0976 (5)	0.3440 (3)	0.0974 (2)	0.0655 (7)
C2	0.0177 (6)	0.4177 (4)	0.0148 (3)	0.0787 (9)
H2	−0.121009	0.475688	0.018249	0.094*
C3	0.1379 (6)	0.4075 (4)	−0.0723 (2)	0.0817 (9)
H3	0.081007	0.457479	−0.127286	0.098*
C4	0.3412 (5)	0.3233 (4)	−0.0769 (2)	0.0761 (8)
C5	0.4257 (5)	0.2472 (4)	0.0028 (3)	0.0803 (9)
H5	0.564010	0.189009	−0.001640	0.096*
C6	0.3029 (5)	0.2578 (4)	0.0903 (2)	0.0737 (8)
H6	0.359586	0.206240	0.144757	0.088*
C7	−0.0352 (6)	0.3630 (4)	0.1930 (2)	0.0787 (9)
H7	−0.202014	0.381664	0.179750	0.094*
C8	0.0618 (11)	0.5022 (5)	0.2504 (3)	0.1252 (17)
H8A	0.222867	0.482028	0.266844	0.188*
H8B	−0.030054	0.516170	0.308868	0.188*
H8C	0.053493	0.595577	0.211571	0.188*
C9	−0.1914 (6)	0.1824 (4)	0.3011 (2)	0.0663 (7)
H9	−0.329443	0.240387	0.295643	0.080*
C10	−0.1902 (5)	0.0462 (3)	0.36642 (19)	0.0594 (6)
C11	−0.0015 (5)	−0.0557 (4)	0.3716 (2)	0.0669 (7)
H11	0.132864	−0.040192	0.333388	0.080*
C12	−0.0170 (6)	−0.1810 (4)	0.4350 (2)	0.0814 (9)
H12	0.106259	−0.252454	0.439271	0.098*
C13	−0.2142 (6)	−0.1989 (4)	0.4910 (3)	0.0869 (10)
H13	−0.227604	−0.281927	0.534612	0.104*
C14	−0.3901 (6)	−0.0935 (5)	0.4818 (3)	0.0886 (11)
H14	−0.524419	−0.107066	0.520363	0.106*
Cl1	0.4936 (2)	0.31179 (16)	−0.18694 (8)	0.1191 (5)
N1	−0.0140 (5)	0.2236 (3)	0.25224 (19)	0.0705 (7)
N2	−0.3844 (4)	0.0290 (4)	0.42131 (19)	0.0780 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0727 (17)	0.0552 (16)	0.0689 (16)	−0.0081 (14)	−0.0095 (13)	0.0102 (13)
C2	0.0786 (19)	0.0687 (19)	0.089 (2)	0.0115 (17)	−0.0045 (17)	0.0194 (17)
C3	0.083 (2)	0.084 (2)	0.078 (2)	0.0062 (18)	−0.0061 (16)	0.0253 (18)
C4	0.0718 (19)	0.079 (2)	0.0778 (19)	−0.0078 (17)	0.0008 (14)	0.0155 (19)
C5	0.0637 (18)	0.085 (2)	0.092 (2)	0.0029 (16)	−0.0035 (16)	0.0198 (19)

C6	0.0710 (18)	0.073 (2)	0.077 (2)	−0.0041 (16)	−0.0151 (15)	0.0194 (16)
C7	0.098 (2)	0.0607 (19)	0.078 (2)	0.0026 (16)	−0.0048 (18)	0.0099 (16)
C8	0.207 (5)	0.075 (3)	0.094 (3)	−0.023 (3)	0.015 (3)	−0.006 (2)
C9	0.0741 (18)	0.0676 (18)	0.0571 (16)	0.0094 (14)	−0.0010 (14)	−0.0044 (14)
C10	0.0662 (16)	0.0598 (15)	0.0521 (14)	−0.0023 (14)	−0.0023 (12)	−0.0068 (13)
C11	0.0653 (16)	0.0674 (18)	0.0679 (18)	0.0005 (15)	0.0007 (13)	−0.0045 (14)
C12	0.086 (2)	0.0700 (19)	0.088 (2)	0.0046 (18)	−0.0147 (17)	0.0074 (19)
C13	0.088 (2)	0.083 (2)	0.090 (2)	−0.013 (2)	−0.0135 (18)	0.026 (2)
C14	0.077 (2)	0.112 (3)	0.077 (2)	−0.013 (2)	0.0066 (16)	0.025 (2)
Cl1	0.1121 (8)	0.1502 (11)	0.0944 (7)	0.0124 (7)	0.0247 (5)	0.0234 (7)
N1	0.0841 (17)	0.0614 (14)	0.0660 (16)	−0.0001 (13)	−0.0015 (13)	0.0072 (12)
N2	0.0670 (15)	0.0952 (19)	0.0717 (16)	0.0036 (14)	0.0064 (12)	0.0052 (16)

Geometric parameters (Å, º)

C1—C2	1.380 (4)	C8—H8B	0.9600
C1—C6	1.380 (4)	C8—H8C	0.9600
C1—C7	1.516 (4)	C9—H9	0.9300
C2—H2	0.9300	C9—C10	1.467 (4)
C2—C3	1.374 (5)	C9—N1	1.253 (4)
C3—H3	0.9300	C10—C11	1.381 (4)
C3—C4	1.359 (5)	C10—N2	1.336 (3)
C4—C5	1.366 (4)	C11—H11	0.9300
C4—Cl1	1.737 (3)	C11—C12	1.380 (5)
C5—H5	0.9300	C12—H12	0.9300
C5—C6	1.386 (5)	C12—C13	1.359 (4)
C6—H6	0.9300	C13—H13	0.9300
C7—H7	0.9800	C13—C14	1.350 (5)
C7—C8	1.531 (6)	C14—H14	0.9300
C7—N1	1.446 (4)	C14—N2	1.334 (5)
C8—H8A	0.9600		
C2—C1—C7	120.1 (3)	C7—C8—H8B	109.5
C6—C1—C2	118.0 (3)	C7—C8—H8C	109.5
C6—C1—C7	121.9 (3)	H8A—C8—H8B	109.5
C1—C2—H2	119.2	H8A—C8—H8C	109.5
C3—C2—C1	121.7 (3)	H8B—C8—H8C	109.5
C3—C2—H2	119.2	C10—C9—H9	118.7
C2—C3—H3	120.5	N1—C9—H9	118.7
C4—C3—C2	119.0 (3)	N1—C9—C10	122.7 (3)
C4—C3—H3	120.5	C11—C10—C9	122.6 (3)
C3—C4—C5	121.3 (3)	N2—C10—C9	115.0 (3)
C3—C4—Cl1	118.9 (3)	N2—C10—C11	122.4 (3)
C5—C4—Cl1	119.8 (3)	C10—C11—H11	120.8
C4—C5—H5	120.4	C12—C11—C10	118.4 (3)
C4—C5—C6	119.3 (3)	C12—C11—H11	120.8
C6—C5—H5	120.4	C11—C12—H12	120.3
C1—C6—C5	120.7 (3)	C13—C12—C11	119.4 (3)

C1—C6—H6	119.6	C13—C12—H12	120.3
C5—C6—H6	119.6	C12—C13—H13	120.8
C1—C7—H7	109.0	C14—C13—C12	118.5 (3)
C1—C7—C8	110.6 (3)	C14—C13—H13	120.8
C8—C7—H7	109.0	C13—C14—H14	117.8
N1—C7—C1	110.9 (3)	N2—C14—C13	124.5 (3)
N1—C7—H7	109.0	N2—C14—H14	117.8
N1—C7—C8	108.2 (3)	C9—N1—C7	117.4 (3)
C7—C8—H8A	109.5	C14—N2—C10	116.9 (3)

C1—C2—C3—C4	−0.3 (5)	C8—C7—N1—C9	96.1 (4)
C1—C7—N1—C9	−142.4 (3)	C9—C10—C11—C12	−179.7 (3)
C2—C1—C6—C5	0.6 (5)	C9—C10—N2—C14	−179.9 (3)
C2—C1—C7—C8	−91.5 (4)	C10—C9—N1—C7	−177.9 (3)
C2—C1—C7—N1	148.5 (3)	C10—C11—C12—C13	−1.0 (5)
C2—C3—C4—C5	0.9 (5)	C11—C10—N2—C14	−0.6 (5)
C2—C3—C4—Cl1	−179.6 (3)	C11—C12—C13—C14	0.7 (5)
C3—C4—C5—C6	−0.8 (5)	C12—C13—C14—N2	−0.2 (6)
C4—C5—C6—C1	0.0 (5)	C13—C14—N2—C10	0.2 (5)
C6—C1—C2—C3	−0.4 (5)	Cl1—C4—C5—C6	179.7 (3)
C6—C1—C7—C8	86.6 (4)	N1—C9—C10—C11	−6.7 (4)
C6—C1—C7—N1	−33.4 (4)	N1—C9—C10—N2	172.7 (3)
C7—C1—C2—C3	177.7 (3)	N2—C10—C11—C12	1.0 (4)
C7—C1—C6—C5	−177.5 (3)		

cis-Dichlorido{(*S*)-(-)-1-(4-chlorophenyl)-*N*-[(pyridin-2-yl)methylidene]ethan-1-amine}palladium(II) complex (imilpd_1_mo)

Crystal data

$[PdCl_2(C_{14}H_{13}ClN_2)]$
$M_r = 422.01$
Orthorhombic, $P2_12_12_1$
$a = 10.2429$ (9) Å
$b = 11.4188$ (14) Å
$c = 12.9466$ (17) Å
$V = 1514.3$ (3) Å^3
$Z = 4$
$F(000) = 832$
$D_x = 1.851$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3623 reflections
$\theta = 3.6$–$26.7°$
$\mu = 1.74$ mm^{-1}
$T = 150$ K
Plate, translucent orange
0.62 × 0.24 × 0.12 mm

Data collection

Xcalibur, Atlas, Gemini diffractometer
Detector resolution: 10.5564 pixels mm^{-1}
ω scans
Absorption correction: analytical [CrysAlisPro (Rigaku OD, 2015) using a multifaceted crystal model based on expressions derived by Clark & Reid (1995)]
$T_{min} = 0.870$, $T_{max} = 0.966$
16724 measured reflections
3328 independent reflections
2665 reflections with $I > 2\sigma(I)$
$R_{int} = 0.064$
$\theta_{max} = 27.1°$, $\theta_{min} = 3.1°$
$h = -13 \rightarrow 13$
$k = -14 \rightarrow 14$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.092$
$S = 1.07$
3328 reflections
182 parameters
0 restraints
Primary atom site location: iterative
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 8.4403P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.38$ e Å^{-3}
$\Delta\rho_{min} = -0.67$ e Å^{-3}
Absolute structure: Flack *x* determined using 1011 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.06 (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}
C1	0.4453 (10)	0.5307 (9)	0.7078 (7)	0.033 (2)
C2	0.4209 (10)	0.4661 (9)	0.7983 (7)	0.033 (2)
H2	0.483692	0.410719	0.821343	0.040*
C3	0.3073 (10)	0.4815 (9)	0.8542 (7)	0.033 (2)
H3	0.291881	0.437210	0.915123	0.039*
C4	0.2163 (9)	0.5625 (9)	0.8203 (8)	0.032 (2)
C5	0.2377 (9)	0.6267 (9)	0.7300 (8)	0.038 (3)
H5	0.174424	0.681322	0.706440	0.046*
C6	0.3530 (10)	0.6095 (9)	0.6748 (8)	0.037 (3)
H6	0.367948	0.653067	0.613396	0.044*
C7	0.5713 (10)	0.5176 (8)	0.6472 (8)	0.031 (2)
H7	0.549819	0.533739	0.573198	0.038*
C8	0.6299 (10)	0.3943 (9)	0.6513 (9)	0.039 (3)
H8A	0.706730	0.390586	0.606362	0.059*
H8B	0.564812	0.337268	0.627834	0.059*
H8C	0.655573	0.376058	0.722453	0.059*
C9	0.6734 (9)	0.6515 (8)	0.7680 (6)	0.0279 (17)
H9	0.605894	0.634992	0.816155	0.033*
C10	0.7778 (9)	0.7307 (9)	0.7950 (8)	0.031 (2)
C11	0.7857 (10)	0.7891 (9)	0.8896 (8)	0.040 (3)
H11	0.722366	0.775686	0.941951	0.049*
C12	0.8873 (9)	0.8666 (9)	0.9058 (10)	0.044 (3)
H12	0.895917	0.906679	0.969730	0.053*
C13	0.9756 (11)	0.8846 (9)	0.8274 (9)	0.042 (3)
H13	1.044741	0.939019	0.836551	0.050*
C14	0.9644 (9)	0.8235 (8)	0.7345 (8)	0.034 (2)
H14	1.027010	0.836022	0.681529	0.041*
Cl1	0.7729 (3)	0.5439 (3)	0.4479 (2)	0.0410 (6)

Cl2	1.0184 (2)	0.7101 (2)	0.51194 (19)	0.0354 (6)
Cl3	0.0736 (2)	0.5835 (2)	0.8907 (2)	0.0430 (7)
N1	0.6727 (8)	0.6036 (6)	0.6781 (5)	0.0281 (16)
N2	0.8678 (7)	0.7481 (6)	0.7191 (6)	0.0265 (17)
Pd1	0.82980 (7)	0.65153 (6)	0.59030 (5)	0.02722 (17)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.034 (6)	0.038 (6)	0.028 (5)	−0.004 (4)	−0.008 (4)	−0.004 (4)
C2	0.027 (5)	0.044 (6)	0.028 (5)	−0.002 (5)	−0.003 (4)	−0.003 (5)
C3	0.030 (6)	0.045 (6)	0.023 (5)	−0.010 (5)	0.002 (4)	0.002 (4)
C4	0.024 (5)	0.039 (6)	0.033 (5)	−0.004 (4)	0.003 (4)	−0.001 (5)
C5	0.028 (5)	0.046 (7)	0.042 (6)	0.000 (4)	−0.004 (4)	0.016 (5)
C6	0.034 (6)	0.040 (6)	0.036 (5)	−0.005 (5)	−0.003 (5)	0.007 (4)
C7	0.031 (5)	0.032 (6)	0.031 (5)	−0.005 (4)	−0.003 (4)	0.000 (4)
C8	0.035 (6)	0.035 (6)	0.048 (7)	−0.003 (5)	0.006 (5)	0.003 (5)
C9	0.021 (4)	0.035 (5)	0.027 (4)	0.008 (5)	0.000 (4)	0.002 (4)
C10	0.025 (5)	0.034 (6)	0.036 (6)	0.007 (4)	0.000 (4)	−0.002 (5)
C11	0.037 (6)	0.043 (6)	0.042 (7)	0.002 (5)	0.006 (5)	−0.009 (5)
C12	0.044 (6)	0.044 (6)	0.043 (6)	0.006 (5)	0.003 (6)	−0.013 (7)
C13	0.033 (6)	0.035 (6)	0.058 (7)	−0.003 (5)	−0.009 (5)	−0.003 (5)
C14	0.026 (5)	0.029 (6)	0.047 (6)	0.008 (4)	0.005 (4)	0.006 (5)
Cl1	0.0353 (13)	0.0519 (17)	0.0358 (13)	−0.0044 (12)	0.0051 (11)	−0.0131 (12)
Cl2	0.0282 (13)	0.0432 (15)	0.0350 (13)	−0.0025 (11)	0.0019 (10)	0.0007 (11)
Cl3	0.0304 (13)	0.0540 (17)	0.0447 (17)	0.0026 (12)	0.0069 (12)	0.0025 (13)
N1	0.027 (4)	0.032 (4)	0.025 (4)	0.009 (4)	0.006 (4)	0.002 (3)
N2	0.028 (4)	0.021 (4)	0.031 (4)	0.007 (3)	0.000 (3)	−0.001 (3)
Pd1	0.0225 (3)	0.0317 (3)	0.0274 (3)	0.0018 (3)	0.0002 (3)	−0.0006 (3)

Geometric parameters (Å, º)

C1—C2	1.407 (14)	C9—H9	0.9500
C1—C6	1.374 (14)	C9—C10	1.443 (13)
C1—C7	1.518 (14)	C9—N1	1.287 (10)
C2—H2	0.9500	C10—C11	1.397 (13)
C2—C3	1.382 (13)	C10—N2	1.362 (12)
C3—H3	0.9500	C11—H11	0.9500
C3—C4	1.385 (13)	C11—C12	1.382 (14)
C4—C5	1.398 (13)	C12—H12	0.9500
C4—Cl3	1.739 (10)	C12—C13	1.375 (15)
C5—H5	0.9500	C13—H13	0.9500
C5—C6	1.394 (14)	C13—C14	1.395 (14)
C6—H6	0.9500	C14—H14	0.9500
C7—H7	1.0000	C14—N2	1.327 (12)
C7—C8	1.531 (13)	Cl1—Pd1	2.291 (3)
C7—N1	1.484 (12)	Cl2—Pd1	2.282 (3)
C8—H8A	0.9800	N1—Pd1	2.045 (8)

C8—H8B	0.9800	N2—Pd1	2.036 (8)
C8—H8C	0.9800		
C2—C1—C7	122.0 (9)	C10—C9—H9	120.3
C6—C1—C2	118.7 (10)	N1—C9—H9	120.3
C6—C1—C7	119.3 (9)	N1—C9—C10	119.3 (9)
C1—C2—H2	119.4	C11—C10—C9	123.6 (9)
C3—C2—C1	121.3 (10)	N2—C10—C9	114.7 (8)
C3—C2—H2	119.4	N2—C10—C11	121.6 (9)
C2—C3—H3	120.5	C10—C11—H11	120.6
C2—C3—C4	119.1 (9)	C12—C11—C10	118.8 (10)
C4—C3—H3	120.5	C12—C11—H11	120.6
C3—C4—C5	120.6 (9)	C11—C12—H12	120.7
C3—C4—Cl3	119.5 (8)	C13—C12—C11	118.6 (11)
C5—C4—Cl3	119.9 (8)	C13—C12—H12	120.7
C4—C5—H5	120.4	C12—C13—H13	119.7
C6—C5—C4	119.2 (9)	C12—C13—C14	120.5 (10)
C6—C5—H5	120.4	C14—C13—H13	119.7
C1—C6—C5	121.1 (9)	C13—C14—H14	119.5
C1—C6—H6	119.5	N2—C14—C13	121.0 (9)
C5—C6—H6	119.5	N2—C14—H14	119.5
C1—C7—H7	106.8	C7—N1—Pd1	125.3 (6)
C1—C7—C8	114.0 (8)	C9—N1—C7	122.0 (8)
C8—C7—H7	106.8	C9—N1—Pd1	112.6 (7)
N1—C7—C1	112.9 (8)	C10—N2—Pd1	112.5 (6)
N1—C7—H7	106.8	C14—N2—C10	119.4 (8)
N1—C7—C8	109.0 (8)	C14—N2—Pd1	128.1 (7)
C7—C8—H8A	109.5	Cl2—Pd1—Cl1	90.85 (9)
C7—C8—H8B	109.5	N1—Pd1—Cl1	95.9 (2)
C7—C8—H8C	109.5	N1—Pd1—Cl2	172.6 (2)
H8A—C8—H8B	109.5	N2—Pd1—Cl1	176.3 (2)
H8A—C8—H8C	109.5	N2—Pd1—Cl2	92.5 (2)
H8B—C8—H8C	109.5	N2—Pd1—N1	80.8 (3)
C1—C2—C3—C4	−0.1 (15)	C9—C10—C11—C12	−177.5 (9)
C1—C7—N1—C9	24.3 (12)	C9—C10—N2—C14	177.0 (8)
C1—C7—N1—Pd1	−159.7 (6)	C9—C10—N2—Pd1	−1.8 (10)
C2—C1—C6—C5	0.7 (15)	C10—C9—N1—C7	177.4 (8)
C2—C1—C7—C8	32.0 (13)	C10—C9—N1—Pd1	0.9 (10)
C2—C1—C7—N1	−93.0 (11)	C10—C11—C12—C13	0.9 (15)
C2—C3—C4—C5	0.9 (15)	C11—C10—N2—C14	−1.0 (13)
C2—C3—C4—Cl3	−179.5 (7)	C11—C10—N2—Pd1	−179.8 (7)
C3—C4—C5—C6	−0.9 (15)	C11—C12—C13—C14	−1.6 (16)
C4—C5—C6—C1	0.1 (16)	C12—C13—C14—N2	0.9 (15)
C6—C1—C2—C3	−0.7 (15)	C13—C14—N2—C10	0.4 (13)
C6—C1—C7—C8	−149.2 (10)	C13—C14—N2—Pd1	178.9 (7)
C6—C1—C7—N1	85.8 (11)	Cl3—C4—C5—C6	179.5 (8)
C7—C1—C2—C3	178.1 (9)	N1—C9—C10—C11	178.5 (9)

C7—C1—C6—C5	−178.1 (9)	N1—C9—C10—N2	0.6 (13)
C8—C7—N1—C9	−103.4 (10)	N2—C10—C11—C12	0.3 (15)
C8—C7—N1—Pd1	72.6 (9)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Cl2^{i}	0.95	2.83	3.4765 (5)	126
C6—H6···Cl2^{ii}	0.95	2.73	3.5996 (5)	153
C7—H7···Cl1	1.00	2.80	3.318 (10)	113
C8—H8*A*···Cl1	0.98	2.78	3.464 (11)	127
C14—H14···Cl2	0.95	2.63	3.207 (11)	120

Symmetry codes: (i) −*x*+3/2, −*y*+1, *z*+1/2; (ii) *x*−1/2, −*y*+3/2, −*z*+1.