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Bis[2-phenyl-1-(phenyliminio)isoindoline] di- μ -chlorido-bis[dichlorido-palladate(II)] benzene disolvate

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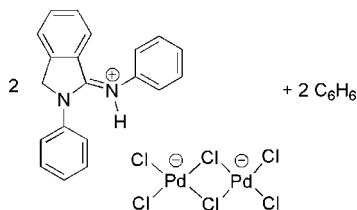
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 Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.039; wR factor = 0.094; data-to-parameter ratio = 22.3.

In the title compound, $(\text{C}_{20}\text{H}_{17}\text{N}_2)_2[\text{Pd}_2\text{Cl}_6] \cdot 2\text{C}_6\text{H}_6$, the dichlorido-bridged $[\text{Pd}_2\text{Cl}_6]^{2-}$ anion lies across an inversion center with each Pd^{II} ion in a slightly distorted square-planar environment. In the crystal structure, two cations and an anion are connected *via* $\text{N}-\text{H} \cdots \text{Cl}$ hydrogen bonds between the NH groups of the iminioisoindoline cations and terminal Cl atoms of a hexachloridodipalladate(II) anion. The Pd–Cl distance of the terminal chloride engaged in hydrogen bonding is slightly longer than the Pd–Cl distance of the adjacent terminal chloride which is not involved in hydrogen bonding.

Related literature

For related literature, see: Bartczak *et al.* (2001); Chitanda *et al.* (2008); Fábry *et al.* (2004); Lassahn *et al.* (2003); Ojwach *et al.* (2007); Schupp *et al.* (2001); Yang *et al.* (2008).



Experimental

Crystal data

$(\text{C}_{20}\text{H}_{17}\text{N}_2)_2[\text{Pd}_2\text{Cl}_6] \cdot 2\text{C}_6\text{H}_6$
 $M_r = 1152.46$
 Triclinic, $P\bar{1}$
 $a = 9.5457$ (3) Å
 $b = 9.9754$ (3) Å
 $c = 14.8002$ (5) Å

$\alpha = 74.270$ (2)°
 $\beta = 80.615$ (2)°
 $\gamma = 63.228$ (2)°
 $V = 1209.74$ (7) Å³
 $Z = 1$
 Mo $K\alpha$ radiation

$\mu = 1.11$ mm⁻¹
 $T = 173$ (2) K

0.22 × 0.18 × 0.05 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
 Absorption correction: ψ scan (SHELXTL; Sheldrick, 2008)
 $T_{\text{min}} = 0.791$, $T_{\text{max}} = 0.946$

18458 measured reflections
 6458 independent reflections
 5322 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.038$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.094$
 $S = 1.04$
 6458 reflections

290 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.82$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.94$ e Å⁻³

Table 1
 Selected geometric parameters (Å, °).

| | | | |
|--------------------------|------------|---------------------------|------------|
| Pd1—Cl2 | 2.2635 (7) | Pd1—Cl3 ⁱ | 2.3292 (7) |
| Pd1—Cl1 | 2.2929 (7) | Pd1—Cl3 | 2.3374 (7) |
| Cl2—Pd1—Cl1 | 91.32 (3) | Cl2—Pd1—Cl3 | 176.86 (3) |
| Cl2—Pd1—Cl3 ⁱ | 91.00 (3) | Cl1—Pd1—Cl3 | 91.47 (3) |
| Cl1—Pd1—Cl3 ⁱ | 177.33 (3) | Cl3 ⁱ —Pd1—Cl3 | 86.25 (3) |

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

Table 2
 Hydrogen-bond geometry (Å, °).

| $D-\text{H} \cdots A$ | $D-\text{H}$ | $\text{H} \cdots A$ | $D \cdots A$ | $D-\text{H} \cdots A$ |
|---|--------------|---------------------|--------------|-----------------------|
| $\text{N2}-\text{H2} \cdots \text{Cl1}$ | 0.88 | 2.37 | 3.242 (2) | 171 |

Symmetry codes: .

Data collection: COLLECT (Nonius, 1998); cell refinement: SCALEPACK (Otwinowski & Minor, 1997); data reduction: DENZO (Otwinowski & Minor 1997) and SCALEPACK; program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2628).

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supporting information

Acta Cryst. (2008). E64, m907–m908 [doi:10.1107/S1600536808017005]

Bis[2-phenyl-1-(phenyliminio)isoindoline] di- μ -chlorido-bis-[dichloridopalladate(II)] benzene disolvate

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S1. Comment

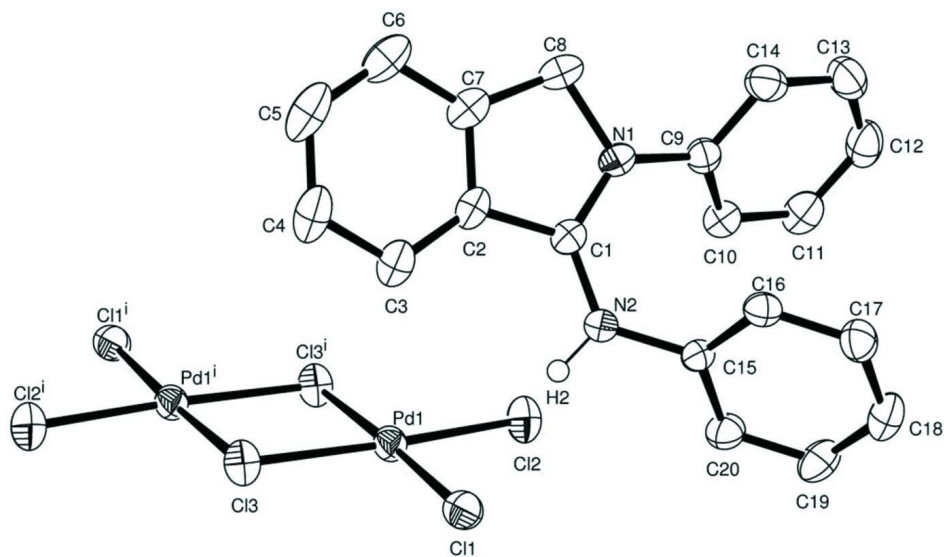
As part of the ongoing research in our laboratory directed at the synthesis of substituted palladacycles incorporating iminoisoindolines (Chitanda *et al.*, 2008), the title compound, **I**, was obtained by reaction of 1-phenylimino-2-phenylisoindoline with dichloropalladium(II) in the presence of HCl. The bis-iminoisoindolinium hexachlorodipalladate complex crystallizes with two molecules of benzene in the unit cell of the triclinic space group $P\bar{1}$. The crystal structure of **I** is stabilized by a system of intermolecular hydrogen bonds between the imine NH atoms of the iminoisoindolinium cation and the terminal chloride atoms in the hexachlorodipalladate(II) anion. The $\text{Pd}_2\text{Cl}_6^{2-}$ anion lies across an inversion center and has the expected planar dichloro-bridged structure with the Pd—Cl distance of the terminal chloride engaged in hydrogen bonding being slightly longer at 2.2929 (7) Å than the Pd—Cl distance of the adjacent terminal chloride at 2.2635 (7) Å which does not show any H-bonding. In previously reported structures incorporating a $\text{Pd}_2\text{Cl}_6^{2-}$ anion, the anion most often lies across an inversion center (Bartczak *et al.*, 2001; Fábry *et al.*, 2004; Lassahn *et al.*, 2003; Ojwach *et al.*, 2007; Schupp *et al.*, 2001; Yang *et al.*, 2008). The molecular structure and packing of the title compound is shown in Figs. 1 and 2.

S2. Experimental

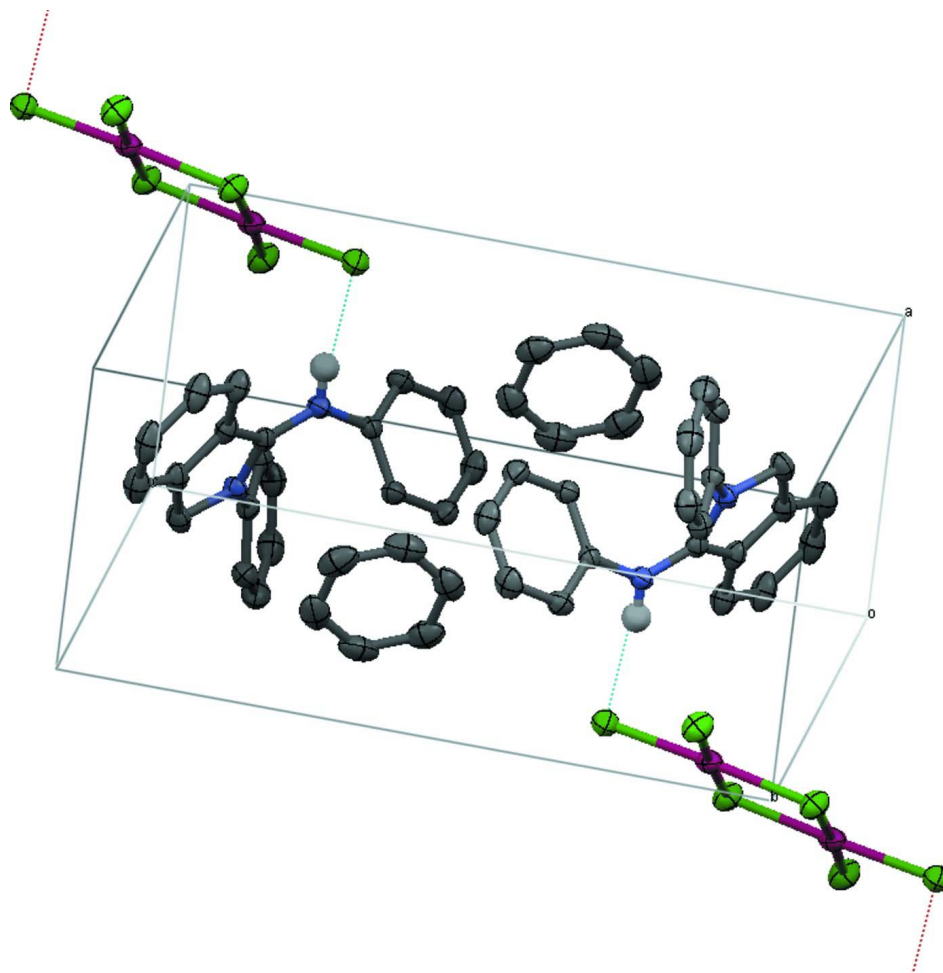
The title compound was synthesized by reaction of 1-phenylimino-2-phenylisoindoline with dichloropalladium(II) in the presence of HCl in dichloromethane. Single crystals were obtained by slow evaporation from a benzene solution at ambient temperature.

S3. Refinement

H atoms were placed in calculated positions with U_{iso} constrained to be 1.2 times U_{eq} of the carrier atom for all hydrogen atoms.

**Figure 1**

Molecular structure of the title compound with thermal ellipsoids at the 50% probability level. H atoms not participating in H-bonding are omitted for clarity. Only the symmetry unique cation is shown [symmetry code: (i) $-x, -y+2, z$].

**Figure 2**

Packing of the title compound with hydrogen bonds shown with dashed lines. H atoms not participating in H-bonding are omitted for clarity.

Bis[2-phenyl-1-(phenyliminio)isoindoline] di- μ -chlorido-bis[dichloridopalladate(II)] benzene disolvate

Crystal data

$(C_{20}H_{17}N_2)_2[Pd_2Cl_6] \cdot 2C_6H_6$

$M_r = 1152.46$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 9.5457(3)\ \text{\AA}$

$b = 9.9754(3)\ \text{\AA}$

$c = 14.8002(5)\ \text{\AA}$

$\alpha = 74.270(2)^\circ$

$\beta = 80.615(2)^\circ$

$\gamma = 63.228(2)^\circ$

$V = 1209.74(7)\ \text{\AA}^3$

$Z = 1$

$F(000) = 580$

$D_x = 1.582\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5512 reflections

$\theta = 1.0\text{--}29.1^\circ$

$\mu = 1.12\ \text{mm}^{-1}$

$T = 173\ \text{K}$

Plate, orange

$0.22 \times 0.18 \times 0.05\ \text{mm}$

Data collection

Bruker–Nonius KappaCCD
diffractometer

Radiation source: fine-focus sealed tube

Horizontally mounted graphite crystal
monochromator

Detector resolution: 9 pixels mm⁻¹

φ scans and ω scans with κ offsets

Absorption correction: ψ scan

(*SHELXTL*; Sheldrick, 2008)

$T_{\min} = 0.791$, $T_{\max} = 0.946$

18458 measured reflections

6458 independent reflections

5322 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$

$\theta_{\max} = 29.1^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -13 \rightarrow 11$

$k = -13 \rightarrow 13$

$l = -20 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.094$

$S = 1.04$

6458 reflections

290 parameters

0 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

$w = 1/[\sigma^2(F_o^2) + (0.0328P)^2 + 1.4367P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.82 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.94 \text{ e } \text{\AA}^{-3}$

Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kFc[1 + 0.001xkFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0061 (7)

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. 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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|-------------|---------------|----------------------------------|
| Pd1 | 0.00603 (2) | 0.87175 (2) | 0.103892 (15) | 0.02846 (8) |
| Cl1 | 0.05538 (8) | 0.85027 (8) | 0.25493 (5) | 0.03459 (15) |
| Cl2 | -0.03111 (9) | 0.65391 (8) | 0.14749 (5) | 0.03895 (17) |
| Cl3 | 0.04870 (8) | 1.09399 (8) | 0.05063 (5) | 0.03515 (15) |
| N1 | 0.5133 (2) | 0.3157 (3) | 0.18312 (15) | 0.0261 (4) |
| N2 | 0.3165 (2) | 0.4983 (2) | 0.26541 (15) | 0.0263 (4) |
| H2 | 0.2504 | 0.5964 | 0.2559 | 0.032* |
| C1 | 0.4296 (3) | 0.4577 (3) | 0.19937 (17) | 0.0243 (5) |
| C2 | 0.4887 (3) | 0.5622 (3) | 0.13560 (18) | 0.0284 (5) |
| C3 | 0.4427 (4) | 0.7181 (4) | 0.1276 (2) | 0.0355 (6) |
| H3 | 0.3529 | 0.7768 | 0.1619 | 0.043* |
| C4 | 0.5329 (4) | 0.7844 (4) | 0.0678 (2) | 0.0435 (7) |
| H4 | 0.5049 | 0.8908 | 0.0608 | 0.052* |
| C5 | 0.6646 (4) | 0.6971 (4) | 0.0176 (2) | 0.0471 (8) |

| | | | | |
|-----|------------|-------------|--------------|------------|
| H5 | 0.7254 | 0.7453 | -0.0223 | 0.057* |
| C6 | 0.7087 (4) | 0.5426 (4) | 0.0246 (2) | 0.0418 (7) |
| H6 | 0.7979 | 0.4843 | -0.0103 | 0.050* |
| C7 | 0.6181 (3) | 0.4753 (3) | 0.08448 (19) | 0.0317 (6) |
| C8 | 0.6411 (3) | 0.3118 (3) | 0.1107 (2) | 0.0332 (6) |
| H8A | 0.6299 | 0.2787 | 0.0560 | 0.040* |
| H8B | 0.7455 | 0.2421 | 0.1366 | 0.040* |
| C9 | 0.4809 (3) | 0.1840 (3) | 0.21669 (18) | 0.0267 (5) |
| C10 | 0.3283 (3) | 0.1986 (3) | 0.22435 (19) | 0.0300 (5) |
| H10 | 0.2433 | 0.2972 | 0.2072 | 0.036* |
| C11 | 0.3010 (4) | 0.0682 (4) | 0.2573 (2) | 0.0381 (6) |
| H11 | 0.1967 | 0.0770 | 0.2640 | 0.046* |
| C12 | 0.4264 (4) | -0.0752 (4) | 0.2804 (2) | 0.0428 (7) |
| H12 | 0.4072 | -0.1643 | 0.3037 | 0.051* |
| C13 | 0.5781 (4) | -0.0902 (3) | 0.2699 (2) | 0.0425 (7) |
| H13 | 0.6633 | -0.1894 | 0.2840 | 0.051* |
| C14 | 0.6063 (3) | 0.0394 (3) | 0.2387 (2) | 0.0352 (6) |
| H14 | 0.7109 | 0.0299 | 0.2324 | 0.042* |
| C15 | 0.2902 (3) | 0.4009 (3) | 0.34982 (17) | 0.0233 (5) |
| C16 | 0.4162 (3) | 0.2904 (3) | 0.40237 (18) | 0.0269 (5) |
| H16 | 0.5201 | 0.2780 | 0.3821 | 0.032* |
| C17 | 0.3886 (3) | 0.1979 (3) | 0.4851 (2) | 0.0338 (6) |
| H17 | 0.4743 | 0.1212 | 0.5216 | 0.041* |
| C18 | 0.2376 (4) | 0.2166 (4) | 0.5149 (2) | 0.0379 (6) |
| H18 | 0.2198 | 0.1519 | 0.5713 | 0.045* |
| C19 | 0.1122 (3) | 0.3291 (4) | 0.4628 (2) | 0.0381 (7) |
| H19 | 0.0083 | 0.3422 | 0.4839 | 0.046* |
| C20 | 0.1372 (3) | 0.4233 (3) | 0.3796 (2) | 0.0314 (6) |
| H20 | 0.0512 | 0.5014 | 0.3439 | 0.038* |
| C21 | 0.6984 (4) | 0.4602 (4) | 0.4106 (3) | 0.0488 (8) |
| H21 | 0.6432 | 0.5641 | 0.4167 | 0.059* |
| C22 | 0.7139 (4) | 0.3430 (4) | 0.4878 (3) | 0.0457 (8) |
| H22 | 0.6699 | 0.3660 | 0.5472 | 0.055* |
| C23 | 0.7927 (4) | 0.1921 (4) | 0.4801 (3) | 0.0455 (8) |
| H23 | 0.8031 | 0.1110 | 0.5338 | 0.055* |
| C24 | 0.8565 (4) | 0.1594 (4) | 0.3940 (3) | 0.0480 (8) |
| H24 | 0.9110 | 0.0553 | 0.3883 | 0.058* |
| C25 | 0.8418 (4) | 0.2765 (5) | 0.3164 (3) | 0.0532 (9) |
| H25 | 0.8862 | 0.2535 | 0.2571 | 0.064* |
| C26 | 0.7618 (4) | 0.4292 (5) | 0.3246 (3) | 0.0523 (9) |
| H26 | 0.7514 | 0.5109 | 0.2712 | 0.063* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Pd1 | 0.02505 (11) | 0.02529 (12) | 0.03109 (13) | -0.00905 (8) | -0.00203 (8) | -0.00290 (8) |
| Cl1 | 0.0361 (3) | 0.0310 (3) | 0.0325 (3) | -0.0106 (3) | -0.0012 (3) | -0.0077 (3) |
| Cl2 | 0.0451 (4) | 0.0345 (4) | 0.0398 (4) | -0.0227 (3) | -0.0061 (3) | 0.0001 (3) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C13 | 0.0404 (4) | 0.0322 (3) | 0.0349 (4) | -0.0187 (3) | -0.0071 (3) | -0.0019 (3) |
| N1 | 0.0222 (10) | 0.0309 (11) | 0.0263 (11) | -0.0128 (9) | 0.0024 (8) | -0.0077 (9) |
| N2 | 0.0240 (10) | 0.0234 (10) | 0.0266 (11) | -0.0076 (8) | 0.0017 (8) | -0.0045 (8) |
| C1 | 0.0226 (11) | 0.0292 (12) | 0.0228 (12) | -0.0124 (10) | -0.0016 (9) | -0.0058 (10) |
| C2 | 0.0307 (13) | 0.0370 (14) | 0.0221 (12) | -0.0210 (11) | -0.0017 (10) | -0.0016 (10) |
| C3 | 0.0442 (16) | 0.0407 (16) | 0.0283 (14) | -0.0262 (14) | 0.0002 (12) | -0.0045 (12) |
| C4 | 0.066 (2) | 0.0516 (19) | 0.0290 (15) | -0.0426 (17) | -0.0017 (14) | -0.0026 (13) |
| C5 | 0.061 (2) | 0.075 (2) | 0.0286 (15) | -0.053 (2) | 0.0020 (14) | -0.0060 (15) |
| C6 | 0.0392 (16) | 0.068 (2) | 0.0314 (15) | -0.0353 (16) | 0.0045 (12) | -0.0124 (14) |
| C7 | 0.0310 (13) | 0.0457 (16) | 0.0257 (13) | -0.0222 (12) | 0.0001 (10) | -0.0100 (12) |
| C8 | 0.0266 (13) | 0.0446 (16) | 0.0312 (14) | -0.0168 (12) | 0.0067 (11) | -0.0145 (12) |
| C9 | 0.0309 (13) | 0.0267 (12) | 0.0231 (12) | -0.0122 (11) | -0.0012 (10) | -0.0069 (10) |
| C10 | 0.0305 (13) | 0.0334 (14) | 0.0291 (13) | -0.0158 (11) | -0.0002 (10) | -0.0087 (11) |
| C11 | 0.0462 (17) | 0.0453 (17) | 0.0333 (15) | -0.0279 (14) | 0.0031 (13) | -0.0128 (13) |
| C12 | 0.069 (2) | 0.0345 (15) | 0.0322 (15) | -0.0291 (15) | 0.0032 (14) | -0.0091 (12) |
| C13 | 0.0541 (19) | 0.0277 (14) | 0.0371 (16) | -0.0095 (13) | -0.0034 (14) | -0.0075 (12) |
| C14 | 0.0335 (14) | 0.0338 (14) | 0.0334 (15) | -0.0079 (12) | -0.0008 (11) | -0.0119 (12) |
| C15 | 0.0239 (11) | 0.0238 (11) | 0.0218 (11) | -0.0102 (9) | 0.0020 (9) | -0.0063 (9) |
| C16 | 0.0230 (11) | 0.0279 (12) | 0.0283 (13) | -0.0088 (10) | -0.0011 (10) | -0.0079 (10) |
| C17 | 0.0376 (15) | 0.0306 (14) | 0.0286 (14) | -0.0117 (12) | -0.0057 (11) | -0.0023 (11) |
| C18 | 0.0493 (17) | 0.0413 (16) | 0.0288 (14) | -0.0287 (14) | 0.0013 (12) | -0.0017 (12) |
| C19 | 0.0328 (14) | 0.0503 (18) | 0.0358 (15) | -0.0254 (14) | 0.0069 (12) | -0.0079 (13) |
| C20 | 0.0234 (12) | 0.0349 (14) | 0.0321 (14) | -0.0103 (11) | 0.0003 (10) | -0.0062 (11) |
| C21 | 0.0351 (16) | 0.0365 (17) | 0.079 (3) | -0.0153 (14) | -0.0067 (16) | -0.0175 (17) |
| C22 | 0.0331 (15) | 0.064 (2) | 0.0496 (19) | -0.0235 (15) | 0.0041 (14) | -0.0259 (17) |
| C23 | 0.0314 (15) | 0.0464 (18) | 0.056 (2) | -0.0190 (14) | -0.0093 (14) | 0.0010 (15) |
| C24 | 0.0276 (14) | 0.0388 (17) | 0.078 (3) | -0.0059 (13) | -0.0101 (15) | -0.0242 (17) |
| C25 | 0.0315 (15) | 0.089 (3) | 0.047 (2) | -0.0249 (18) | 0.0012 (14) | -0.031 (2) |
| C26 | 0.0394 (17) | 0.059 (2) | 0.058 (2) | -0.0292 (17) | -0.0142 (16) | 0.0092 (17) |

Geometric parameters (Å, °)

| | | | |
|----------------------|------------|---------|-----------|
| Pd1—C12 | 2.2635 (7) | C11—C12 | 1.386 (5) |
| Pd1—C11 | 2.2929 (7) | C11—H11 | 0.9500 |
| Pd1—C13 ⁱ | 2.3292 (7) | C12—C13 | 1.374 (5) |
| Pd1—C13 | 2.3374 (7) | C12—H12 | 0.9500 |
| Pd1—Pd1 ⁱ | 3.4060 (4) | C13—C14 | 1.381 (4) |
| C13—Pd1 ⁱ | 2.3292 (7) | C13—H13 | 0.9500 |
| N1—C1 | 1.343 (3) | C14—H14 | 0.9500 |
| N1—C9 | 1.426 (3) | C15—C16 | 1.383 (3) |
| N1—C8 | 1.481 (3) | C15—C20 | 1.388 (3) |
| N2—C1 | 1.327 (3) | C16—C17 | 1.386 (4) |
| N2—C15 | 1.424 (3) | C16—H16 | 0.9500 |
| N2—H2 | 0.8800 | C17—C18 | 1.380 (4) |
| C1—C2 | 1.456 (4) | C17—H17 | 0.9500 |
| C2—C3 | 1.388 (4) | C18—C19 | 1.382 (4) |
| C2—C7 | 1.391 (4) | C18—H18 | 0.9500 |
| C3—C4 | 1.381 (4) | C19—C20 | 1.390 (4) |

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| C3—H3 | 0.9500 | C19—H19 | 0.9500 |
| C4—C5 | 1.397 (5) | C20—H20 | 0.9500 |
| C4—H4 | 0.9500 | C21—C22 | 1.367 (5) |
| C5—C6 | 1.381 (5) | C21—C26 | 1.369 (5) |
| C5—H5 | 0.9500 | C21—H21 | 0.9500 |
| C6—C7 | 1.391 (4) | C22—C23 | 1.374 (5) |
| C6—H6 | 0.9500 | C22—H22 | 0.9500 |
| C7—C8 | 1.490 (4) | C23—C24 | 1.377 (5) |
| C8—H8A | 0.9900 | C23—H23 | 0.9500 |
| C8—H8B | 0.9900 | C24—C25 | 1.371 (5) |
| C9—C10 | 1.385 (4) | C24—H24 | 0.9500 |
| C9—C14 | 1.392 (4) | C25—C26 | 1.393 (5) |
| C10—C11 | 1.386 (4) | C25—H25 | 0.9500 |
| C10—H10 | 0.9500 | C26—H26 | 0.9500 |
| | | | |
| C12—Pd1—C11 | 91.32 (3) | C11—C10—H10 | 120.3 |
| C12—Pd1—C13 ⁱ | 91.00 (3) | C10—C11—C12 | 119.8 (3) |
| C11—Pd1—C13 ⁱ | 177.33 (3) | C10—C11—H11 | 120.1 |
| C12—Pd1—C13 | 176.86 (3) | C12—C11—H11 | 120.1 |
| C11—Pd1—C13 | 91.47 (3) | C13—C12—C11 | 120.9 (3) |
| C13 ⁱ —Pd1—C13 | 86.25 (3) | C13—C12—H12 | 119.6 |
| C12—Pd1—Pd1 ⁱ | 134.20 (2) | C11—C12—H12 | 119.6 |
| C11—Pd1—Pd1 ⁱ | 134.48 (2) | C12—C13—C14 | 119.8 (3) |
| C13 ⁱ —Pd1—Pd1 ⁱ | 43.218 (17) | C12—C13—H13 | 120.1 |
| C13—Pd1—Pd1 ⁱ | 43.030 (18) | C14—C13—H13 | 120.1 |
| Pd1 ⁱ —C13—Pd1 | 93.75 (3) | C13—C14—C9 | 119.6 (3) |
| C1—N1—C9 | 128.5 (2) | C13—C14—H14 | 120.2 |
| C1—N1—C8 | 111.3 (2) | C9—C14—H14 | 120.2 |
| C9—N1—C8 | 119.7 (2) | C16—C15—C20 | 121.3 (2) |
| C1—N2—C15 | 127.3 (2) | C16—C15—N2 | 119.6 (2) |
| C1—N2—H2 | 116.3 | C20—C15—N2 | 119.0 (2) |
| C15—N2—H2 | 116.4 | C15—C16—C17 | 119.0 (2) |
| N2—C1—N1 | 126.8 (2) | C15—C16—H16 | 120.5 |
| N2—C1—C2 | 124.2 (2) | C17—C16—H16 | 120.5 |
| N1—C1—C2 | 108.9 (2) | C18—C17—C16 | 120.5 (3) |
| C3—C2—C7 | 122.0 (3) | C18—C17—H17 | 119.8 |
| C3—C2—C1 | 130.0 (3) | C16—C17—H17 | 119.8 |
| C7—C2—C1 | 107.7 (2) | C17—C18—C19 | 120.1 (3) |
| C4—C3—C2 | 117.3 (3) | C17—C18—H18 | 120.0 |
| C4—C3—H3 | 121.3 | C19—C18—H18 | 120.0 |
| C2—C3—H3 | 121.3 | C18—C19—C20 | 120.4 (3) |
| C3—C4—C5 | 120.9 (3) | C18—C19—H19 | 119.8 |
| C3—C4—H4 | 119.5 | C20—C19—H19 | 119.8 |
| C5—C4—H4 | 119.5 | C15—C20—C19 | 118.7 (3) |
| C6—C5—C4 | 121.7 (3) | C15—C20—H20 | 120.6 |
| C6—C5—H5 | 119.2 | C19—C20—H20 | 120.6 |
| C4—C5—H5 | 119.2 | C22—C21—C26 | 120.6 (3) |
| C5—C6—C7 | 117.7 (3) | C22—C21—H21 | 119.7 |

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| C5—C6—H6 | 121.2 | C26—C21—H21 | 119.7 |
| C7—C6—H6 | 121.2 | C21—C22—C23 | 120.4 (3) |
| C2—C7—C6 | 120.4 (3) | C21—C22—H22 | 119.8 |
| C2—C7—C8 | 109.5 (2) | C23—C22—H22 | 119.8 |
| C6—C7—C8 | 130.0 (3) | C22—C23—C24 | 119.6 (3) |
| N1—C8—C7 | 102.4 (2) | C22—C23—H23 | 120.2 |
| N1—C8—H8A | 111.3 | C24—C23—H23 | 120.2 |
| C7—C8—H8A | 111.3 | C25—C24—C23 | 120.3 (3) |
| N1—C8—H8B | 111.3 | C25—C24—H24 | 119.9 |
| C7—C8—H8B | 111.3 | C23—C24—H24 | 119.9 |
| H8A—C8—H8B | 109.2 | C24—C25—C26 | 119.9 (3) |
| C10—C9—C14 | 120.6 (3) | C24—C25—H25 | 120.0 |
| C10—C9—N1 | 120.8 (2) | C26—C25—H25 | 120.0 |
| C14—C9—N1 | 118.6 (2) | C21—C26—C25 | 119.2 (3) |
| C9—C10—C11 | 119.3 (3) | C21—C26—H26 | 120.4 |
| C9—C10—H10 | 120.3 | C25—C26—H26 | 120.4 |
| | | | |
| Cl1—Pd1—Cl3—Pd1 ⁱ | -178.61 (3) | C8—N1—C9—C10 | -133.0 (3) |
| Cl3 ⁱ —Pd1—Cl3—Pd1 ⁱ | 0.0 | C1—N1—C9—C14 | -144.4 (3) |
| C15—N2—C1—N1 | 21.0 (4) | C8—N1—C9—C14 | 44.9 (3) |
| C15—N2—C1—C2 | -155.2 (2) | C14—C9—C10—C11 | 2.1 (4) |
| C9—N1—C1—N2 | 15.2 (4) | N1—C9—C10—C11 | -180.0 (2) |
| C8—N1—C1—N2 | -173.5 (2) | C9—C10—C11—C12 | -1.2 (4) |
| C9—N1—C1—C2 | -168.2 (2) | C10—C11—C12—C13 | -0.9 (5) |
| C8—N1—C1—C2 | 3.1 (3) | C11—C12—C13—C14 | 2.0 (5) |
| N2—C1—C2—C3 | -1.4 (5) | C12—C13—C14—C9 | -1.1 (4) |
| N1—C1—C2—C3 | -178.2 (3) | C10—C9—C14—C13 | -1.0 (4) |
| N2—C1—C2—C7 | 173.0 (2) | N1—C9—C14—C13 | -178.9 (2) |
| N1—C1—C2—C7 | -3.8 (3) | C1—N2—C15—C16 | 42.8 (4) |
| C7—C2—C3—C4 | -1.3 (4) | C1—N2—C15—C20 | -139.8 (3) |
| C1—C2—C3—C4 | 172.4 (3) | C20—C15—C16—C17 | 1.7 (4) |
| C2—C3—C4—C5 | 0.1 (5) | N2—C15—C16—C17 | 179.1 (2) |
| C3—C4—C5—C6 | 0.9 (5) | C15—C16—C17—C18 | -0.4 (4) |
| C4—C5—C6—C7 | -0.7 (5) | C16—C17—C18—C19 | -0.7 (5) |
| C3—C2—C7—C6 | 1.6 (4) | C17—C18—C19—C20 | 0.6 (5) |
| C1—C2—C7—C6 | -173.4 (3) | C16—C15—C20—C19 | -1.8 (4) |
| C3—C2—C7—C8 | 177.9 (3) | N2—C15—C20—C19 | -179.2 (2) |
| C1—C2—C7—C8 | 3.0 (3) | C18—C19—C20—C15 | 0.6 (4) |
| C5—C6—C7—C2 | -0.5 (4) | C26—C21—C22—C23 | -0.4 (5) |
| C5—C6—C7—C8 | -176.0 (3) | C21—C22—C23—C24 | 0.1 (5) |
| C1—N1—C8—C7 | -1.3 (3) | C22—C23—C24—C25 | 0.1 (5) |
| C9—N1—C8—C7 | 170.9 (2) | C23—C24—C25—C26 | -0.1 (5) |
| C2—C7—C8—N1 | -1.1 (3) | C22—C21—C26—C25 | 0.3 (5) |
| C6—C7—C8—N1 | 174.7 (3) | C24—C25—C26—C21 | -0.1 (5) |
| C1—N1—C9—C10 | 37.6 (4) | | |

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

Hydrogen-bond geometry (Å, °)

| <i>D—H...A</i> | <i>D—H</i> | <i>H...A</i> | <i>D...A</i> | <i>D—H...A</i> |
|----------------|------------|--------------|--------------|----------------|
| N2—H2...C11 | 0.88 | 2.37 | 3.242 (2) | 171 |