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# *trans*-Bis{1-[2-(2,6-diisopropylanilino)-phenyl]-3-isopropylimidazolin-2-yl-idenyl-$\kappa C^2$}diiodidopalladium(II) benzene disolvate

**Christopher G. Daly, Kuldip Singh and Warren B. Cross***

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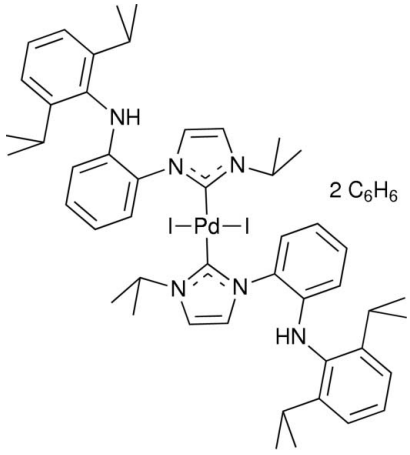
Key indicators: single-crystal X-ray study; $T$ = 150 K; mean $\sigma$(C–C) = 0.012 Å; $R$ factor = 0.063; $wR$ factor = 0.128; data-to-parameter ratio = 17.2.

In the title complex, $[PdI_2(C_{24}H_{31}N_3)_2]\cdot 2C_6H_6$, the $Pd^{2+}$ ion is located on an inversion centre in a slightly distorted square-planar geometry. The angle between the $I_2C_2$ square plane and the mean plane of the *N*-heterocyclic carbene ring is 79.8 (2)°, with I—Pd—C—N torsion angles of −81.1 (6) and −78.2 (5)°. The Pd—carbene and Pd—I distances are 2.016 (6) and 2.5971 (10) Å, respectively.

## Related literature

For a review of *N*-heterocyclic carbenes in late transition metal catalysis, see: Díez-González *et al.* (2009). For the synthesis of the pro-ligand and crystal structures of related complexes, see: Cross *et al.* (2011).




## Experimental

### Crystal data

$[PdI_2(C_{24}H_{31}N_3)_2]\cdot 2C_6H_6$
$M_r$ = 1239.45
Triclinic, $P\overline{1}$
$a$ = 8.998 (4) Å
$b$ = 12.000 (5) Å
$c$ = 13.839 (6) Å
$\alpha$ = 81.572 (8)°
$\beta$ = 78.819 (9)°
$\gamma$ = 76.411 (8)°
$V$ = 1417.0 (10) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 1.46 mm$^{-1}$
$T$ = 150 K
0.16 × 0.11 × 0.06 mm

### Data collection

Bruker APEX 2000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min}$ = 0.338, $T_{max}$ = 0.831
11207 measured reflections
5500 independent reflections
3317 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.106

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.128
$S$ = 0.88
5500 reflections
319 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.92 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.27 e Å$^{-3}$

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* and *SHELXTL* (Sheldrick, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The University of Leicester is thanked for a graduate studentship to CGD.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2410).

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# supporting information

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## *trans*-Bis{1-[2-(2,6-diisopropylanilino)phenyl]-3-isopropylimidazolin-2-ylidenyl-$\kappa C^2$}diiodidopalladium(II) benzene disolvate

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### S1. Comment

Bifunctional catalysis, in which an electrophilic metal and a nucleophilic ligand act together to activate a substrate, can enable reactions that are not possible using classical catalytic transformations that occur only at the metal centre. We are interested in catalysts in which an *N*-heterocyclic carbene ligand tethers a nucleophilic amido donor to the metal. Previously, we have reported tridentate amido-bis(NHC) (CNC) complexes of palladium and platinum, a bidentate amido-NHC (C,*N*-dipp) complex of palladium and a complex [*trans*-($C_{24}H_{31}N_3$)$PdI_2$(py)], in which the amine-NHC ligand binds to Pd only through the carbene (Cross *et al.*, 2011). In the synthesis of [*trans*-($C_{24}H_{31}N_3$)$PdI_2$(py)], we isolated a single-crystal of the title complex.

The solid state structure of the title complex is shown in Fig. 1. Two NHC and two iodide ligands are coordinated to the square planar Pd, which is located at an inversion centre. The Pd-carbene distance of 2.016 (6) Å is *ca* 0.05 Å longer than in the corresponding complex [*trans*-($C_{24}H_{31}N_3$)$PdI_2$(py)] (Cross *et al.*, 2011), as a consequence of the strong *trans*-influence of the NHC ligand.

### S2. Experimental

The title complex was an unexpected by-product in the synthesis of [*trans*-($C_{24}H_{31}N_3$)$PdI_2$(py)] (Cross *et al.*, 2011). Crystals of the title complex were grown by slow evaporation from benzene.

### S3. Refinement

Hydrogen atoms were included in calculated positions at distances C—H = 0.95 to 1.00 Å and N—H = 0.88 Å in riding mode on the bonded atoms with $U_{iso}$(H) set to 1.5 $U_{eq}$(C) for methyl H atoms and 1.2 $U_{eq}$(C/N) for all other H atoms. The final difference map was essentially featureless with some residual electron density in the close proximity of iodine atom.

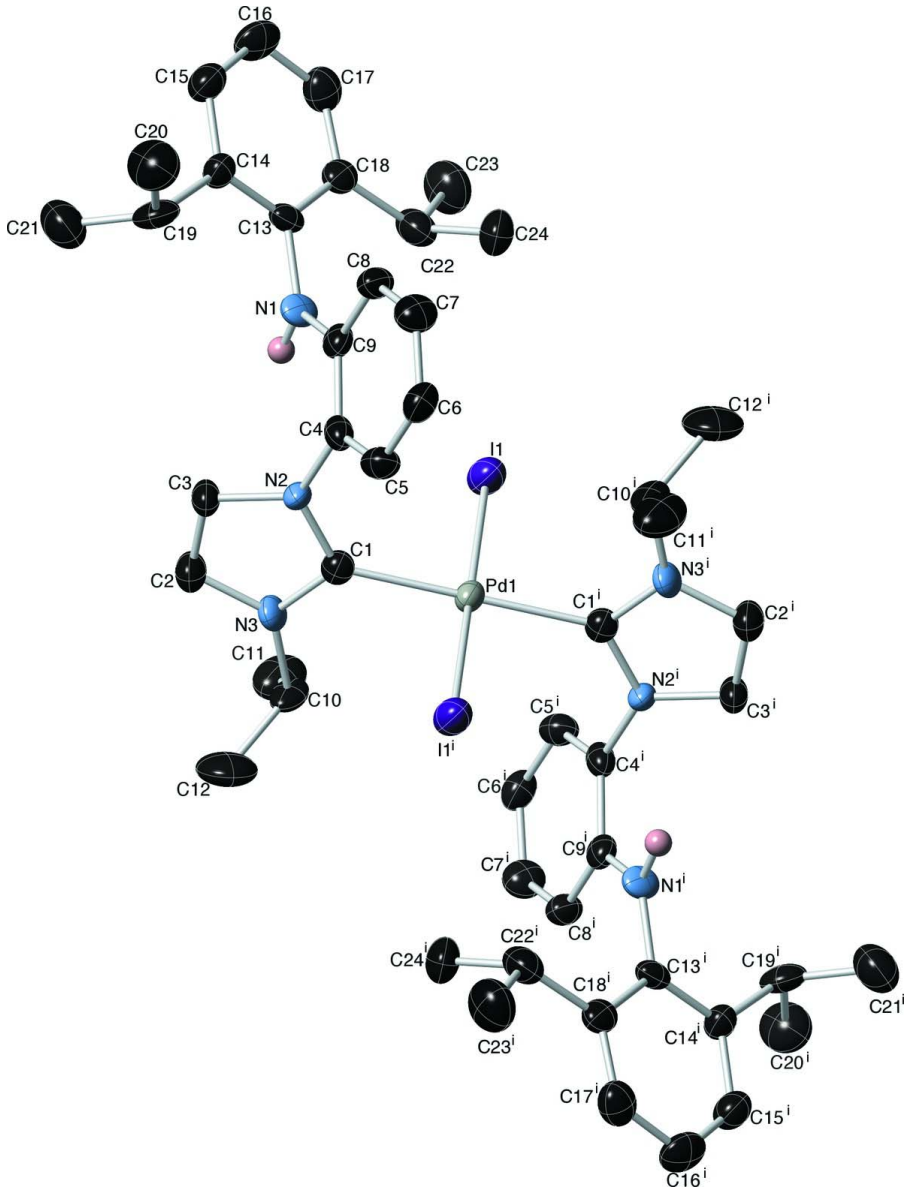


**Figure 1**

The molecular structure of the title complex, with 50% probablity ellipsoids. Two molecules of benzene and H atoms except N—H have been omitted for clarity. Symmetry operation $^{i}$ = -*x* + 2, -*y*, -*z*.

## ***trans*-Bis{1-[2-(2,6-diisopropylanilino)phenyl]-3- isopropylimidazolin-2-ylidenyl-$\kappa C^2$}diiodidopalladium(II) benzene disolvate**

*Crystal data*

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Triclinic, $P\overline{1}$
Hall symbol: -P 1
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$\alpha$ = 81.572 (8)°
$\beta$ = 78.819 (9)°
$\gamma$ = 76.411 (8)°
*V* = 1417.0 (10) Å$^3$
*Z* = 1
*F*(000) = 628
$D_x$ = 1.452 Mg m$^{-3}$

Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 580 reflections
$\theta$ = 2.4–23.4°
$\mu$ = 1.46 mm$^{-1}$
$T$ = 150 K
Block, yellow
0.16 × 0.11 × 0.06 mm

*Data collection*

Bruker APEX 2000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min}$ = 0.338, $T_{max}$ = 0.831
11207 measured reflections
5500 independent reflections
3317 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.106
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 1.8°
$h$ = −11→11
$k$ = −14→14
$l$ = −17→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.128
$S$ = 0.88
5500 reflections
319 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
$w = 1/[\sigma^2(F_o^2) + (0.035P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.92 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.27 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**. 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Pd1 | 1.0000 | 0.0000 | 0.0000 | 0.0245 (2) |
| I1 | 1.08790 (6) | 0.17737 (4) | 0.03915 (4) | 0.03773 (18) |
| N1 | 0.7871 (6) | 0.1906 (5) | 0.3084 (4) | 0.0291 (14) |
| H1 | 0.7552 | 0.2298 | 0.2546 | 0.035* |
| N2 | 0.7258 (6) | 0.0747 (5) | 0.1601 (4) | 0.0245 (13) |
| N3 | 0.6700 (6) | 0.1348 (5) | 0.0142 (4) | 0.0292 (14) |
| C1 | 0.7838 (7) | 0.0734 (5) | 0.0618 (5) | 0.0262 (16) |
| C2 | 0.5403 (8) | 0.1765 (6) | 0.0799 (5) | 0.0382 (19) |
| H2 | 0.4453 | 0.2227 | 0.0639 | 0.046* |
| C3 | 0.5740 (7) | 0.1388 (6) | 0.1722 (5) | 0.0296 (17) |
| H3 | 0.5071 | 0.1533 | 0.2332 | 0.036* |
| C4 | 0.8000 (7) | 0.0118 (6) | 0.2392 (5) | 0.0275 (16) |

| | | | | |
|---|---|---|---|---|
| C5 | 0.8455 (8) | −0.1079 (6) | 0.2430 (5) | 0.0305 (17) |
| H5 | 0.8274 | −0.1468 | 0.1927 | 0.037* |
| C6 | 0.9170 (8) | −0.1699 (6) | 0.3198 (5) | 0.0338 (18) |
| H6 | 0.9530 | −0.2510 | 0.3204 | 0.041* |
| C7 | 0.9359 (8) | −0.1155 (6) | 0.3943 (5) | 0.0370 (19) |
| H7 | 0.9790 | −0.1591 | 0.4491 | 0.044* |
| C8 | 0.8928 (8) | 0.0033 (6) | 0.3907 (5) | 0.0319 (17) |
| H8 | 0.9082 | 0.0398 | 0.4433 | 0.038* |
| C9 | 0.8277 (7) | 0.0710 (6) | 0.3129 (5) | 0.0265 (16) |
| C10 | 0.6882 (8) | 0.1564 (6) | −0.0949 (5) | 0.0354 (19) |
| H10 | 0.7875 | 0.1056 | −0.1231 | 0.043* |
| C11 | 0.6985 (10) | 0.2798 (7) | −0.1303 (6) | 0.059 (3) |
| H11A | 0.5979 | 0.3307 | −0.1104 | 0.088* |
| H11B | 0.7263 | 0.2885 | −0.2026 | 0.088* |
| H11C | 0.7778 | 0.3002 | −0.1008 | 0.088* |
| C12 | 0.5553 (11) | 0.1221 (9) | −0.1295 (6) | 0.071 (3) |
| H12A | 0.5662 | 0.0382 | −0.1172 | 0.107* |
| H12B | 0.5585 | 0.1460 | −0.2006 | 0.107* |
| H12C | 0.4561 | 0.1599 | −0.0930 | 0.107* |
| C13 | 0.7948 (8) | 0.2525 (6) | 0.3867 (5) | 0.0264 (16) |
| C14 | 0.6834 (8) | 0.2513 (6) | 0.4726 (5) | 0.0293 (17) |
| C15 | 0.6914 (8) | 0.3156 (6) | 0.5452 (5) | 0.0370 (19) |
| H15 | 0.6181 | 0.3148 | 0.6047 | 0.044* |
| C16 | 0.8014 (9) | 0.3811 (6) | 0.5353 (6) | 0.043 (2) |
| H16 | 0.8035 | 0.4250 | 0.5866 | 0.052* |
| C17 | 0.9087 (9) | 0.3814 (6) | 0.4490 (6) | 0.041 (2) |
| H17 | 0.9838 | 0.4273 | 0.4415 | 0.049* |
| C18 | 0.9109 (8) | 0.3185 (6) | 0.3745 (5) | 0.0308 (17) |
| C19 | 0.5504 (9) | 0.1905 (6) | 0.4850 (5) | 0.039 (2) |
| H19 | 0.5708 | 0.1432 | 0.4282 | 0.047* |
| C20 | 0.5396 (10) | 0.1076 (7) | 0.5800 (6) | 0.060 (3) |
| H20A | 0.6394 | 0.0533 | 0.5819 | 0.090* |
| H20B | 0.4587 | 0.0649 | 0.5814 | 0.090* |
| H20C | 0.5139 | 0.1514 | 0.6376 | 0.090* |
| C21 | 0.3993 (9) | 0.2773 (7) | 0.4780 (6) | 0.057 (2) |
| H21A | 0.3738 | 0.3240 | 0.5338 | 0.086* |
| H21B | 0.3162 | 0.2366 | 0.4799 | 0.086* |
| H21C | 0.4103 | 0.3276 | 0.4156 | 0.086* |
| C22 | 1.0365 (8) | 0.3122 (7) | 0.2834 (6) | 0.042 (2) |
| H22 | 0.9868 | 0.3124 | 0.2247 | 0.051* |
| C23 | 1.1199 (9) | 0.4138 (7) | 0.2635 (6) | 0.057 (2) |
| H23A | 1.0434 | 0.4866 | 0.2581 | 0.086* |
| H23B | 1.1940 | 0.4070 | 0.2015 | 0.086* |
| H23C | 1.1752 | 0.4124 | 0.3182 | 0.086* |
| C24 | 1.1573 (9) | 0.1988 (7) | 0.2928 (6) | 0.053 (2) |
| H24A | 1.2033 | 0.1944 | 0.3523 | 0.079* |
| H24B | 1.2388 | 0.1961 | 0.2342 | 0.079* |
| H24C | 1.1071 | 0.1336 | 0.2978 | 0.079* |

| | | | | |
|---|---|---|---|---|
| C25 | 0.5767 (11) | 0.4395 (7) | 0.2054 (8) | 0.060 (3) |
| H25 | 0.5044 | 0.3906 | 0.2232 | 0.072* |
| C26 | 0.6599 (13) | 0.4465 (9) | 0.1094 (8) | 0.078 (3) |
| H26 | 0.6473 | 0.4008 | 0.0623 | 0.093* |
| C27 | 0.7615 (12) | 0.5211 (9) | 0.0835 (8) | 0.079 (3) |
| H27 | 0.8176 | 0.5285 | 0.0181 | 0.095* |
| C28 | 0.7792 (12) | 0.5832 (8) | 0.1533 (9) | 0.071 (3) |
| H28 | 0.8497 | 0.6335 | 0.1365 | 0.085* |
| C29 | 0.6973 (12) | 0.5746 (8) | 0.2475 (8) | 0.071 (3) |
| H29 | 0.7099 | 0.6198 | 0.2950 | 0.085* |
| C30 | 0.5984 (10) | 0.5019 (7) | 0.2729 (7) | 0.056 (3) |
| H30 | 0.5439 | 0.4948 | 0.3388 | 0.067* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pd1 | 0.0217 (4) | 0.0279 (4) | 0.0209 (4) | −0.0004 (3) | −0.0016 (3) | −0.0040 (3) |
| I1 | 0.0378 (3) | 0.0405 (3) | 0.0365 (3) | −0.0119 (2) | 0.0001 (2) | −0.0124 (2) |
| N1 | 0.036 (4) | 0.024 (3) | 0.025 (3) | 0.003 (3) | −0.016 (3) | 0.003 (3) |
| N2 | 0.019 (3) | 0.035 (3) | 0.018 (3) | −0.002 (3) | −0.002 (2) | −0.008 (3) |
| N3 | 0.021 (3) | 0.033 (3) | 0.030 (4) | 0.005 (3) | −0.009 (3) | −0.003 (3) |
| C1 | 0.026 (4) | 0.025 (4) | 0.028 (4) | −0.006 (3) | −0.003 (3) | −0.004 (3) |
| C2 | 0.024 (4) | 0.049 (5) | 0.037 (5) | 0.003 (4) | −0.004 (4) | −0.008 (4) |
| C3 | 0.019 (4) | 0.041 (4) | 0.026 (4) | 0.000 (3) | −0.002 (3) | −0.003 (3) |
| C4 | 0.020 (4) | 0.040 (4) | 0.020 (4) | −0.007 (3) | −0.002 (3) | 0.003 (3) |
| C5 | 0.034 (4) | 0.035 (4) | 0.027 (4) | −0.013 (3) | −0.005 (3) | −0.006 (3) |
| C6 | 0.035 (4) | 0.029 (4) | 0.032 (5) | −0.003 (3) | 0.002 (4) | −0.005 (4) |
| C7 | 0.044 (5) | 0.036 (5) | 0.029 (4) | −0.006 (4) | −0.010 (4) | 0.003 (4) |
| C8 | 0.031 (4) | 0.035 (4) | 0.029 (4) | 0.000 (3) | −0.009 (3) | −0.011 (4) |
| C9 | 0.026 (4) | 0.029 (4) | 0.020 (4) | −0.002 (3) | 0.002 (3) | −0.001 (3) |
| C10 | 0.040 (5) | 0.045 (5) | 0.013 (4) | 0.006 (4) | −0.005 (3) | 0.000 (3) |
| C11 | 0.074 (7) | 0.061 (6) | 0.033 (5) | 0.004 (5) | −0.013 (5) | 0.001 (4) |
| C12 | 0.086 (8) | 0.103 (8) | 0.033 (5) | −0.019 (6) | −0.024 (5) | −0.015 (5) |
| C13 | 0.029 (4) | 0.023 (4) | 0.029 (4) | −0.002 (3) | −0.015 (3) | −0.005 (3) |
| C14 | 0.028 (4) | 0.029 (4) | 0.032 (4) | −0.003 (3) | −0.002 (3) | −0.011 (3) |
| C15 | 0.039 (5) | 0.037 (5) | 0.032 (5) | −0.003 (4) | 0.000 (4) | −0.009 (4) |
| C16 | 0.055 (5) | 0.027 (4) | 0.045 (5) | 0.002 (4) | −0.008 (4) | −0.015 (4) |
| C17 | 0.035 (5) | 0.034 (4) | 0.052 (6) | −0.003 (4) | −0.009 (4) | −0.005 (4) |
| C18 | 0.032 (4) | 0.032 (4) | 0.026 (4) | 0.002 (3) | −0.011 (3) | −0.002 (3) |
| C19 | 0.052 (5) | 0.047 (5) | 0.020 (4) | −0.015 (4) | −0.002 (4) | −0.012 (4) |
| C20 | 0.063 (6) | 0.070 (7) | 0.047 (6) | −0.026 (5) | −0.003 (5) | 0.004 (5) |
| C21 | 0.042 (5) | 0.075 (7) | 0.057 (6) | −0.013 (5) | −0.016 (5) | −0.003 (5) |
| C22 | 0.036 (5) | 0.062 (6) | 0.034 (5) | −0.017 (4) | −0.011 (4) | −0.003 (4) |
| C23 | 0.047 (5) | 0.065 (6) | 0.062 (6) | −0.024 (5) | −0.005 (5) | 0.001 (5) |
| C24 | 0.031 (5) | 0.070 (6) | 0.051 (6) | 0.004 (4) | −0.001 (4) | −0.020 (5) |
| C25 | 0.063 (6) | 0.041 (6) | 0.069 (7) | 0.004 (5) | −0.014 (6) | −0.002 (5) |
| C26 | 0.094 (9) | 0.064 (7) | 0.075 (8) | −0.001 (6) | −0.019 (7) | −0.025 (6) |
| C27 | 0.075 (8) | 0.077 (8) | 0.065 (8) | −0.003 (6) | 0.016 (6) | 0.000 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C28 | 0.078 (8) | 0.053 (7) | 0.082 (8) | −0.023 (6) | −0.019 (7) | 0.018 (6) |
| C29 | 0.084 (8) | 0.050 (6) | 0.073 (8) | 0.000 (6) | −0.023 (6) | 0.002 (6) |
| C30 | 0.058 (6) | 0.032 (5) | 0.062 (7) | 0.005 (4) | 0.002 (5) | 0.002 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Pd1—C1 | 2.016 (6) | C14—C19 | 1.513 (9) |
| Pd1—C1$^{i}$ | 2.016 (6) | C15—C16 | 1.377 (9) |
| Pd1—I1$^{i}$ | 2.5971 (10) | C15—H15 | 0.9500 |
| Pd1—I1 | 2.5971 (10) | C16—C17 | 1.382 (10) |
| N1—C9 | 1.390 (8) | C16—H16 | 0.9500 |
| N1—C13 | 1.421 (8) | C17—C18 | 1.359 (9) |
| N1—H1 | 0.8800 | C17—H17 | 0.9500 |
| N2—C1 | 1.359 (8) | C18—C22 | 1.518 (9) |
| N2—C3 | 1.393 (8) | C19—C21 | 1.517 (10) |
| N2—C4 | 1.421 (8) | C19—C20 | 1.530 (10) |
| N3—C1 | 1.338 (8) | C19—H19 | 1.0000 |
| N3—C2 | 1.373 (8) | C20—H20A | 0.9800 |
| N3—C10 | 1.478 (8) | C20—H20B | 0.9800 |
| C2—C3 | 1.359 (9) | C20—H20C | 0.9800 |
| C2—H2 | 0.9500 | C21—H21A | 0.9800 |
| C3—H3 | 0.9500 | C21—H21B | 0.9800 |
| C4—C5 | 1.395 (9) | C21—H21C | 0.9800 |
| C4—C9 | 1.414 (9) | C22—C24 | 1.536 (10) |
| C5—C6 | 1.380 (9) | C22—C23 | 1.542 (10) |
| C5—H5 | 0.9500 | C22—H22 | 1.0000 |
| C6—C7 | 1.355 (9) | C23—H23A | 0.9800 |
| C6—H6 | 0.9500 | C23—H23B | 0.9800 |
| C7—C8 | 1.382 (9) | C23—H23C | 0.9800 |
| C7—H7 | 0.9500 | C24—H24A | 0.9800 |
| C8—C9 | 1.389 (9) | C24—H24B | 0.9800 |
| C8—H8 | 0.9500 | C24—H24C | 0.9800 |
| C10—C11 | 1.508 (10) | C25—C30 | 1.348 (11) |
| C10—C12 | 1.531 (10) | C25—C26 | 1.394 (12) |
| C10—H10 | 1.0000 | C25—H25 | 0.9500 |
| C11—H11A | 0.9800 | C26—C27 | 1.389 (13) |
| C11—H11B | 0.9800 | C26—H26 | 0.9500 |
| C11—H11C | 0.9800 | C27—C28 | 1.355 (13) |
| C12—H12A | 0.9800 | C27—H27 | 0.9500 |
| C12—H12B | 0.9800 | C28—C29 | 1.371 (12) |
| C12—H12C | 0.9800 | C28—H28 | 0.9500 |
| C13—C14 | 1.399 (9) | C29—C30 | 1.353 (12) |
| C13—C18 | 1.425 (9) | C29—H29 | 0.9500 |
| C14—C15 | 1.375 (9) | C30—H30 | 0.9500 |
| | | | |
| C1—Pd1—C1$^{i}$ | 180.0 (5) | C14—C15—C16 | 122.7 (7) |
| C1—Pd1—I1$^{i}$ | 92.78 (18) | C14—C15—H15 | 118.7 |
| C1$^{i}$—Pd1—I1$^{i}$ | 87.22 (18) | C16—C15—H15 | 118.7 |

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| C1—Pd1—I1 | 87.22 (18) | C15—C16—C17 | 118.5 (7) |
| C1$^{i}$—Pd1—I1 | 92.78 (18) | C15—C16—H16 | 120.7 |
| I1$^{i}$—Pd1—I1 | 180.00 (2) | C17—C16—H16 | 120.7 |
| C9—N1—C13 | 123.0 (6) | C18—C17—C16 | 122.6 (7) |
| C9—N1—H1 | 118.5 | C18—C17—H17 | 118.7 |
| C13—N1—H1 | 118.5 | C16—C17—H17 | 118.7 |
| C1—N2—C3 | 109.4 (5) | C17—C18—C13 | 117.5 (7) |
| C1—N2—C4 | 126.2 (5) | C17—C18—C22 | 122.2 (7) |
| C3—N2—C4 | 124.0 (5) | C13—C18—C22 | 120.2 (6) |
| C1—N3—C2 | 111.1 (6) | C14—C19—C21 | 110.5 (6) |
| C1—N3—C10 | 122.9 (6) | C14—C19—C20 | 112.6 (6) |
| C2—N3—C10 | 125.9 (6) | C21—C19—C20 | 112.0 (7) |
| N3—C1—N2 | 106.0 (6) | C14—C19—H19 | 107.1 |
| N3—C1—Pd1 | 126.8 (5) | C21—C19—H19 | 107.1 |
| N2—C1—Pd1 | 127.1 (5) | C20—C19—H19 | 107.1 |
| C3—C2—N3 | 106.8 (6) | C19—C20—H20A | 109.5 |
| C3—C2—H2 | 126.6 | C19—C20—H20B | 109.5 |
| N3—C2—H2 | 126.6 | H20A—C20—H20B | 109.5 |
| C2—C3—N2 | 106.7 (6) | C19—C20—H20C | 109.5 |
| C2—C3—H3 | 126.7 | H20A—C20—H20C | 109.5 |
| N2—C3—H3 | 126.7 | H20B—C20—H20C | 109.5 |
| C5—C4—C9 | 120.7 (6) | C19—C21—H21A | 109.5 |
| C5—C4—N2 | 119.4 (6) | C19—C21—H21B | 109.5 |
| C9—C4—N2 | 119.9 (6) | H21A—C21—H21B | 109.5 |
| C6—C5—C4 | 119.9 (7) | C19—C21—H21C | 109.5 |
| C6—C5—H5 | 120.0 | H21A—C21—H21C | 109.5 |
| C4—C5—H5 | 120.0 | H21B—C21—H21C | 109.5 |
| C7—C6—C5 | 120.2 (7) | C18—C22—C24 | 110.1 (6) |
| C7—C6—H6 | 119.9 | C18—C22—C23 | 113.9 (7) |
| C5—C6—H6 | 119.9 | C24—C22—C23 | 108.9 (6) |
| C6—C7—C8 | 120.2 (7) | C18—C22—H22 | 107.9 |
| C6—C7—H7 | 119.9 | C24—C22—H22 | 107.9 |
| C8—C7—H7 | 119.9 | C23—C22—H22 | 107.9 |
| C7—C8—C9 | 122.3 (7) | C22—C23—H23A | 109.5 |
| C7—C8—H8 | 118.9 | C22—C23—H23B | 109.5 |
| C9—C8—H8 | 118.9 | H23A—C23—H23B | 109.5 |
| C8—C9—N1 | 122.3 (6) | C22—C23—H23C | 109.5 |
| C8—C9—C4 | 116.5 (6) | H23A—C23—H23C | 109.5 |
| N1—C9—C4 | 121.3 (6) | H23B—C23—H23C | 109.5 |
| N3—C10—C11 | 111.4 (6) | C22—C24—H24A | 109.5 |
| N3—C10—C12 | 109.1 (6) | C22—C24—H24B | 109.5 |
| C11—C10—C12 | 112.4 (7) | H24A—C24—H24B | 109.5 |
| N3—C10—H10 | 107.9 | C22—C24—H24C | 109.5 |
| C11—C10—H10 | 107.9 | H24A—C24—H24C | 109.5 |
| C12—C10—H10 | 107.9 | H24B—C24—H24C | 109.5 |
| C10—C11—H11A | 109.5 | C30—C25—C26 | 120.2 (10) |
| C10—C11—H11B | 109.5 | C30—C25—H25 | 119.9 |
| H11A—C11—H11B | 109.5 | C26—C25—H25 | 119.9 |

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| C10—C11—H11C | 109.5 | C27—C26—C25 | 119.2 (10) |
| H11A—C11—H11C | 109.5 | C27—C26—H26 | 120.4 |
| H11B—C11—H11C | 109.5 | C25—C26—H26 | 120.4 |
| C10—C12—H12A | 109.5 | C28—C27—C26 | 118.8 (10) |
| C10—C12—H12B | 109.5 | C28—C27—H27 | 120.6 |
| H12A—C12—H12B | 109.5 | C26—C27—H27 | 120.6 |
| C10—C12—H12C | 109.5 | C27—C28—C29 | 121.2 (10) |
| H12A—C12—H12C | 109.5 | C27—C28—H28 | 119.4 |
| H12B—C12—H12C | 109.5 | C29—C28—H28 | 119.4 |
| C14—C13—N1 | 119.1 (6) | C30—C29—C28 | 120.1 (10) |
| C14—C13—C18 | 121.4 (6) | C30—C29—H29 | 120.0 |
| N1—C13—C18 | 119.5 (6) | C28—C29—H29 | 120.0 |
| C15—C14—C13 | 117.3 (6) | C25—C30—C29 | 120.4 (9) |
| C15—C14—C19 | 119.5 (6) | C25—C30—H30 | 119.8 |
| C13—C14—C19 | 123.0 (6) | C29—C30—H30 | 119.8 |

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| C2—N3—C1—N2 | 0.5 (8) | C1—N3—C10—C11 | −107.3 (8) |
| C10—N3—C1—N2 | 178.5 (6) | C2—N3—C10—C11 | 70.3 (9) |
| C2—N3—C1—Pd1 | −177.1 (5) | C1—N3—C10—C12 | 128.0 (7) |
| C10—N3—C1—Pd1 | 0.9 (9) | C2—N3—C10—C12 | −54.3 (9) |
| C3—N2—C1—N3 | −0.4 (7) | C9—N1—C13—C14 | −73.6 (8) |
| C4—N2—C1—N3 | 173.8 (6) | C9—N1—C13—C18 | 109.2 (7) |
| C3—N2—C1—Pd1 | 177.2 (5) | N1—C13—C14—C15 | −177.7 (6) |
| C4—N2—C1—Pd1 | −8.6 (9) | C18—C13—C14—C15 | −0.6 (10) |
| $I1^{i}$—Pd1—C1—N3 | −81.1 (6) | N1—C13—C14—C19 | −2.4 (10) |
| I1—Pd1—C1—N3 | 98.9 (6) | C18—C13—C14—C19 | 174.7 (7) |
| $I1^{i}$—Pd1—C1—N2 | 101.8 (5) | C13—C14—C15—C16 | 1.1 (11) |
| I1—Pd1—C1—N2 | −78.2 (5) | C19—C14—C15—C16 | −174.3 (7) |
| C1—N3—C2—C3 | −0.5 (8) | C14—C15—C16—C17 | −0.5 (12) |
| C10—N3—C2—C3 | −178.4 (6) | C15—C16—C17—C18 | −0.9 (12) |
| N3—C2—C3—N2 | 0.3 (8) | C16—C17—C18—C13 | 1.4 (11) |
| C1—N2—C3—C2 | 0.0 (8) | C16—C17—C18—C22 | −175.2 (7) |
| C4—N2—C3—C2 | −174.2 (6) | C14—C13—C18—C17 | −0.6 (10) |
| C1—N2—C4—C5 | −57.2 (9) | N1—C13—C18—C17 | 176.4 (6) |
| C3—N2—C4—C5 | 116.1 (7) | C14—C13—C18—C22 | 176.0 (7) |
| C1—N2—C4—C9 | 122.4 (7) | N1—C13—C18—C22 | −6.9 (10) |
| C3—N2—C4—C9 | −64.3 (8) | C15—C14—C19—C21 | 68.8 (9) |
| C9—C4—C5—C6 | 0.7 (10) | C13—C14—C19—C21 | −106.4 (8) |
| N2—C4—C5—C6 | −179.7 (6) | C15—C14—C19—C20 | −57.4 (9) |
| C4—C5—C6—C7 | 3.4 (10) | C13—C14—C19—C20 | 127.4 (7) |
| C5—C6—C7—C8 | −4.1 (10) | C17—C18—C22—C24 | 100.7 (8) |
| C6—C7—C8—C9 | 0.7 (11) | C13—C18—C22—C24 | −75.9 (8) |
| C7—C8—C9—N1 | −178.7 (6) | C17—C18—C22—C23 | −22.0 (10) |
| C7—C8—C9—C4 | 3.2 (10) | C13—C18—C22—C23 | 161.5 (7) |
| C13—N1—C9—C8 | −6.2 (10) | C30—C25—C26—C27 | −2.0 (14) |
| C13—N1—C9—C4 | 171.8 (6) | C25—C26—C27—C28 | 1.4 (16) |
| C5—C4—C9—C8 | −3.9 (9) | C26—C27—C28—C29 | −1.0 (16) |
| N2—C4—C9—C8 | 176.5 (6) | C27—C28—C29—C30 | 1.1 (15) |

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| C5—C4—C9—N1 | 178.0 (6) | C26—C25—C30—C29 | 2.1 (14) |
| N2—C4—C9—N1 | −1.6 (9) | C28—C29—C30—C25 | −1.6 (14) |

Symmetry code: (i) −*x*+2, −*y*, −*z*.