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# Bis[*S*-hexyl (*E*)-3-(4-methoxybenzylidene)dithiocarbazato-$\kappa^2N^3,S$]palladium(II)

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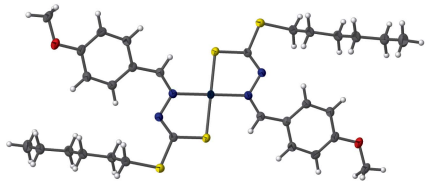
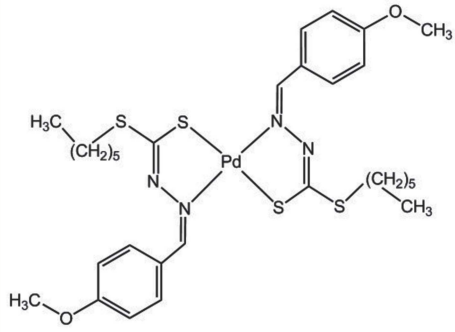
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title complex, $[Pd(C_{15}H_{21}N_2OS_2)_2]$, the $Pd^{II}$ ion is located on a crystallographic inversion center. The two Schiff base ligands in a deprotonated imino thiolate form chelate the metal atom *via* the azomithine N and thiolate S atoms in a *trans*-square-planar configuration as imposed by the crystal symmetry. The complex has an approximately planar geometry with the exception of the hexyl chains; the mean plane of the five-membered chelate ring makes a dihedral angle of 15.43 (5)° with the benzene ring. In the crystal, the complex molecules are stacked along the *a* axis.

**3D view**



**Chemical scheme**




## Structure description

The molecular structure of the title compound is illustrated in Fig. 1. In the complex, the Pd—S and Pd—N bond lengths are 2.2949 (5) and 2.0358 (14) Å, respectively, with the S1—Pd1—N1 chelating angle of 83.13 (5)°. These values are in agreement with those observed in similar bis(dithiocarbazato)$Pd^{II}$ complexes, either with a *trans* configuration of ligands (Khaledi & Mohd Ali, 2011; Tampouris *et al.*, 2007; Tarafder *et al.*, 2010) or with a *cis* configuration (Begum, Howlader, Sheikh *et al.*, 2015; Ali *et al.*, 2002; Liu *et al.*, 2011; Duan *et al.*, 1998; Tampouris *et al.*, 2007). The ligand recently reported (Begum, Howlader, Miyatake *et al.*, 2015) rotates about the C9—N2 bond by 180° in order to allow the *N*,*S* chelating behavior towards the metal. Upon coordination some salient features are observed, compared to the free ligand The most significant one is an elongation of the C9—S1 bond length; the C9—S1 distance of 1.7311 (17) Å in the present $PdL_2$ complex is longer than that of 1.6713 (19) Å in the ligand H*L*, validating the coordination with the deprotonated thiolate S atom. Correspondingly, the present N2—C9 and N1—N2 bond

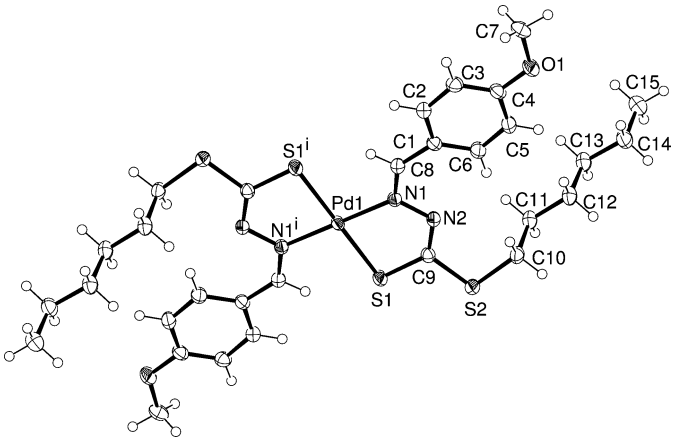



**Figure 1**
The molecular structure of the title compound, showing displacement ellipsoids at the 50% probability level [symmetry code: (i) $-x, -y, -z$].

lengths of 1.284 (3) and 1.411 (3) Å, respectively, are shorter and slightly longer than the values of 1.343 (3) and 1.377 (2) Å in the free ligand. In the crystal, the molecules are stacked along the *a* axis (Fig. 2).

## Synthesis and crystallization

A solution of $PdCl_2$ (0.044 g, 0.25 mmol) in 25 ml methanol was added to a solution of *S*-hexyl (*E*)-3-(4-methoxybenzylidene)dithiocarbazate (0.155 g, 0.5 mmol) in 10 ml methanol. The resulting mixture was refluxed with constant stirring for 4 h. The orange–red precipitate formed was filtered off, washed with methanol and dried *in vacuo* over anhydrous $CaCl_2$. Orange–red single crystals of the title compound suitable for X-ray diffraction were obtained by slow evaporation from a solution in a mixture of dichloromethane and acetonitrile (2:1) (m.p. 457 K).

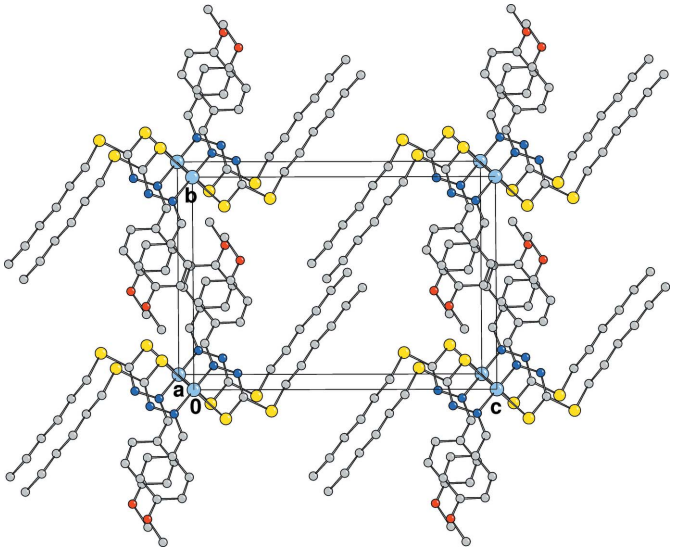



**Figure 2**
A packing view of the title compound along the *a* axis.

**Table 1**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[Pd(C_{15}H_{21}N_2OS_2)_2]$ |
| $M_r$ | 725.33 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 173 |
| $a, b, c$ (Å) | 4.54371 (18), 11.6697 (6), 15.5677 (8) |
| $\alpha, \beta, \gamma$ (°) | 90.8429 (14), 98.1733 (18), 100.3441 (11) |
| $V$ (Å$^3$) | 803.10 (7) |
| $Z$ | 1 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.87 |
| Crystal size (mm) | 0.20 × 0.09 × 0.02 |
| | |
| Data collection | |
| Diffractometer | Rigaku R-AXIS RAPID |
| Absorption correction | Multi-scan (*ABSCOR*; Higashi, 1995) |
| $T_{min}$, $T_{max}$ | 0.891, 0.983 |
| No. of measured, independent and observed [$F^2 > 2\sigma(F^2)$] reflections | 6642, 2935, 2802 |
| $R_{int}$ | 0.017 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.602 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.021, 0.057, 1.15 |
| No. of reflections | 2935 |
| No. of parameters | 189 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.43, −0.23 |

Computer programs: *RAPID-AUTO* (Rigaku, 2001), *SIR92* (Altomare *et al.*, 1993), *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

## Acknowledgements

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# full crystallographic data

*IUCrData* (2016). **1**, x160521 [doi:10.1107/S2414314616005216]

## Bis[*S*-hexyl (*E*)-3-(4-methoxybenzylidene)dithiocarbazato-$\kappa^2N^3$,*S*]palladium(II)

**E. Zangrando, M. S. Begum, M. B. H. Howlader, M. C. Sheikh and R. Miyatake**

**Bis[*S*-hexyl (*E*)-3-(4-methoxybenzylidene)dithiocarbazato-$\kappa^2N^3$,*S*]palladium(II)**

*Crystal data*

$[Pd(C_{15}H_{21}N_2OS_2)_2]$
$M_r$ = 725.33
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 4.54371 (18) Å
$b$ = 11.6697 (6) Å
$c$ = 15.5677 (8) Å
$\alpha$ = 90.8429 (14)°
$\beta$ = 98.1733 (18)°
$\gamma$ = 100.3441 (11)°
$V$ = 803.10 (7) Å$^3$
$Z$ = 1
$F$(000) = 376.00
$D_x$ = 1.500 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71075 Å
Cell parameters from 7004 reflections
$\theta$ = 3.1–27.5°
$\mu$ = 0.87 mm$^{-1}$
$T$ = 173 K
Platelet, orange
0.20 × 0.09 × 0.02 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.000 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.891, $T_{max}$ = 0.983
6642 measured reflections
2935 independent reflections
2802 reflections with $F^2 > 2\sigma(F^2)$
$R_{int}$ = 0.017
$\theta_{max}$ = 25.3°
$h$ = −5→5
$k$ = −14→14
$l$ = −18→18

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.057
$S$ = 1.15
2935 reflections
189 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
$w = 1/[\sigma^2(F_o^2) + (0.0251P)^2 + 0.3967P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$

*Special details*

**Geometry**. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY
**Refinement**. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on $F^2$. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma($F^2$) is used only for calculating R-factor (gt).

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Pd1 | 0.0000 | 0.0000 | 0.0000 | 0.02080 (8) |
| S1 | −0.00459 (11) | −0.13653 (4) | 0.10464 (3) | 0.02995 (12) |
| S2 | 0.36335 (11) | −0.12720 (4) | 0.27412 (3) | 0.02920 (12) |
| O1 | 1.5353 (4) | 0.49771 (13) | 0.23168 (10) | 0.0379 (4) |
| N1 | 0.3597 (4) | 0.08710 (13) | 0.08319 (10) | 0.0223 (4) |
| N2 | 0.4365 (4) | 0.04560 (14) | 0.16655 (10) | 0.0239 (4) |
| C1 | 0.7997 (4) | 0.25574 (16) | 0.11173 (12) | 0.0235 (4) |
| C2 | 0.9437 (5) | 0.34306 (17) | 0.06407 (12) | 0.0270 (4) |
| C3 | 1.1907 (5) | 0.42501 (17) | 0.10040 (13) | 0.0282 (4) |
| C4 | 1.2993 (5) | 0.42088 (17) | 0.18824 (13) | 0.0280 (4) |
| C5 | 1.1622 (5) | 0.33362 (18) | 0.23675 (13) | 0.0330 (5) |
| C6 | 0.9169 (5) | 0.25205 (18) | 0.19998 (13) | 0.0297 (5) |
| C7 | 1.6597 (5) | 0.59746 (18) | 0.18742 (15) | 0.0383 (5) |
| C8 | 0.5364 (4) | 0.17987 (16) | 0.06361 (12) | 0.0241 (4) |
| C9 | 0.2833 (4) | −0.05543 (16) | 0.17755 (11) | 0.0229 (4) |
| C10 | 0.6641 (5) | −0.02298 (18) | 0.33661 (12) | 0.0281 (4) |
| C11 | 0.5519 (5) | 0.07304 (18) | 0.38258 (12) | 0.0283 (5) |
| C12 | 0.8067 (5) | 0.15415 (18) | 0.44003 (12) | 0.0297 (5) |
| C13 | 0.6976 (5) | 0.24810 (19) | 0.48976 (13) | 0.0320 (5) |
| C14 | 0.9466 (5) | 0.32555 (19) | 0.55097 (14) | 0.0349 (5) |
| C15 | 0.8324 (6) | 0.4187 (2) | 0.59973 (16) | 0.0448 (6) |
| H1 | 0.8693 | 0.3465 | 0.0041 | 0.0325* |
| H2 | 1.2847 | 0.4832 | 0.0659 | 0.0339* |
| H3 | 1.2389 | 0.3300 | 0.2965 | 0.0396* |
| H4 | 0.8266 | 0.1930 | 0.2344 | 0.0356* |
| H5 | 1.5003 | 0.6415 | 0.1674 | 0.0460* |
| H6 | 1.7440 | 0.5720 | 0.1374 | 0.0460* |
| H7 | 1.8201 | 0.6472 | 0.2272 | 0.0460* |
| H8 | 0.4834 | 0.2032 | 0.0061 | 0.0289* |
| H9 | 0.7793 | −0.0649 | 0.3805 | 0.0337* |
| H10 | 0.8044 | 0.0130 | 0.2973 | 0.0337* |
| H11 | 0.4001 | 0.0372 | 0.4187 | 0.0340* |
| H12 | 0.4508 | 0.1192 | 0.3386 | 0.0340* |
| H13 | 0.9539 | 0.1922 | 0.4033 | 0.0357* |
| H14 | 0.9133 | 0.1072 | 0.4821 | 0.0357* |
| H15 | 0.6007 | 0.2975 | 0.4475 | 0.0384* |
| H16 | 0.5417 | 0.2100 | 0.5238 | 0.0384* |
| H17 | 1.1027 | 0.3639 | 0.5171 | 0.0418* |
| H18 | 1.0433 | 0.2764 | 0.5936 | 0.0418* |
| H19 | 0.6890 | 0.3813 | 0.6368 | 0.0537* |
| H20 | 0.7311 | 0.4663 | 0.5580 | 0.0537* |
| H21 | 1.0035 | 0.4684 | 0.6358 | 0.0537* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pd1 | 0.02019 (11) | 0.02079 (12) | 0.01926 (11) | −0.00035 (8) | 0.00101 (7) | −0.00108 (7) |
| S1 | 0.0326 (3) | 0.0252 (3) | 0.0254 (3) | −0.0065 (2) | −0.00314 (19) | 0.00252 (19) |
| S2 | 0.0342 (3) | 0.0249 (3) | 0.0250 (3) | 0.0003 (2) | −0.00123 (19) | 0.00403 (19) |
| O1 | 0.0355 (8) | 0.0308 (8) | 0.0380 (9) | −0.0094 (7) | −0.0067 (7) | 0.0002 (7) |
| N1 | 0.0230 (8) | 0.0230 (8) | 0.0203 (8) | 0.0034 (7) | 0.0022 (6) | 0.0000 (6) |
| N2 | 0.0255 (8) | 0.0242 (9) | 0.0202 (8) | 0.0023 (7) | 0.0000 (6) | 0.0011 (6) |
| C1 | 0.0220 (9) | 0.0219 (10) | 0.0256 (10) | 0.0031 (8) | 0.0019 (7) | −0.0016 (8) |
| C2 | 0.0291 (10) | 0.0265 (10) | 0.0240 (10) | 0.0044 (8) | −0.0005 (8) | 0.0005 (8) |
| C3 | 0.0278 (10) | 0.0241 (10) | 0.0316 (11) | 0.0012 (8) | 0.0046 (8) | 0.0026 (8) |
| C4 | 0.0242 (9) | 0.0227 (10) | 0.0343 (11) | 0.0013 (8) | −0.0005 (8) | −0.0034 (8) |
| C5 | 0.0362 (11) | 0.0311 (11) | 0.0259 (10) | −0.0019 (9) | −0.0049 (9) | 0.0012 (9) |
| C6 | 0.0312 (10) | 0.0277 (11) | 0.0266 (10) | −0.0023 (9) | 0.0014 (8) | 0.0032 (8) |
| C7 | 0.0358 (11) | 0.0259 (11) | 0.0464 (13) | −0.0089 (9) | 0.0019 (10) | −0.0016 (10) |
| C8 | 0.0237 (9) | 0.0253 (10) | 0.0225 (9) | 0.0041 (8) | 0.0010 (7) | 0.0008 (8) |
| C9 | 0.0239 (9) | 0.0240 (10) | 0.0207 (9) | 0.0050 (8) | 0.0030 (7) | −0.0015 (7) |
| C10 | 0.0248 (9) | 0.0315 (11) | 0.0251 (10) | 0.0029 (9) | −0.0029 (8) | 0.0030 (8) |
| C11 | 0.0241 (9) | 0.0353 (11) | 0.0236 (10) | 0.0024 (9) | 0.0008 (8) | 0.0008 (8) |
| C12 | 0.0246 (9) | 0.0371 (12) | 0.0250 (10) | 0.0019 (9) | 0.0002 (8) | 0.0011 (9) |
| C13 | 0.0273 (10) | 0.0373 (12) | 0.0285 (11) | 0.0024 (9) | −0.0008 (8) | −0.0007 (9) |
| C14 | 0.0330 (11) | 0.0353 (12) | 0.0319 (11) | −0.0007 (9) | −0.0009 (9) | −0.0013 (9) |
| C15 | 0.0492 (14) | 0.0371 (13) | 0.0427 (13) | 0.0045 (11) | −0.0062 (11) | −0.0071 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Pd1—S1 | 2.2949 (5) | C14—C15 | 1.522 (4) |
| Pd1—S1$^{i}$ | 2.2949 (5) | C2—H1 | 0.950 |
| Pd1—N1 | 2.0358 (14) | C3—H2 | 0.950 |
| Pd1—N1$^{i}$ | 2.0358 (14) | C5—H3 | 0.950 |
| S1—C9 | 1.7311 (17) | C6—H4 | 0.950 |
| S2—C9 | 1.7564 (19) | C7—H5 | 0.980 |
| S2—C10 | 1.8119 (18) | C7—H6 | 0.980 |
| O1—C4 | 1.357 (3) | C7—H7 | 0.980 |
| O1—C7 | 1.431 (3) | C8—H8 | 0.950 |
| N1—N2 | 1.411 (3) | C10—H9 | 0.990 |
| N1—C8 | 1.295 (3) | C10—H10 | 0.990 |
| N2—C9 | 1.284 (3) | C11—H11 | 0.990 |
| C1—C2 | 1.392 (3) | C11—H12 | 0.990 |
| C1—C6 | 1.405 (3) | C12—H13 | 0.990 |
| C1—C8 | 1.457 (3) | C12—H14 | 0.990 |
| C2—C3 | 1.383 (3) | C13—H15 | 0.990 |
| C3—C4 | 1.391 (3) | C13—H16 | 0.990 |
| C4—C5 | 1.387 (3) | C14—H17 | 0.990 |
| C5—C6 | 1.377 (3) | C14—H18 | 0.990 |
| C10—C11 | 1.521 (3) | C15—H19 | 0.980 |
| C11—C12 | 1.524 (3) | C15—H20 | 0.980 |

| | | | |
|---|---|---|---|
| C12—C13 | 1.525 (4) | C15—H21 | 0.980 |
| C13—C14 | 1.519 (3) | | |

| | | | |
|---|---|---|---|
| S1—Pd1—S1$^{i}$ | 180.00 (3) | O1—C7—H5 | 109.469 |
| S1—Pd1—N1 | 83.13 (5) | O1—C7—H6 | 109.467 |
| S1—Pd1—N1$^{i}$ | 96.87 (5) | O1—C7—H7 | 109.464 |
| S1$^{i}$—Pd1—N1 | 96.87 (5) | H5—C7—H6 | 109.479 |
| S1$^{i}$—Pd1—N1$^{i}$ | 83.13 (5) | H5—C7—H7 | 109.470 |
| N1—Pd1—N1$^{i}$ | 180.00 (9) | H6—C7—H7 | 109.477 |
| Pd1—S1—C9 | 95.72 (7) | N1—C8—H8 | 113.450 |
| C9—S2—C10 | 102.89 (9) | C1—C8—H8 | 113.448 |
| C4—O1—C7 | 118.18 (16) | S2—C10—H9 | 108.858 |
| Pd1—N1—N2 | 120.58 (11) | S2—C10—H10 | 108.853 |
| Pd1—N1—C8 | 123.64 (13) | C11—C10—H9 | 108.859 |
| N2—N1—C8 | 115.75 (14) | C11—C10—H10 | 108.849 |
| N1—N2—C9 | 112.98 (14) | H9—C10—H10 | 107.706 |
| C2—C1—C6 | 117.37 (16) | C10—C11—H11 | 109.100 |
| C2—C1—C8 | 115.14 (16) | C10—C11—H12 | 109.105 |
| C6—C1—C8 | 127.46 (17) | C12—C11—H11 | 109.106 |
| C1—C2—C3 | 122.68 (17) | C12—C11—H12 | 109.103 |
| C2—C3—C4 | 118.89 (18) | H11—C11—H12 | 107.845 |
| O1—C4—C3 | 124.42 (18) | C11—C12—H13 | 108.895 |
| O1—C4—C5 | 116.13 (18) | C11—C12—H14 | 108.898 |
| C3—C4—C5 | 119.45 (17) | C13—C12—H13 | 108.898 |
| C4—C5—C6 | 121.28 (19) | C13—C12—H14 | 108.893 |
| C1—C6—C5 | 120.31 (19) | H13—C12—H14 | 107.732 |
| N1—C8—C1 | 133.10 (18) | C12—C13—H15 | 108.748 |
| S1—C9—S2 | 112.82 (10) | C12—C13—H16 | 108.753 |
| S1—C9—N2 | 127.04 (14) | C14—C13—H15 | 108.757 |
| S2—C9—N2 | 120.13 (13) | C14—C13—H16 | 108.759 |
| S2—C10—C11 | 113.56 (14) | H15—C13—H16 | 107.646 |
| C10—C11—C12 | 112.47 (17) | C13—C14—H17 | 108.973 |
| C11—C12—C13 | 113.37 (17) | C13—C14—H18 | 108.975 |
| C12—C13—C14 | 114.00 (18) | C15—C14—H17 | 108.977 |
| C13—C14—C15 | 113.04 (19) | C15—C14—H18 | 108.973 |
| C1—C2—H1 | 118.658 | H17—C14—H18 | 107.774 |
| C3—C2—H1 | 118.661 | C14—C15—H19 | 109.470 |
| C2—C3—H2 | 120.558 | C14—C15—H20 | 109.468 |
| C4—C3—H2 | 120.548 | C14—C15—H21 | 109.470 |
| C4—C5—H3 | 119.366 | H19—C15—H20 | 109.477 |
| C6—C5—H3 | 119.354 | H19—C15—H21 | 109.472 |
| C1—C6—H4 | 119.844 | H20—C15—H21 | 109.470 |
| C5—C6—H4 | 119.851 | | |

| | | | |
|---|---|---|---|
| S1—Pd1—N1—N2 | −7.46 (11) | N2—N1—C8—C1 | −2.8 (3) |
| S1—Pd1—N1—C8 | 170.36 (13) | C8—N1—N2—C9 | −170.01 (16) |
| N1—Pd1—S1—C9 | 4.28 (5) | N1—N2—C9—S1 | −3.2 (3) |
| S1—Pd1—N1$^{i}$—N2$^{i}$ | −172.54 (11) | N1—N2—C9—S2 | 175.43 (14) |

| | | | |
|---|---|---|---|
| S1—Pd1—N1$^{i}$—C8$^{i}$ | 9.64 (13) | C2—C1—C6—C5 | 0.9 (3) |
| N1$^{i}$—Pd1—S1—C9 | −175.72 (5) | C6—C1—C2—C3 | −0.7 (3) |
| S1$^{i}$—Pd1—N1—N2 | 172.54 (11) | C2—C1—C8—N1 | 174.9 (2) |
| S1$^{i}$—Pd1—N1—C8 | −9.64 (13) | C8—C1—C2—C3 | 177.76 (17) |
| N1—Pd1—S1$^{i}$—C9$^{i}$ | 175.72 (5) | C6—C1—C8—N1 | −6.8 (4) |
| S1$^{i}$—Pd1—N1$^{i}$—N2$^{i}$ | 7.46 (11) | C8—C1—C6—C5 | −177.33 (18) |
| S1$^{i}$—Pd1—N1$^{i}$—C8$^{i}$ | −170.36 (13) | C1—C2—C3—C4 | −0.4 (4) |
| N1$^{i}$—Pd1—S1$^{i}$—C9$^{i}$ | −4.28 (5) | C2—C3—C4—O1 | −178.54 (19) |
| Pd1—S1—C9—S2 | 179.30 (10) | C2—C3—C4—C5 | 1.4 (3) |
| Pd1—S1—C9—N2 | −2.01 (17) | O1—C4—C5—C6 | 178.75 (18) |
| C9—S2—C10—C11 | 80.84 (13) | C3—C4—C5—C6 | −1.2 (4) |
| C10—S2—C9—S1 | −179.47 (11) | C4—C5—C6—C1 | 0.0 (4) |
| C10—S2—C9—N2 | 1.74 (18) | S2—C10—C11—C12 | 175.70 (11) |
| C7—O1—C4—C3 | 7.6 (3) | C10—C11—C12—C13 | −177.57 (14) |
| C7—O1—C4—C5 | −172.30 (17) | C11—C12—C13—C14 | 176.88 (15) |
| Pd1—N1—N2—C9 | 8.0 (2) | C12—C13—C14—C15 | 179.92 (15) |
| Pd1—N1—C8—C1 | 179.34 (14) | | |

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