

## [1,2-Bis(phenylseleno)benzene]-dichloridopalladium(II)

Nobuhiro Takeda,<sup>‡</sup> Toru Isobe, Takahiro Sasamori and Norihiro Tokitoh\*

Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan

Correspondence e-mail: tokitoh@boc.kuicr.kyoto-u.ac.jp

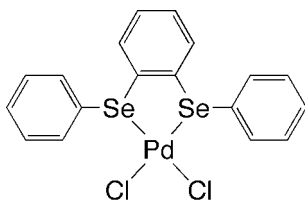
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Key indicators: single-crystal X-ray study;  $T = 103$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.014;  $wR$  factor = 0.037; data-to-parameter ratio = 11.8.

In the title compound,  $[\text{PdCl}_2\{1,2\text{-C}_6\text{H}_4(\text{SePh})_2\}]$ , the two Cl atoms and the two Se atoms are arranged in a square-planar fashion around the Pd atom. The two phenyl groups are on the same side of the  $\text{PdCl}_2\text{Se}_2$  plane. Intermolecular interactions between the Cl and Se atoms are suggested [ $\text{Se}\cdots\text{Cl} = 3.4003$  (4) and  $3.4101$  (4) Å].

### Related literature

For related literature, see: Bondi (1964); Booth *et al.* (1997); Champness *et al.* (1995); Gujadhur & Venkataraman (2003); Gulliver *et al.* (1984); Hartley *et al.* (1979); Nakanishi & Hayashi (2000); Orpen *et al.* (1989); Petragnari & Toscano (1970); Takeda *et al.* (2005); Whitfield (1970).



### Experimental

#### Crystal data

$[\text{PdCl}_2(\text{C}_{18}\text{H}_{14}\text{Se}_2)]$

$M_r = 565.51$

Triclinic,  $P\bar{1}$

$a = 8.7008$  (3) Å

$b = 10.4873$  (2) Å

$c = 10.9779$  (3) Å

$\alpha = 64.1072$  (13)°

$\beta = 78.4779$  (12)°

$\gamma = 74.2744$  (17)°

$V = 863.58$  (4) Å<sup>3</sup>

$Z = 2$

Mo  $K\alpha$  radiation

$\mu = 5.59$  mm<sup>-1</sup>

$T = 103$  (2) K

$0.08 \times 0.08 \times 0.02$  mm

#### Data collection

Rigaku VariMax Saturn diffractometer

Absorption correction: multi-scan (REQAB; Jacobson; 1998)

$T_{\text{min}} = 0.663$ ,  $T_{\text{max}} = 0.896$

7378 measured reflections  
3122 independent reflections

3057 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.015$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.014$

$wR(F^2) = 0.037$

$S = 1.05$

3122 reflections

264 parameters

All H-atom parameters refined

$\Delta\rho_{\text{max}} = 0.63$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.31$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

|             |              |             |             |
|-------------|--------------|-------------|-------------|
| Pd1—Cl2     | 2.3282 (4)   | Se1—C7      | 1.9367 (16) |
| Pd1—Cl1     | 2.3471 (4)   | Se1—C1      | 1.9547 (17) |
| Pd1—Se2     | 2.3790 (2)   | Se2—Cl2     | 1.9301 (16) |
| Pd1—Se1     | 2.38098 (19) | Se2—Cl3     | 1.9515 (17) |
| Cl2—Pd1—Cl1 | 94.066 (15)  | C7—Se1—C1   | 97.24 (7)   |
| Cl2—Pd1—Se2 | 87.714 (12)  | C7—Se1—Pd1  | 102.52 (5)  |
| Cl1—Pd1—Se2 | 176.116 (12) | C1—Se1—Pd1  | 99.60 (5)   |
| Cl2—Pd1—Se1 | 176.146 (12) | Cl2—Se2—Cl3 | 98.11 (7)   |
| Cl1—Pd1—Se1 | 87.742 (11)  | Cl2—Se2—Pd1 | 102.46 (5)  |
| Se2—Pd1—Se1 | 90.279 (7)   | Cl3—Se2—Pd1 | 99.58 (5)   |

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP III* (Burnett & Johnson, 1996); 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: OM2151).

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<sup>‡</sup> Present address: Department of Chemistry and Chemical Biology, Graduate School of Engineering, Gunma University, 1-5-1 Tenjin-cho, Kiryu, Gunma 376-8515, Japan.

**supplementary materials**

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## [1,2-Bis(phenylseleno)benzene]dichloridopalladium(II)

N. Takeda, T. Isobe, T. Sasamori and N. Tokitoh

### Comment

There are no reports on the synthesis of the title compound,  $[\text{PdCl}_2\{1,2\text{-C}_6\text{H}_4(\text{SePh})_2\}]$  (1), although the synthesis and full characterization of the sulfur analog,  $[\text{PdCl}_2\{1,2\text{-C}_6\text{H}_4(\text{SPh})_2\}]$  (2), has already been reported (Hartley *et al.*, 1979; Takeda *et al.*, 2005). This paper presents the first synthesis and X-ray structural analysis of (1).

Compound (1) was prepared by a method similar to that for the sulfur analog (2) (Takeda *et al.*, 2005), *i.e.*, the reaction of the ligand, 1,2-bis(phenylseleno)benzene with  $\text{NaPdCl}_4$ . The X-ray structural analysis of (1) shows features similar to those of (2) (Takeda *et al.*, 2005), *e.g.*, a square planar arrangement of the two chlorine and two chalcogen atoms around the palladium center, and a conformation where the two terminal phenyl groups of the diselenoether ligand are on the same side of the  $\text{PdCl}_2\text{Ch}_2$  plane (Fig. 1). The Pd—Cl bond lengths (Pd1—Cl1 2.3471 (4) and Pd1—Cl2 2.3282 (4) Å) are slightly longer than those of (2) (Pd1—Cl1 2.3159 (6) and Pd1—Cl2 2.3116 (5) Å), although these values are within the range of the reported values for tetracoordinate palladium(II) complexes (2.298–2.354 Å) (Orpen *et al.*, 1989). This result suggests that the coordination of the Se atoms to the Pd center in (1) is slightly stronger than that of the S atoms in (2). The Pd—Se bond lengths (Pd1—Se1 2.38098 (19) and Pd1—Se2 2.3790 (2) Å) are similar to those of the reported *cis*-dichloropalladium(II) complexes with selenoether (2.36–2.40 Å) (Booth *et al.*, 1997; Champness *et al.*, 1995; Whitfield, 1970).

Intermolecular Se—Cl distances (Se1—Cl2 3.4003 (4) and Se2—Cl1 3.4101 (4) Å) are slightly shorter than the sum of the van der Waals radii of chlorine and selenium (3.65 Å) (Bondi, 1964) (Fig. 2). This result suggests there is an intermolecular interaction between the chlorine and selenium atoms as well as between the chlorine and sulfur observed in (2). In addition, there are intermolecular C9—H7—Cl1 (2.94 (2) Å) and C10—H8—Cl2 (3.11 (2) Å) distances, although it is thought that these are weaker than the corresponding interactions in (2).

### Experimental

Sodium tetrachloropalladate (93.8 mg, 0.319 mmol) was added to a solution of 1,2-bis(phenylseleno)benzene,  $1,2\text{-C}_6\text{H}_4(\text{SePh})_2$ , (100 mg, 0.258 mmol) (Gujadhur & Venkataraman, 2003; Nakanishi & Hayashi, 2000; Gulliver *et al.*, 1984; Petragnari & Toscano, 1970) in chloroform (3 ml)/ethanol (20 ml) at room temperature. After stirring for 3 h, the mixture was filtered. The precipitates were washed with ethanol (5 ml  $\times$  3) and then extracted with dichloromethane (300 ml) and chloroform (300 ml). After filtration of the mixture, evaporation of the filtrate gave the title compound,  $[\text{PdCl}_2\{1,2\text{-C}_6\text{H}_4(\text{SePh})_2\}]$  (1) (138.7 mg, 0.245 mmol, 95%). Further purification by recrystallization from chloroform/ethanol provided analytically pure (1) (m.p. 270 °C, decomposition. Analysis found: C 38.08, H 2.65%;  $\text{C}_{18}\text{H}_{14}\text{Cl}_2\text{PdSe}_2$  requires: C 38.23, H 2.50%). Suitable crystals for X-ray crystallography were obtained by slow evaporation of a dichloromethane/chloroform solution.

### Refinement

All H atoms were refined isotropically, while all the other atoms were refined anisotropically.

## Figures

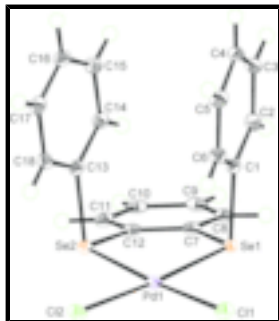


Fig. 1. View of the molecule of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

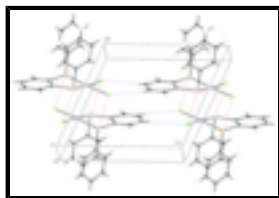


Fig. 2. The molecular packing as viewed down the *a* axis..

## [1,2-Bis(phenylseleno)benzene]dichloridopalladium(II)

### Crystal data

[PdCl<sub>2</sub>(C<sub>18</sub>H<sub>14</sub>Se<sub>2</sub>)]

*M<sub>r</sub>* = 565.51

Triclinic, *P* $\bar{1}$

Hall symbol: -P 1

*a* = 8.7008 (3) Å

*b* = 10.4873 (2) Å

*c* = 10.9779 (3) Å

$\alpha$  = 64.1072 (13)°

$\beta$  = 78.4779 (12)°

$\gamma$  = 74.2744 (17)°

*V* = 863.58 (4) Å<sup>3</sup>

*Z* = 2

*F*<sub>000</sub> = 540

*D<sub>x</sub>* = 2.175 Mg m<sup>-3</sup>

Mo *K*α radiation

$\lambda$  = 0.71069 Å

Cell parameters from 2442 reflections

$\theta$  = 3.1–25.5°

$\mu$  = 5.59 mm<sup>-1</sup>

*T* = 103 (2) K

Prism, orange

0.08 × 0.08 × 0.02 mm

### Data collection

Rigaku VariMax Saturn  
diffractometer

Radiation source: rotating-anode X-ray tube

Monochromator: Confocal

*T* = 103(2) K

$\omega$  scans

Absorption correction: multi-scan  
(REQAB; Jacobson; 1998)

*T<sub>min</sub>* = 0.663, *T<sub>max</sub>* = 0.896

7378 measured reflections

3057 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.015

$\theta_{\text{max}}$  = 25.5°

$\theta_{\text{min}}$  = 3.1°

*h* = -10→10

*k* = -12→12

*l* = -13→13

Standard reflections: ?

3122 independent reflections

*Refinement*

|                                                                |                                                          |
|----------------------------------------------------------------|----------------------------------------------------------|
| Refinement on $F^2$                                            | Secondary atom site location: difference Fourier map     |
| Least-squares matrix: full                                     | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.014$                                | All H-atom parameters refined                            |
| $wR(F^2) = 0.037$                                              | $w = 1/[\sigma^2(F_o^2) + (0.0102P)^2 + 0.541P]$         |
| $S = 1.05$                                                     | where $P = (F_o^2 + 2F_c^2)/3$                           |
| 3122 reflections                                               | $(\Delta/\sigma)_{\max} = 0.002$                         |
| 264 parameters                                                 | $\Delta\rho_{\max} = 0.63 \text{ e } \text{\AA}^{-3}$    |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\min} = -0.31 \text{ e } \text{\AA}^{-3}$   |
|                                                                | Extinction correction: none                              |

*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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

|     | $x$           | $y$           | $z$           | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|---------------|---------------|----------------------------------|
| Pd1 | 0.646899 (14) | 0.363137 (13) | 0.003739 (12) | 0.01048 (5)                      |
| Cl1 | 0.78072 (5)   | 0.46915 (5)   | -0.21221 (4)  | 0.01566 (9)                      |
| Cl2 | 0.47187 (5)   | 0.28911 (5)   | -0.07496 (4)  | 0.01613 (9)                      |
| Se1 | 0.832610 (19) | 0.422118 (17) | 0.093337 (16) | 0.01072 (5)                      |
| Se2 | 0.527966 (19) | 0.244530 (17) | 0.227340 (16) | 0.01141 (5)                      |
| C1  | 0.99842 (19)  | 0.24472 (18)  | 0.13286 (17)  | 0.0128 (3)                       |
| C2  | 1.0948 (2)    | 0.20103 (19)  | 0.23691 (18)  | 0.0153 (3)                       |
| H1  | 1.088 (2)     | 0.254 (2)     | 0.287 (2)     | 0.011 (5)*                       |
| C3  | 1.2088 (2)    | 0.0720 (2)    | 0.26636 (18)  | 0.0169 (4)                       |
| H2  | 1.275 (3)     | 0.042 (2)     | 0.335 (2)     | 0.021 (5)*                       |
| C4  | 1.2279 (2)    | -0.0099 (2)   | 0.19135 (18)  | 0.0167 (4)                       |
| H3  | 1.302 (2)     | -0.097 (2)    | 0.211 (2)     | 0.017 (5)*                       |
| C5  | 1.1351 (2)    | 0.03816 (19)  | 0.08486 (18)  | 0.0169 (4)                       |
| H4  | 1.152 (3)     | -0.019 (2)    | 0.033 (2)     | 0.022 (5)*                       |
| C6  | 1.0194 (2)    | 0.16632 (19)  | 0.05435 (17)  | 0.0155 (3)                       |
| H5  | 0.961 (2)     | 0.197 (2)     | -0.016 (2)    | 0.017 (5)*                       |
| C7  | 0.7402 (2)    | 0.38254 (18)  | 0.27874 (16)  | 0.0125 (3)                       |

## supplementary materials

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|     |            |               |              |            |
|-----|------------|---------------|--------------|------------|
| C8  | 0.8009 (2) | 0.42967 (19)  | 0.35619 (18) | 0.0151 (3) |
| H6  | 0.888 (3)  | 0.480 (2)     | 0.319 (2)    | 0.020 (5)* |
| C9  | 0.7332 (2) | 0.40479 (19)  | 0.48820 (18) | 0.0172 (4) |
| H7  | 0.774 (3)  | 0.434 (2)     | 0.538 (2)    | 0.023 (6)* |
| C10 | 0.6045 (2) | 0.33526 (19)  | 0.54185 (18) | 0.0170 (4) |
| H8  | 0.557 (2)  | 0.326 (2)     | 0.624 (2)    | 0.017 (5)* |
| C11 | 0.5435 (2) | 0.28864 (19)  | 0.46451 (18) | 0.0161 (4) |
| H9  | 0.453 (3)  | 0.240 (2)     | 0.502 (2)    | 0.024 (6)* |
| C12 | 0.6132 (2) | 0.31227 (18)  | 0.33235 (17) | 0.0129 (3) |
| C13 | 0.6685 (2) | 0.05285 (18)  | 0.27761 (17) | 0.0131 (3) |
| C14 | 0.7849 (2) | 0.00403 (19)  | 0.36772 (17) | 0.0146 (3) |
| H10 | 0.799 (2)  | 0.064 (2)     | 0.4087 (19)  | 0.010 (4)* |
| C15 | 0.8820 (2) | -0.1332 (2)   | 0.39744 (18) | 0.0171 (4) |
| H11 | 0.960 (3)  | -0.165 (2)    | 0.458 (2)    | 0.018 (5)* |
| C16 | 0.8626 (2) | -0.2206 (2)   | 0.33869 (18) | 0.0168 (4) |
| H12 | 0.928 (2)  | -0.315 (2)    | 0.358 (2)    | 0.020 (5)* |
| C17 | 0.7451 (2) | -0.17168 (19) | 0.25014 (18) | 0.0154 (3) |
| H13 | 0.732 (2)  | -0.224 (2)    | 0.207 (2)    | 0.015 (5)* |
| C18 | 0.6474 (2) | -0.03441 (19) | 0.21878 (17) | 0.0143 (3) |
| H14 | 0.574 (2)  | -0.002 (2)    | 0.157 (2)    | 0.018 (5)* |

### Atomic displacement parameters ( $\text{\AA}^2$ )

|     | $U^{11}$    | $U^{22}$    | $U^{33}$     | $U^{12}$      | $U^{13}$      | $U^{23}$      |
|-----|-------------|-------------|--------------|---------------|---------------|---------------|
| Pd1 | 0.01126 (8) | 0.01039 (8) | 0.00946 (8)  | -0.00007 (5)  | -0.00263 (5)  | -0.00429 (6)  |
| Cl1 | 0.0179 (2)  | 0.0164 (2)  | 0.01045 (19) | -0.00168 (16) | -0.00059 (15) | -0.00487 (16) |
| Cl2 | 0.0167 (2)  | 0.0168 (2)  | 0.0175 (2)   | -0.00128 (17) | -0.00698 (16) | -0.00834 (17) |
| Se1 | 0.01120 (9) | 0.01027 (9) | 0.01034 (9)  | -0.00178 (7)  | -0.00084 (6)  | -0.00420 (7)  |
| Se2 | 0.01043 (9) | 0.01092 (9) | 0.01232 (9)  | -0.00123 (7)  | -0.00143 (6)  | -0.00464 (7)  |
| C1  | 0.0103 (8)  | 0.0113 (8)  | 0.0143 (8)   | -0.0022 (6)   | 0.0020 (6)    | -0.0041 (7)   |
| C2  | 0.0151 (8)  | 0.0174 (9)  | 0.0158 (8)   | -0.0049 (7)   | -0.0004 (7)   | -0.0085 (7)   |
| C3  | 0.0132 (8)  | 0.0180 (9)  | 0.0168 (9)   | -0.0025 (7)   | -0.0040 (7)   | -0.0041 (7)   |
| C4  | 0.0117 (8)  | 0.0136 (9)  | 0.0204 (9)   | 0.0000 (7)    | 0.0003 (7)    | -0.0052 (7)   |
| C5  | 0.0180 (9)  | 0.0150 (9)  | 0.0175 (9)   | -0.0024 (7)   | 0.0009 (7)    | -0.0080 (7)   |
| C6  | 0.0153 (8)  | 0.0172 (9)  | 0.0124 (8)   | -0.0026 (7)   | -0.0020 (7)   | -0.0049 (7)   |
| C7  | 0.0135 (8)  | 0.0112 (8)  | 0.0099 (8)   | 0.0031 (6)    | -0.0021 (6)   | -0.0045 (7)   |
| C8  | 0.0140 (8)  | 0.0119 (8)  | 0.0190 (9)   | 0.0024 (7)    | -0.0049 (7)   | -0.0076 (7)   |
| C9  | 0.0187 (9)  | 0.0159 (9)  | 0.0180 (9)   | 0.0059 (7)    | -0.0080 (7)   | -0.0106 (8)   |
| C10 | 0.0205 (9)  | 0.0138 (9)  | 0.0108 (8)   | 0.0069 (7)    | -0.0020 (7)   | -0.0055 (7)   |
| C11 | 0.0159 (9)  | 0.0120 (9)  | 0.0159 (8)   | 0.0016 (7)    | -0.0006 (7)   | -0.0045 (7)   |
| C12 | 0.0162 (8)  | 0.0097 (8)  | 0.0124 (8)   | 0.0021 (7)    | -0.0042 (7)   | -0.0057 (7)   |
| C13 | 0.0122 (8)  | 0.0117 (8)  | 0.0128 (8)   | -0.0026 (7)   | 0.0019 (6)    | -0.0039 (7)   |
| C14 | 0.0161 (8)  | 0.0136 (9)  | 0.0143 (8)   | -0.0035 (7)   | -0.0002 (7)   | -0.0060 (7)   |
| C15 | 0.0166 (9)  | 0.0172 (9)  | 0.0157 (8)   | -0.0027 (7)   | -0.0047 (7)   | -0.0040 (7)   |
| C16 | 0.0163 (9)  | 0.0114 (9)  | 0.0188 (9)   | -0.0006 (7)   | 0.0002 (7)    | -0.0048 (7)   |
| C17 | 0.0169 (8)  | 0.0144 (9)  | 0.0168 (8)   | -0.0052 (7)   | 0.0021 (7)    | -0.0085 (7)   |
| C18 | 0.0129 (8)  | 0.0173 (9)  | 0.0127 (8)   | -0.0049 (7)   | -0.0004 (7)   | -0.0055 (7)   |

*Geometric parameters (Å, °)*

|             |              |             |             |
|-------------|--------------|-------------|-------------|
| Pd1—Cl2     | 2.3282 (4)   | C7—C8       | 1.391 (2)   |
| Pd1—Cl1     | 2.3471 (4)   | C8—C9       | 1.388 (3)   |
| Pd1—Se2     | 2.3790 (2)   | C8—H6       | 0.96 (2)    |
| Pd1—Se1     | 2.38098 (19) | C9—C10      | 1.392 (3)   |
| Se1—C7      | 1.9367 (16)  | C9—H7       | 0.89 (2)    |
| Se1—C1      | 1.9547 (17)  | C10—C11     | 1.388 (3)   |
| Se2—C12     | 1.9301 (16)  | C10—H8      | 0.89 (2)    |
| Se2—C13     | 1.9515 (17)  | C11—C12     | 1.396 (2)   |
| C1—C6       | 1.388 (2)    | C11—H9      | 0.97 (2)    |
| C1—C2       | 1.391 (2)    | C13—C14     | 1.394 (2)   |
| C2—C3       | 1.392 (3)    | C13—C18     | 1.394 (2)   |
| C2—H1       | 0.92 (2)     | C14—C15     | 1.391 (3)   |
| C3—C4       | 1.389 (3)    | C14—H10     | 0.96 (2)    |
| C3—H2       | 0.93 (2)     | C15—C16     | 1.389 (3)   |
| C4—C5       | 1.384 (3)    | C15—H11     | 0.94 (2)    |
| C4—H3       | 0.92 (2)     | C16—C17     | 1.389 (3)   |
| C5—C6       | 1.393 (2)    | C16—H12     | 0.95 (2)    |
| C5—H4       | 0.96 (2)     | C17—C18     | 1.391 (3)   |
| C6—H5       | 0.90 (2)     | C17—H13     | 0.91 (2)    |
| C7—C12      | 1.383 (2)    | C18—H14     | 0.91 (2)    |
| Cl2—Pd1—Cl1 | 94.066 (15)  | C9—C8—C7    | 119.29 (17) |
| Cl2—Pd1—Se2 | 87.714 (12)  | C9—C8—H6    | 120.0 (13)  |
| Cl1—Pd1—Se2 | 176.116 (12) | C7—C8—H6    | 120.7 (13)  |
| Cl2—Pd1—Se1 | 176.146 (12) | C8—C9—C10   | 120.37 (16) |
| Cl1—Pd1—Se1 | 87.742 (11)  | C8—C9—H7    | 118.7 (14)  |
| Se2—Pd1—Se1 | 90.279 (7)   | C10—C9—H7   | 121.0 (14)  |
| C7—Se1—C1   | 97.24 (7)    | C11—C10—C9  | 120.38 (17) |
| C7—Se1—Pd1  | 102.52 (5)   | C11—C10—H8  | 119.7 (13)  |
| C1—Se1—Pd1  | 99.60 (5)    | C9—C10—H8   | 119.8 (13)  |
| C12—Se2—C13 | 98.11 (7)    | C10—C11—C12 | 119.08 (17) |
| C12—Se2—Pd1 | 102.46 (5)   | C10—C11—H9  | 120.4 (13)  |
| C13—Se2—Pd1 | 99.58 (5)    | C12—C11—H9  | 120.5 (13)  |
| C6—C1—C2    | 121.35 (16)  | C7—C12—C11  | 120.48 (15) |
| C6—C1—Se1   | 119.04 (13)  | C7—C12—Se2  | 121.14 (12) |
| C2—C1—Se1   | 119.59 (13)  | C11—C12—Se2 | 118.38 (13) |
| C1—C2—C3    | 118.74 (16)  | C14—C13—C18 | 120.97 (16) |
| C1—C2—H1    | 123.1 (12)   | C14—C13—Se2 | 122.29 (13) |
| C3—C2—H1    | 118.2 (12)   | C18—C13—Se2 | 116.74 (12) |
| C4—C3—C2    | 120.52 (16)  | C15—C14—C13 | 119.05 (16) |
| C4—C3—H2    | 119.8 (13)   | C15—C14—H10 | 120.2 (11)  |
| C2—C3—H2    | 119.6 (13)   | C13—C14—H10 | 120.8 (11)  |
| C5—C4—C3    | 119.89 (17)  | C16—C15—C14 | 120.42 (16) |
| C5—C4—H3    | 119.0 (12)   | C16—C15—H11 | 121.0 (13)  |
| C3—C4—H3    | 121.1 (12)   | C14—C15—H11 | 118.5 (12)  |
| C4—C5—C6    | 120.53 (16)  | C15—C16—C17 | 120.13 (17) |
| C4—C5—H4    | 118.4 (13)   | C15—C16—H12 | 121.4 (12)  |

## supplementary materials

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|                 |              |                 |              |
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| C6—C5—H4        | 121.1 (13)   | C17—C16—H12     | 118.5 (12)   |
| C1—C6—C5        | 118.88 (16)  | C16—C17—C18     | 120.24 (16)  |
| C1—C6—H5        | 121.8 (13)   | C16—C17—H13     | 122.3 (13)   |
| C5—C6—H5        | 119.3 (13)   | C18—C17—H13     | 117.4 (13)   |
| C12—C7—C8       | 120.39 (15)  | C17—C18—C13     | 119.20 (16)  |
| C12—C7—Se1      | 120.80 (12)  | C17—C18—H14     | 119.2 (13)   |
| C8—C7—Se1       | 118.78 (13)  | C13—C18—H14     | 121.5 (13)   |
| C11—Pd1—Se1—C7  | 169.73 (5)   | C7—C8—C9—C10    | -0.9 (3)     |
| Se2—Pd1—Se1—C7  | -13.61 (5)   | C8—C9—C10—C11   | 0.7 (3)      |
| C11—Pd1—Se1—C1  | -90.57 (5)   | C9—C10—C11—C12  | 0.1 (3)      |
| Se2—Pd1—Se1—C1  | 86.08 (5)    | C8—C7—C12—C11   | 0.5 (2)      |
| C12—Pd1—Se2—C12 | -168.85 (5)  | Se1—C7—C12—C11  | -177.73 (13) |
| Se1—Pd1—Se2—C12 | 14.44 (5)    | C8—C7—C12—Se2   | -179.51 (12) |
| C12—Pd1—Se2—C13 | 90.55 (5)    | Se1—C7—C12—Se2  | 2.30 (19)    |
| Se1—Pd1—Se2—C13 | -86.16 (5)   | C10—C11—C12—C7  | -0.7 (2)     |
| C7—Se1—C1—C6    | 133.28 (14)  | C10—C11—C12—Se2 | 179.29 (13)  |
| Pd1—Se1—C1—C6   | 29.21 (14)   | C13—Se2—C12—C7  | 88.59 (14)   |
| C7—Se1—C1—C2    | -47.93 (14)  | Pd1—Se2—C12—C7  | -13.16 (14)  |
| Pd1—Se1—C1—C2   | -152.00 (13) | C13—Se2—C12—C11 | -91.38 (14)  |
| C6—C1—C2—C3     | -3.3 (3)     | Pd1—Se2—C12—C11 | 166.87 (12)  |
| Se1—C1—C2—C3    | 177.98 (13)  | C12—Se2—C13—C14 | 1.13 (15)    |
| C1—C2—C3—C4     | 1.3 (3)      | Pd1—Se2—C13—C14 | 105.32 (14)  |
| C2—C3—C4—C5     | 1.2 (3)      | C12—Se2—C13—C18 | -178.82 (13) |
| C3—C4—C5—C6     | -1.7 (3)     | Pd1—Se2—C13—C18 | -74.64 (13)  |
| C2—C1—C6—C5     | 2.7 (3)      | C18—C13—C14—C15 | 0.7 (2)      |
| Se1—C1—C6—C5    | -178.49 (13) | Se2—C13—C14—C15 | -179.21 (13) |
| C4—C5—C6—C1     | -0.2 (3)     | C13—C14—C15—C16 | -0.3 (3)     |
| C1—Se1—C7—C12   | -91.70 (14)  | C14—C15—C16—C17 | -0.4 (3)     |
| Pd1—Se1—C7—C12  | 9.85 (14)    | C15—C16—C17—C18 | 0.6 (3)      |
| C1—Se1—C7—C8    | 90.07 (14)   | C16—C17—C18—C13 | -0.2 (3)     |
| Pd1—Se1—C7—C8   | -168.37 (12) | C14—C13—C18—C17 | -0.5 (2)     |
| C12—C7—C8—C9    | 0.3 (2)      | Se2—C13—C18—C17 | 179.49 (12)  |
| Se1—C7—C8—C9    | 178.56 (12)  |                 |              |



Fig. 1

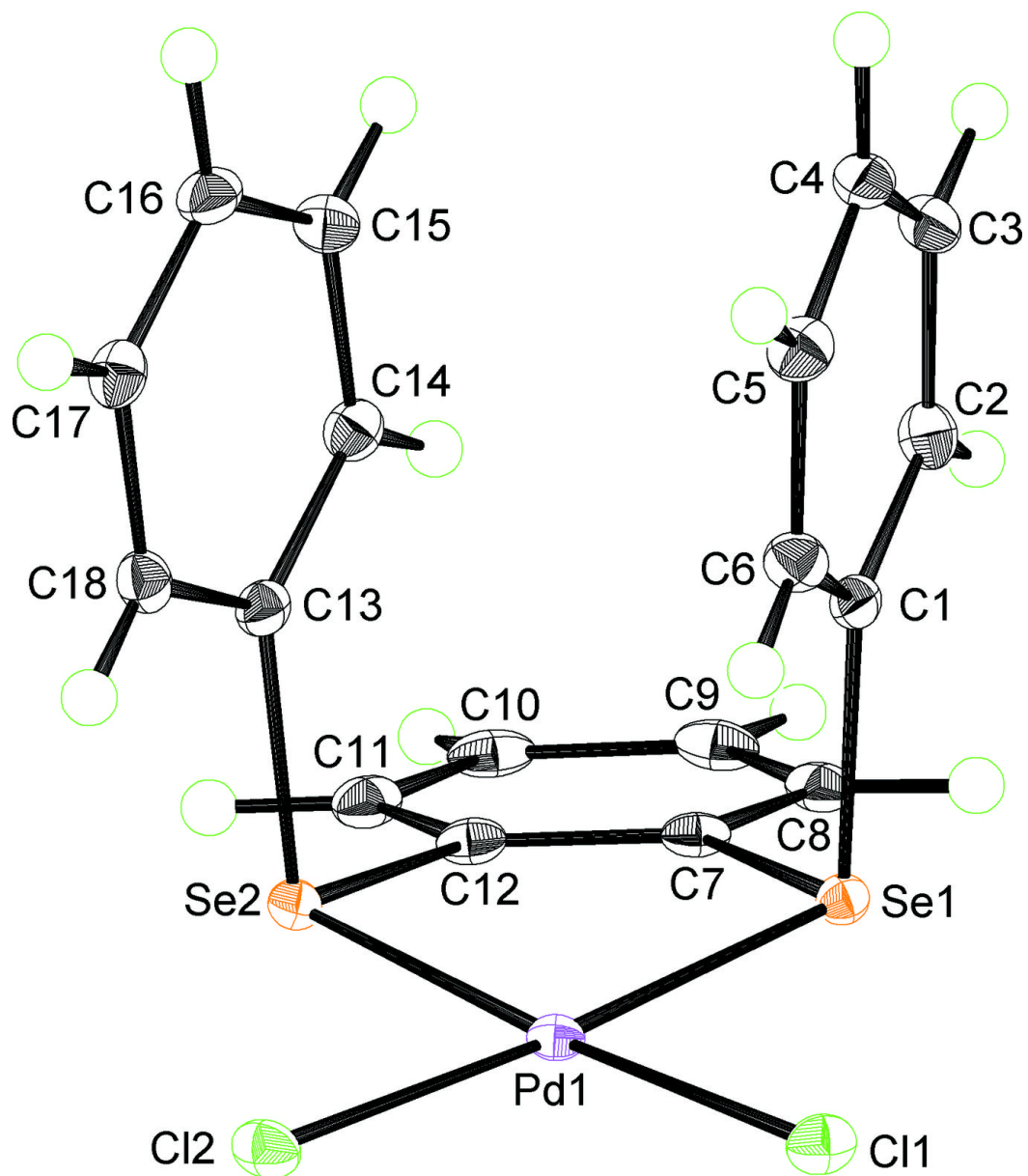


Fig. 2

