

Bis(tetra-*n*-butylammonium) (μ -*N,N'*-diselenium dinitride)bis[tribromo-palladate(II)]

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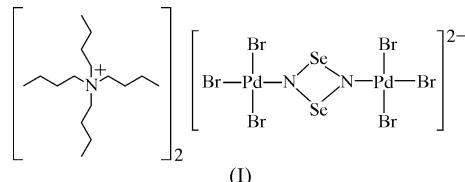
The reaction of Se_4N_4 with $(\text{Bu}_4\text{N})_2[\text{Pd}_2\text{Br}_6]$ gives the title compound, $(\text{C}_{16}\text{H}_{36}\text{N})_2[\text{Pd}_2\text{Br}_6(\text{N}_2\text{Se}_2)]$, in good yield. The $[\text{Pd}_2(\text{Se}_2\text{N}_2)\text{Br}_6]^{2-}$ anion lies on an inversion centre, and therefore the asymmetric unit contains half a formula unit. The crystal structure confirms the coordination of the Se_2N_2 unit to Pd through the N atoms, as previously assigned by IR spectroscopic analysis [Kelly, Slawin & Soriano-Rama (1997). *J. Chem. Soc. Dalton Trans.* pp. 559–562]. The title compound contains the longest Pd–N bond so far observed for such systems.

Comment

During the course of our work on the reactivity of Se_4N_4 towards metal centres, we have successfully demonstrated that, under the right circumstances, adducts of diselenium dinitride, Se_2N_2 , can be generated. Examples so far fully characterized by X-ray crystallography are $(\text{AlBr}_3)_2(\text{Se}_2\text{N}_2)$ (Kelly & Slawin, 1996), $(\text{PPh}_4)_2[\text{Pd}_2(\text{Se}_2\text{N}_2)\text{Br}_6]$ (Kelly *et al.*, 1997) and $(\text{PPh}_4)_2[\text{Pd}_2(\text{Se}_2\text{N}_2)\text{Cl}_6]$ (Kelly & Slawin, 1995). All are of great interest due to the fact that, unlike its sulfur analogue (the four-membered ring S_2N_2), Se_2N_2 is unknown in the free state. Thus, these compounds have the potential to act as sources of the free material *via* appropriate substitution reactions.

In terms of performing such reactions, however, the aluminium compound is hampered by its extreme air-sensitivity, while the tetraphenylphosphonium salts of the air-stable palladium adducts form in rather poor yield. By far the best yield thus far obtained for one of these palladium adducts occurs when Se_4N_4 is reacted with $(\text{Bu}_4\text{N})_2[\text{Pd}_2\text{Br}_6]$ to give $(\text{Bu}_4\text{N})_2[\text{Pd}_2(\text{Se}_2\text{N}_2)\text{Br}_6]$, (I) [typically *ca* 67% yield, compared with *ca* 20% for the tetraphenylphosphonium salts]. However, in our previous report on this compound, we used only IR spectroscopy and microanalysis as characterization techniques (Kelly *et al.*, 1997). Given that, thanks to its high yield, this compound is the obvious starting point for investigations into

the ability of such adducts to act as sources of the free nitride, and in the light of the general lack of structural data on complexes of Se_2N_2 , confirmation of the structure of (I) by X-ray crystallography becomes desirable.



(I)

The X-ray crystal structure of (I) confirms the presence of the four-membered Se_2N_2 ring, N-bound to the Pd centres, with the $[\text{Pd}_2(\text{Se}_2\text{N}_2)\text{Br}_6]^{2-}$ anion situated on an inversion centre. The asymmetric unit therefore contains half a formula unit. The Se–N bond lengths are almost equivalent, in direct contrast with the other examples shown in Table 2. Co-crystallization of the anion with tetraphenylphosphonium cations results in a greater asymmetry in the Se–N bond lengths than seen in (I). In comparison with $(\text{PPh}_4)_2[\text{Pd}_2(\text{Se}_2\text{N}_2)\text{Br}_6]$ (Kelly *et al.*, 1997), the presence of the tetrabutylammonium cations in (I) appears to result in a lengthening of the Pd–N bond, in addition to an increase in the symmetry of the Se_2N_2 unit.

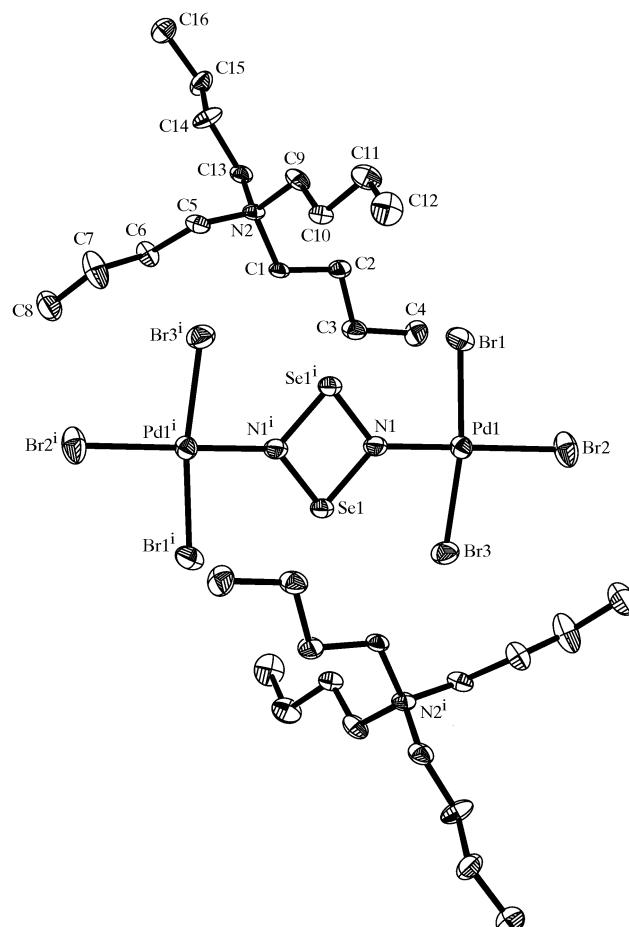


Figure 1

A view of (I), showing the atom-labelling scheme and with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $1 - x, 1 - y, 2 - z$.]

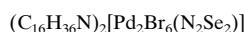
Analysis of the salts $(\text{PPh}_4)_2[\text{Pd}_2(\text{Se}_2\text{N}_2)\text{Br}_6]$ (Kelly *et al.*, 1997) and $(\text{PPh}_4)_2[\text{Pd}_2(\text{Se}_2\text{N}_2)\text{Cl}_6]$ (Kelly & Slawin, 1995) shows that there are interactions between the cations and anions which are absent from compound (I). In the case of $(\text{PPh}_4)_2[\text{Pd}_2(\text{Se}_2\text{N}_2)\text{Br}_6]$, there are C–H···Se interactions having C···Se distances of the order of 4.5 Å and C–H···Br interactions having C···Br distances in the range 3.8–3.95 Å. In addition, there is weak π – π stacking, with the Se_2N_2 unit held between two benzene rings, at a distance of 4.3 Å from each benzene ring. This weak π – π stacking is not observed in $(\text{PPh}_4)_2[\text{Pd}_2(\text{Se}_2\text{N}_2)\text{Cl}_6]$; instead, there are C–H···Se interactions having C···Se distances of the order of 4.3 Å and C–H···Cl interactions having C···Cl distances of the order of 3.6 Å. It is possible that the absence from (I) of relatively acidic C–H donors, such as the aromatic C–H groups of the tetraphenylphosphonium cations, may thus lead to a greater symmetry in the Se_2N_2 unit in the former.

A potentially important feature of (I) is the fact that the Pd–N bond is the longest so far observed for such systems (Tables 1 and 2). This fact, along with the high yield of the compound, suggests that it is likely to be the most effective starting material for studies into the liberation of the Se_2N_2 unit.

Experimental

The title compound was prepared according to the literature method of Kelly *et al.* (1997) and single crystals were grown by slow diffusion of diethyl ether into a CH_2Cl_2 solution.

Crystal data



$M_r = 1363.12$

Triclinic, $P\bar{1}$

$a = 9.081(2)$ Å

$b = 10.671(3)$ Å

$c = 12.415(3)$ Å

$\alpha = 95.131(4)^\circ$

$\beta = 98.598(4)^\circ$

$\gamma = 98.689(4)^\circ$

$V = 1168.1(5)$ Å³

$Z = 1$
 $D_x = 1.938 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 2921
reflections
 $\theta = 2.4\text{--}27.2^\circ$
 $\mu = 7.49 \text{ mm}^{-1}$
 $T = 150(2)$ K
Lath, orange
 $0.30 \times 0.20 \times 0.09$ mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer

ω rotation scans with narrow frames

Absorption correction: multi-scan (SADABS; Sheldrick, 2003)

$T_{\min} = 0.195$, $T_{\max} = 0.508$

8065 measured reflections

4049 independent reflections
3002 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.037$
 $\theta_{\text{max}} = 25.0^\circ$
 $h = -10 \rightarrow 10$
 $k = -12 \rightarrow 12$
 $l = -14 \rightarrow 14$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.131$

$S = 1.04$

4049 reflections

212 parameters

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 10.845P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\text{max}} = 0.85 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\text{min}} = -1.50 \text{ e } \text{\AA}^{-3}$$

Table 1
Selected geometric parameters (Å, °).

Pd1–N1	1.978 (7)	Pd1–Br3	2.4316 (12)
Pd1–Br1	2.4299 (12)	Se1–N1 ⁱ	1.806 (7)
Pd1–Br2	2.4066 (13)	Se1–N1	1.809 (7)
N1–Pd1–Br2	176.6 (2)	Br1–Pd1–Br3	170.88 (5)
N1–Pd1–Br1	85.4 (2)	Se1 ⁱ –N1–Se1	97.9 (3)
Br2–Pd1–Br1	94.39 (4)	Se1 ⁱ –N1–Pd1	130.5 (4)
N1–Pd1–Br3	85.7 (2)	Se1–N1–Pd1	130.2 (4)
Br2–Pd1–Br3	94.61 (4)	N1 ⁱ –Se1–N1	82.1 (3)

Symmetry code: (i) $1 - x$, $1 - y$, $2 - z$.

Table 2
Selected bond lengths (Å) in (I) and related compounds.

Compound	Metal–N	Se–N	Reference
(I)	1.978 (7)	1.806 (7), 1.809 (7)	<i>a</i>
$(\text{AlBr}_3)_2(\text{Se}_2\text{N}_2)$	1.92 (2)	1.77 (1), 1.81 (1)	<i>b</i>
$(\text{PPh}_4)_2[\text{Pd}_2(\text{Se}_2\text{N}_2)\text{Br}_6]$	1.875 (9)	1.809 (10), 1.920 (9)	<i>c</i>
$(\text{PPh}_4)_2[\text{Pd}_2(\text{Se}_2\text{N}_2)\text{Cl}_6]$	1.946 (4)	1.804 (5), 1.779 (4)	<i>d</i>

(a) This work; (b) Kelly & Slawin (1996); (c) Kelly *et al.* (1997); (d) Kelly & Slawin (1995).

Methylene ($\text{C}–\text{H} = 0.99$ Å) and methyl ($\text{C}–\text{H} = 0.98$ Å) H atoms were placed in geometric positions and refined using a riding model. $U_{\text{iso}}(\text{H})$ values were set at $1.2U_{\text{eq}}(\text{C})$ for methylene and $1.5U_{\text{eq}}(\text{C})$ for methyl H atoms. The data set was truncated at $2\theta = 50^\circ$, as only statistically insignificant data were present above this limit.

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

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: BM1591). Services for accessing these data are described at the back of the journal.

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supporting information

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Computing details

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

Bis(tetra-*n*-butylammonium) (μ -*N,N'*-diselenium dinitride)bis[tribromopalladate(II)]

Crystal data

(C ₁₆ H ₃₆ N) ₂ [Pd ₂ Br ₆ (N ₂ Se ₂)]	Z = 1
M _r = 1363.12	F(000) = 662
Triclinic, P1	D _x = 1.938 Mg m ⁻³
Hall symbol: -P 1	Mo K α radiation, λ = 0.71073 Å
<i>a</i> = 9.081 (2) Å	Cell parameters from 2921 reflections
<i>b</i> = 10.671 (3) Å	θ = 2.4–27.2°
<i>c</i> = 12.415 (3) Å	μ = 7.49 mm ⁻¹
α = 95.131 (4)°	T = 150 K
β = 98.598 (4)°	Lath, orange
γ = 98.689 (4)°	0.30 × 0.20 × 0.09 mm
<i>V</i> = 1168.1 (5) Å ³	

Data collection

Bruker SMART 1000 CCD area-detector	8065 measured reflections
diffractometer	4049 independent reflections
Radiation source: sealed tube	3002 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\text{int}} = 0.037$
ω rotation with narrow frames scans	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 1.7^\circ$
Absorption correction: multi-scan	$h = -10 \rightarrow 10$
(SADABS; Sheldrick, 2003)	$k = -12 \rightarrow 12$
$T_{\text{min}} = 0.195$, $T_{\text{max}} = 0.508$	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.050$	Hydrogen site location: inferred from neighbouring sites
wR(F^2) = 0.131	H-atom parameters constrained
S = 1.04	
4049 reflections	
212 parameters	
0 restraints	

$$w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 10.845P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.85 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.50 \text{ e } \text{\AA}^{-3}$$

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.

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	0.38454 (7)	0.27271 (7)	0.81142 (5)	0.0250 (2)
Br1	0.60510 (11)	0.35536 (10)	0.73407 (8)	0.0389 (3)
Br2	0.31511 (11)	0.08397 (11)	0.68135 (9)	0.0453 (3)
Br3	0.17092 (11)	0.22292 (10)	0.90619 (8)	0.0355 (3)
N1	0.4496 (8)	0.4223 (7)	0.9237 (6)	0.0273 (17)
Se1	0.37705 (10)	0.46360 (9)	1.04779 (7)	0.0267 (2)
N2	0.7449 (7)	0.8942 (7)	0.7313 (6)	0.0203 (15)
C1	0.5911 (9)	0.8135 (8)	0.7296 (7)	0.0214 (18)
H1A	0.5967	0.7689	0.7963	0.026*
H1B	0.5170	0.8720	0.7349	0.026*
C2	0.5298 (9)	0.7150 (9)	0.6320 (7)	0.027 (2)
H2A	0.5990	0.6522	0.6265	0.032*
H2B	0.5212	0.7568	0.5638	0.032*
C3	0.3748 (10)	0.6478 (9)	0.6468 (7)	0.029 (2)
H3A	0.3040	0.7100	0.6451	0.035*
H3B	0.3826	0.6156	0.7195	0.035*
C4	0.3115 (10)	0.5358 (10)	0.5569 (8)	0.036 (2)
H4A	0.2969	0.5682	0.4853	0.053*
H4B	0.2145	0.4925	0.5712	0.053*
H4C	0.3828	0.4755	0.5569	0.053*
C5	0.7997 (9)	0.9643 (9)	0.8442 (7)	0.0229 (19)
H5A	0.9027	1.0117	0.8458	0.027*
H5B	0.8079	0.9004	0.8969	0.027*
C6	0.7015 (9)	1.0590 (9)	0.8844 (7)	0.0242 (19)
H6A	0.7015	1.1291	0.8373	0.029*
H6B	0.5961	1.0146	0.8779	0.029*
C7	0.7581 (12)	1.1130 (12)	0.9996 (8)	0.047 (3)
H7A	0.8588	1.1655	1.0034	0.056*
H7B	0.7716	1.0417	1.0440	0.056*
C8	0.6588 (11)	1.1934 (11)	1.0505 (9)	0.045 (3)
H8A	0.6814	1.2810	1.0323	0.067*
H8B	0.6777	1.1934	1.1303	0.067*
H8C	0.5526	1.1583	1.0220	0.067*
C9	0.8593 (10)	0.8099 (9)	0.7057 (7)	0.027 (2)
H9A	0.8295	0.7710	0.6286	0.032*
H9B	0.9589	0.8650	0.7116	0.032*

C10	0.8776 (10)	0.7057 (9)	0.7764 (8)	0.029 (2)
H10A	0.7794	0.6483	0.7698	0.035*
H10B	0.9077	0.7432	0.8539	0.035*
C11	0.9946 (10)	0.6288 (10)	0.7454 (8)	0.034 (2)
H11A	1.0883	0.6880	0.7418	0.041*
H11B	0.9575	0.5826	0.6712	0.041*
C12	1.0323 (11)	0.5326 (10)	0.8245 (9)	0.042 (3)
H12A	1.0741	0.5777	0.8975	0.063*
H12B	1.1067	0.4849	0.7984	0.063*
H12C	0.9403	0.4732	0.8286	0.063*
C13	0.7294 (9)	0.9863 (9)	0.6456 (7)	0.025 (2)
H13A	0.6426	1.0297	0.6554	0.030*
H13B	0.7053	0.9363	0.5722	0.030*
C14	0.8670 (10)	1.0875 (9)	0.6474 (8)	0.031 (2)
H14A	0.9558	1.0455	0.6411	0.037*
H14B	0.8879	1.1423	0.7185	0.037*
C15	0.8441 (11)	1.1703 (9)	0.5546 (8)	0.033 (2)
H15A	0.8322	1.1169	0.4834	0.040*
H15B	0.7504	1.2066	0.5571	0.040*
C16	0.9753 (10)	1.2765 (9)	0.5632 (8)	0.032 (2)
H16A	0.9837	1.3320	0.6319	0.047*
H16B	0.9596	1.3262	0.5011	0.047*
H16C	1.0684	1.2406	0.5624	0.047*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.0231 (4)	0.0280 (4)	0.0221 (4)	0.0029 (3)	0.0017 (3)	-0.0002 (3)
Br1	0.0377 (6)	0.0458 (6)	0.0350 (5)	0.0040 (5)	0.0167 (4)	0.0014 (5)
Br2	0.0327 (6)	0.0482 (7)	0.0475 (6)	0.0093 (5)	-0.0050 (5)	-0.0194 (5)
Br3	0.0291 (5)	0.0411 (6)	0.0322 (5)	-0.0064 (4)	0.0053 (4)	0.0025 (4)
N1	0.028 (4)	0.031 (4)	0.021 (4)	-0.003 (3)	0.007 (3)	0.002 (3)
Se1	0.0243 (5)	0.0294 (5)	0.0255 (5)	-0.0028 (4)	0.0093 (4)	0.0007 (4)
N2	0.013 (3)	0.025 (4)	0.025 (4)	0.004 (3)	0.007 (3)	0.005 (3)
C1	0.014 (4)	0.029 (5)	0.022 (4)	-0.001 (4)	0.008 (3)	0.001 (4)
C2	0.015 (4)	0.036 (5)	0.028 (5)	-0.003 (4)	0.008 (4)	-0.002 (4)
C3	0.021 (5)	0.038 (6)	0.027 (5)	0.001 (4)	0.007 (4)	0.003 (4)
C4	0.021 (5)	0.040 (6)	0.040 (6)	-0.002 (4)	0.001 (4)	-0.006 (5)
C5	0.019 (4)	0.032 (5)	0.018 (4)	0.004 (4)	0.005 (3)	0.004 (4)
C6	0.017 (4)	0.032 (5)	0.022 (4)	0.012 (4)	-0.005 (3)	-0.002 (4)
C7	0.044 (6)	0.061 (8)	0.035 (6)	0.028 (6)	-0.001 (5)	-0.012 (5)
C8	0.035 (6)	0.056 (7)	0.041 (6)	0.010 (5)	0.010 (5)	-0.015 (5)
C9	0.022 (4)	0.035 (5)	0.027 (5)	0.011 (4)	0.009 (4)	0.001 (4)
C10	0.027 (5)	0.029 (5)	0.032 (5)	0.000 (4)	0.015 (4)	0.004 (4)
C11	0.025 (5)	0.046 (6)	0.035 (5)	0.012 (4)	0.007 (4)	0.006 (5)
C12	0.030 (5)	0.048 (7)	0.049 (6)	0.018 (5)	-0.001 (5)	0.009 (5)
C13	0.016 (4)	0.035 (5)	0.024 (5)	0.003 (4)	0.007 (4)	0.000 (4)
C14	0.017 (4)	0.033 (5)	0.040 (5)	-0.005 (4)	-0.002 (4)	0.016 (4)

C15	0.040 (6)	0.023 (5)	0.033 (5)	-0.005 (4)	0.005 (4)	0.007 (4)
C16	0.029 (5)	0.031 (5)	0.032 (5)	0.002 (4)	-0.002 (4)	0.005 (4)

Geometric parameters (\AA , $^{\circ}$)

Pd1—N1	1.978 (7)	C7—H7A	0.9900
Pd1—Br1	2.4299 (12)	C7—H7B	0.9900
Pd1—Br2	2.4066 (13)	C8—H8A	0.9800
Pd1—Br3	2.4316 (12)	C8—H8B	0.9800
Se1—N1 ⁱ	1.806 (7)	C8—H8C	0.9800
Se1—N1	1.809 (7)	C9—C10	1.491 (13)
N2—C5	1.504 (10)	C9—H9A	0.9900
N2—C13	1.517 (11)	C9—H9B	0.9900
N2—C1	1.522 (10)	C10—C11	1.510 (12)
N2—C9	1.522 (10)	C10—H10A	0.9900
C1—C2	1.508 (12)	C10—H10B	0.9900
C1—H1A	0.9900	C11—C12	1.524 (13)
C1—H1B	0.9900	C11—H11A	0.9900
C2—C3	1.525 (11)	C11—H11B	0.9900
C2—H2A	0.9900	C12—H12A	0.9800
C2—H2B	0.9900	C12—H12B	0.9800
C3—C4	1.539 (12)	C12—H12C	0.9800
C3—H3A	0.9900	C13—C14	1.519 (11)
C3—H3B	0.9900	C13—H13A	0.9900
C4—H4A	0.9800	C13—H13B	0.9900
C4—H4B	0.9800	C14—C15	1.522 (12)
C4—H4C	0.9800	C14—H14A	0.9900
C5—C6	1.544 (11)	C14—H14B	0.9900
C5—H5A	0.9900	C15—C16	1.500 (12)
C5—H5B	0.9900	C15—H15A	0.9900
C6—C7	1.478 (12)	C15—H15B	0.9900
C6—H6A	0.9900	C16—H16A	0.9800
C6—H6B	0.9900	C16—H16B	0.9800
C7—C8	1.502 (14)	C16—H16C	0.9800
N1—Pd1—Br2	176.6 (2)	C8—C7—H7B	108.5
N1—Pd1—Br1	85.4 (2)	H7A—C7—H7B	107.5
Br2—Pd1—Br1	94.39 (4)	C7—C8—H8A	109.5
N1—Pd1—Br3	85.7 (2)	C7—C8—H8B	109.5
Br2—Pd1—Br3	94.61 (4)	H8A—C8—H8B	109.5
Br1—Pd1—Br3	170.88 (5)	C7—C8—H8C	109.5
Se1 ⁱ —N1—Se1	97.9 (3)	H8A—C8—H8C	109.5
Se1 ⁱ —N1—Pd1	130.5 (4)	H8B—C8—H8C	109.5
Se1—N1—Pd1	130.2 (4)	C10—C9—N2	116.2 (7)
N1 ⁱ —Se1—N1	82.1 (3)	C10—C9—H9A	108.2
C5—N2—C13	111.3 (7)	N2—C9—H9A	108.2
C5—N2—C1	108.9 (6)	C10—C9—H9B	108.2
C13—N2—C1	108.7 (6)	N2—C9—H9B	108.2

C5—N2—C9	108.1 (6)	H9A—C9—H9B	107.4
C13—N2—C9	109.3 (6)	C9—C10—C11	112.1 (7)
C1—N2—C9	110.6 (6)	C9—C10—H10A	109.2
C2—C1—N2	117.6 (6)	C11—C10—H10A	109.2
C2—C1—H1A	107.9	C9—C10—H10B	109.2
N2—C1—H1A	107.9	C11—C10—H10B	109.2
C2—C1—H1B	107.9	H10A—C10—H10B	107.9
N2—C1—H1B	107.9	C10—C11—C12	114.0 (8)
H1A—C1—H1B	107.2	C10—C11—H11A	108.8
C1—C2—C3	108.5 (7)	C12—C11—H11A	108.8
C1—C2—H2A	110.0	C10—C11—H11B	108.8
C3—C2—H2A	110.0	C12—C11—H11B	108.8
C1—C2—H2B	110.0	H11A—C11—H11B	107.7
C3—C2—H2B	110.0	C11—C12—H12A	109.5
H2A—C2—H2B	108.4	C11—C12—H12B	109.5
C2—C3—C4	111.8 (7)	H12A—C12—H12B	109.5
C2—C3—H3A	109.2	C11—C12—H12C	109.5
C4—C3—H3A	109.2	H12A—C12—H12C	109.5
C2—C3—H3B	109.2	H12B—C12—H12C	109.5
C4—C3—H3B	109.2	N2—C13—C14	115.7 (7)
H3A—C3—H3B	107.9	N2—C13—H13A	108.4
C3—C4—H4A	109.5	C14—C13—H13A	108.4
C3—C4—H4B	109.5	N2—C13—H13B	108.4
H4A—C4—H4B	109.5	C14—C13—H13B	108.4
C3—C4—H4C	109.5	H13A—C13—H13B	107.4
H4A—C4—H4C	109.5	C13—C14—C15	111.8 (7)
H4B—C4—H4C	109.5	C13—C14—H14A	109.3
N2—C5—C6	116.2 (7)	C15—C14—H14A	109.3
N2—C5—H5A	108.2	C13—C14—H14B	109.3
C6—C5—H5A	108.2	C15—C14—H14B	109.3
N2—C5—H5B	108.2	H14A—C14—H14B	107.9
C6—C5—H5B	108.2	C16—C15—C14	111.1 (8)
H5A—C5—H5B	107.4	C16—C15—H15A	109.4
C7—C6—C5	111.4 (7)	C14—C15—H15A	109.4
C7—C6—H6A	109.3	C16—C15—H15B	109.4
C5—C6—H6A	109.3	C14—C15—H15B	109.4
C7—C6—H6B	109.3	H15A—C15—H15B	108.0
C5—C6—H6B	109.3	C15—C16—H16A	109.5
H6A—C6—H6B	108.0	C15—C16—H16B	109.5
C6—C7—C8	115.3 (8)	H16A—C16—H16B	109.5
C6—C7—H7A	108.5	C15—C16—H16C	109.5
C8—C7—H7A	108.5	H16A—C16—H16C	109.5
C6—C7—H7B	108.5	H16B—C16—H16C	109.5
Br1—Pd1—N1—Se1 ⁱ	-10.2 (5)	C9—N2—C5—C6	178.0 (7)
Br3—Pd1—N1—Se1 ⁱ	171.8 (5)	N2—C5—C6—C7	174.7 (8)
Br1—Pd1—N1—Se1	-173.1 (5)	C5—C6—C7—C8	-172.6 (10)
Br3—Pd1—N1—Se1	9.0 (5)	C5—N2—C9—C10	64.2 (9)

Se1 ⁱ —N1—Se1—N1 ⁱ	0.0	C13—N2—C9—C10	−174.6 (7)
Pd1—N1—Se1—N1 ⁱ	166.9 (8)	C1—N2—C9—C10	−54.9 (10)
Pd1—N1—Se1—Se1 ⁱ	166.9 (8)	N2—C9—C10—C11	−179.3 (8)
C5—N2—C1—C2	−167.7 (8)	C9—C10—C11—C12	172.4 (8)
C13—N2—C1—C2	71.0 (9)	C5—N2—C13—C14	51.4 (9)
C9—N2—C1—C2	−49.1 (10)	C1—N2—C13—C14	171.3 (7)
N2—C1—C2—C3	−179.0 (7)	C9—N2—C13—C14	−67.9 (9)
C1—C2—C3—C4	−173.8 (8)	N2—C13—C14—C15	176.7 (7)
C13—N2—C5—C6	58.0 (9)	C13—C14—C15—C16	175.2 (8)
C1—N2—C5—C6	−61.8 (9)		

Symmetry code: (i) $-x+1, -y+1, -z+2$.