Crystal structure of a dicationic Pd\textsuperscript{II} dimer containing a 2-[(diisopropylphosphanyl)methyl]-quinoline-8-thiolate pincer ligand

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A dicationic Pd\textsuperscript{II} dimer, bis[2-[(diisopropylphosphanyl)methyl]quinoline-8-thiolato]palladium(II) bis(hexafluoridoantimonate) dichloromethane monosolvate, \([\text{Pd}_2(\text{C}_{32}\text{H}_{42}\text{N}_2\text{P}_2\text{S}_2))(\text{SbF}_6)_2\cdot\text{CH}_2\text{Cl}_2]\), containing a 2-[(diisopropylphosphanyl)methyl]quinoline-8-thiolate pincer ligand, was isolated and its crystal structure determined. The title compound crystallizes in the orthorhombic space group \(Pbca\). A dimeric structure is formed by bridging coordination of the S atoms. The geometry of the butterfly-shaped Pd\textsubscript{2}S\textsubscript{2} core is bent, with a hinge angle of 108.0 (1)° and a short Pd···Pd distance of 2.8425 (7) Å. These values are the lowest measured compared to ten dicationic dimers with a Pd\textsubscript{2}S\textsubscript{2} core featuring sulfur atoms embedded in a chelating ligand. One of the two hexafluoridoantimonate anions is disordered over two sets of positions with site-occupancy factors of 0.711 (5) and 0.289 (5). The crystal structure is stabilized by many C—H···F and C—H···π interactions, forming a supramolecular network.

1. Chemical context
The stereoelectronic properties of transition-metal complexes can be finely modulated thanks to the ligands introduced on the metal coordination sphere, and this plays a fundamental role in organometallic chemistry. Over the past two decades, impressive developments have been achieved with pincer complexes, which nicely illustrate how the properties and reactivity of a complex can be adjusted through ligand modifications (Morales-Morales, 2018). In pincer complexes, the central \(M—X\) bond is enforced by the coordination of two peripheral donor groups (\(D\)), and the chelating rigid nature of the monoanionic \(DXD\) pincer ligand bestows a unique balance between stability and reactivity. This has led to spectacular catalytic developments, including with pincer complexes based on Pd, a transition metal that occupies a central place in organometallic catalysis. As far as Pd is concerned, the main topology of the used monoanionic pincer ligands consists of an aryl central moiety featuring two coordinating side arms, as illustrated in Fig. 1 (model I). These complexes have been successfully applied to C—C or C—X bond-forming catalytic transformations. The impact of the side groups (coordinating atom and linker) on the catalytic performances has been explored (Selander et al., 2011). We have developed new models of Pd pincer complexes varying the aromatic central ring, introducing indenyl and indolyl moieties (model II in Fig. 1). The nature of the central ring was found to significantly
impact the catalytic activity of the Pd complexes in the allylation of amines (Lisena et al., 2013).

Seeking to further modify the structure of the Pd pincer complexes so that the catalytic activity can be modulated, we now aim to incorporate an extended π-system as the central moiety (so that rigidity is increased). We have thus designed and prepared a pincer PNS Pd complex based on a 8-thiolate-quinoline featuring a methylenephosphine side arm (model III in Fig. 1). We report herein that when cationizing the corresponding chloro palladium pincer complex \( \text{I} \) with AgSbF\(_6\), a dimeric dicationic species \( \text{II} \) crystallized with a tight S-bridging assembly of the two quinoline-based PNS Pd pincer fragments. The structural features are discussed. It is worth noting that we have previously reported S-bridged homo and heteropolymetallic species derived from Pd pincer complexes of type \( \text{II} \) (Nebra et al., 2011, 2012).

2. Structural commentary

X-ray diffraction of the yellow crystals obtained from \( 2\text{(SbF}_6\text{)}_2 \) revealed a dimeric structure, composed of two cationic PNSPd fragments, that crystallizes in the orthorhombic system and \( Pbcn \) space group (Figs. 2 and 3; selected bond lengths and bond angles are given in Table 1). The dicationic nature of the structure is confirmed by the presence of two SbF\(_6^-\) units per dimer. The two PNSPd fragments are connected to each other by two bridging S atoms. The S donor atom of each PNSPd fragment completes the coordination sphere of the other, forming a Pd\(_2\)S\(_2\) diamond core.

For each PNSPd fragment, besides the two bridging S atoms, the Pd atom is coordinated by one N atom and one P atom, completing a tetracoordinate sphere that deviates

![Figure 1](image1.png)

Schematic representation of Pd pincer complexes \( \text{I} \text{- III} \)

![Figure 2](image2.png)

The molecular structure of the title compound with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

![Figure 3](image3.png)

Detail of the molecular structure of \( 2^{2+} \), showing the main atom-numbering scheme and displacement ellipsoids at the 50% probability level. H atoms and \('i'Pr groups have been omitted for clarity.

Table 1

| Selected geometric parameters (Å, °) |
|-------------------------------------|
| Pd1—N1 2.027 (5) Pd2—S1 2.3184 (16) |
| Pd1—P1 2.2455 (18) Pd2—S2 2.3602 (17) |
| Pd1—S1 2.3349 (16) P1—C1 1.825 (6) |
| Pd1—S2 2.3657 (17) P2—C17 1.836 (6) |
| Pd1—Pd2 2.8425 (7) S1—C4 1.784 (7) |
| Pd2—N2 2.027 (5) S2—C25 1.774 (7) |
| Pd2—P2 2.2417 (18) N1—Pd1—P1 83.86 (15) |
| N1—Pd1—S2 168.93 (15) P2—Pd2—S1 106.34 (6) |
| N1—Pd1—S1 86.49 (15) P2—Pd2—S2 170.20 (6) |
| N1—Pd1—Pd2 117.54 (14) S2—Pd1—S1 74.71 (5) |
| N1—Pd1—S1 51.89 (15) P1—Pd1—Pd2 129.40 (5) |
| Pd1—Pd2 53.28 (4) S2—Pd1—S1 114.86 (14) |
| N1—Pd1—Pd2 136.83 (5) S2—Pd1—Pd2 53.40 (4) |
| N1—Pd1—S2 51.83 (4) Pd2—S1—Pd1 74.88 (5) |
| Pd2—S2—Pd1 53.84 (4) Pd1—S2—Pd2 74.88 (5) |

Acta Cryst. (2022). E78, 18–22 Clerc et al. • \[\text{Pd}_2(\text{C}_{19}\text{H}_{27}\text{N}_2\text{P}_2\text{S}_2)^{2+}\text{(SbF}_6\text{)}_2\cdot\text{CH}_2\text{Cl}_2\]
slightly from square-planar geometry (deviation estimated by the \( /C_28\) index, with values of 0.15 and 0.16 for Pd1 and Pd2, respectively) (Yang et al., 2007). The Pd—N and the Pd—P bond lengths are almost identical for the two fragments \([\text{Pd1—N1} = 2.027 (5), \text{Pd2—N2} = 2.027 (5) \text{Å} \text{ and } \text{Pd1—P1} = 2.2455 (18), \text{Pd2—P2} = 2.2417 (18) \text{Å}]\), and the values are in the range of those observed for quinoline/phosphine chelate Pd complexes (Mori et al., 2021; Scharf et al., 2014 for example). The coordination environment around each Pd atom and the quinoline moiety is approximately planar [dihedral angles of 13.1 (1)° for Pd1 and 2.3 (1)° for Pd2, as estimated by the dihedral angle between the mean planes of the two fragments].

As for the Pd\(_2\)S\(_2\) core, the two Pd—S bond lengths for each Pd atom are slightly different and, interestingly, the bonds between the Pd atoms and the bridging S atom of the other fragment are shorter [2.3149 (16) and 2.3184 (16) for Pd1—S2 and Pd2—S1, respectively] than the bonds between the Pd atoms and the chelating S atom of the pincer ligand [2.3657 (17) and 2.3602 (17) for Pd1—S1 and Pd2—S2, respectively]. This is most likely due to the rigidity of the 8-thio-quinoline moiety (the C3—C4—S1 and C26—C27—S2 angles deviate from 120° by less than 2°). The two S atoms are noticeably pyramidalized (\( /C_6\) S = 287 and 290° for S1 and S2, respectively). The hinge angle of the core unit (involving the two [S,Pd,S] planes) has a value of 108.0 (1)°, which is in fact the lowest value reported for such kind of dicaticion species with a Pd\(_2\)S\(_2\) core (see the Database survey section). This results in a rather short Pd1—Pd2 distance of 2.8425 (7) Å, which is significantly shorter than the sum of van der Waals radii (4.10 Å; Batsanov et al., 2001) and exceeds the sum of the covalent radii (2.78 Å; Cordero et al., 2008) by only 2%.

3. Supramolecular features

The crystal packing of the title compound, illustrated in Fig. 4, involves weak intramolecular C—H···Cg contacts, and intermolecular C—H···F contacts between the cations and anions, which link the components in a three-dimensional network (Table 2, Figs. 5 and 6). No classical hydrogen-bonding interactions were found.

Each dicationic unit is surrounded by eight SbF\(_6^-\) anions, engaged in weak C—H···F contacts with C···F distances in the range 3.128 (9)—3.172 (13) Å (associated with H···F distances in the range 2.27—2.54 Å) (Fig. 5). As for the SbF\(_6^-\) anions, two different situations can be observed. One of the anions (containing Sb1) displays weak C—H···F contacts with
C—H bonds from five different dicaticonic units, while the other one (containing Sb2), interacts weakly with C—H bonds from three dicaticonic units and from a CH2Cl2 solvent molecule. Finally, an intramolecular C—H⋯C short contact is observed between one of the CH3 of the Pr groups of one PNSPd pincer fragment (Pd2) and the benzo ring of the quinoline moiety of the other fragment [C16⋯Cg1 = 3.701 (8) Å, associated with a H16A⋯Cg1 distance of 2.93 Å] (Fig. 6). It should be noted that a significantly longer distance (H28B⋯Cg2 of 3.2 Å) is observed for the other part of the unit (CH3 group of the Pd2 fragment with the benzo ring of the other), indicating a non-symmetrical organization of the dimer.

4. Database survey

To the best of our knowledge, structures of quinoline-based PNSPd dicaticonic dimers as described herein have not been reported previously. A structure survey was carried out in the Cambridge Structural Database (CSD version 5.42, update of November 2020; Groom et al., 2016). It revealed 28 hits for dicaticonic dimers with a Pd2S2 core, of which ten can be compared with the title compound as they feature the sulfur atoms embedded in a chelating ligand [refcodes CUYLIT (Kouno et al., 2015), NORGEG (Albinati et al., 1997), NOXVAZ (Chen et al., 2015), POTMUG (Kersting, 1998), QOCCUG (Su et al., 2000), SELGUL (Leung et al., 1998), TEGWUY (Cabeza et al., 2006), TIXLOE (Mane et al., 2019), XAHBUI (Nayan Sharma et al., 2015), XULYUZ (Azizpoor Fard et al., 2015)]. Hinge angles in the range 115.3–156.6° were measured for these compounds, all values higher than that measured for the title compound [108.0 (1)°].

5. Synthesis and crystallization

A solution of PNS-Pd-Cl 1 (Scharf et al., 2014) (1.0 equiv., 0.1 M) was added dropwise over 5 min to a suspension of AgSbF6 (1.0 equiv.) in CH2Cl2 (0.1 M) at 195 K. After the addition, the reaction mixture was allowed to quickly warm up to room temperature and was stirred for 2 h. The reaction was then filtered via canula, and the solvent was removed in vacuo to yield the corresponding dicaticonic complex as a reddish powder (95%). X-ray quality crystals were grown by slow diffusion at 273 K of pentane into a concentrated solution of 2 in CH2Cl2. 1H NMR (300 MHz, CD2Cl2): δ = 8.60 (d, J = 8.5 Hz, 2H), 8.23 (dd, J = 7.5, 1.2 Hz, 2H), 8.13 (dd, J = 8.5, 1.2 Hz, 2H), 7.87–7.75 (m, 4H), 4.16 (dd, J = 18.9, 9.7 Hz, 2H), 3.86 (dd, J = 18.9, 11.2 Hz, 2H), 2.47 (m, 2H), 1.79 (dd, J = 20.1, 7.1 Hz, 6H), 1.49 (dd, J = 17.4, 6.9 Hz, 6H), 1.28 (m, 2H), 0.82 (dd, J = 16.1, 6.9 Hz, 6H), 0.08 (dd, J = 19.7, 7.1 Hz, 6H).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. One of the two hexafluoroantimonate anions is disordered over two positions, for which occupancies were refined, converging to 0.711 (5) and 0.289 (5). SAME, DELU and SIMU restraints were applied (Sheldrick, 2015b). All H atoms were fixed geometrically and treated as riding with C—H = 0.95 Å (aromatic), 0.98 Å (CH3), 0.99 Å (CH2) or 1.0 Å (CH), with Uiso(H) = 1.2Ueq(CH, CH2) or 1.5Ueq(CH3).

Table 2

| Cg1 is the centroid of the C21–C26 ring. | D—H⋯A | D—H | H⋯A | D—A | D—H⋯A |
|---|---|---|---|---|---|
| C1—H1A⋯F3 | 0.99 | 2.34 | 3.305 (9) | 166 |
| C7—H7⋯F1u | 0.95 | 2.37 | 3.229 (8) | 151 |
| C11—H11⋯F2nu | 1.00 | 2.27 | 3.128 (9) | 143 |
| C17—H17A⋯F11u | 0.99 | 2.41 | 3.279 (10) | 147 |
| C22—H22⋯F8w | 0.95 | 2.33 | 3.190 (11) | 150 |
| C23—H23⋯F1u | 0.95 | 2.53 | 3.396 (9) | 152 |
| C27—H27⋯F12a | 1.00 | 2.43 | 3.322 (10) | 148 |
| C31—H31C⋯F3w | 0.98 | 2.50 | 3.399 (9) | 152 |
| C33—H33A⋯F10l | 0.99 | 2.54 | 3.172 (13) | 122 |
| C16—H16A⋯Cg1 | 0.98 | 2.93 | 3.701 (8) | 136 |

Symmetry codes: (i) x, y, z + 1/2; (ii) x, −y+2, −z+1; (iii) x+1, −y+2, −z+1; (iv) x, y, z + 1; (v) x−1/2, −y+1, z + 1/2; (vi) x+1, −y+2, z + 1/2.

Table 3

| Experimental details. | Crystal data | Chemical formula | M | Crystal system, space group | Temperature (K) | V (Å³) | Z | µ (mm⁻¹) | Crystal size (mm) |
|---|---|---|---|---|---|---|---|---|---|
| | [Pd2(C3H4N2P2S2)](SbF6)2 | CH2Cl2 | 1349.86 | Orthorhombic, Pbca | 23.5167 (19), 16.1492 (14), 24.0414 (18) | 30261 | 8 | 2.30 | 0.10 × 0.08 × 0.04 |

Data collection

Diffractometer: Bruker Kappa APEXII CCD Quazar

Absorption correction: Multi-scan (SADABS; Bruker, 2014)

Tmax, Tmax = 0.677, 0.728

No. of measured, independent and observed | H > 2σ(I) | reflections | Rint | (sin θ/λ)max (Å⁻¹) | R | S |
|---|---|---|---|---|---|---|
| | | | | | | |

Refinement

R[F² > 2σ(F²)], wR(F²), S | 0.046, 0.113, 1.01 | 9812 | 577 | 213 | H-atom parameters constrained | Δρmax, Δρmin (e Å⁻³) | 1.50, −1.07 |

Computer programs: APEX2 (Bruker, 2014) and SHELXT (Sheldrick, 2015a), SHELXL2016/3 (Sheldrick, 2015b), SHELXTL (Sheldrick, 2008) and Mercury (Macrae et al., 2020), PLATON (Spek, 2020) and publICIF (Westrip, 2010).

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Crystal structure of a dicationic Pd^{II} dimer containing a 2-[(diisopropylphosphanyl)methyl]quinoline-8-thiolate pincer ligand

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Computing details

Data collection: APEX2 (Bruker, 2014); cell refinement: SAINT (Bruker, 2014); data reduction: SAINT (Bruker, 2014); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: SHELXL2018/3 (Sheldrick, 2015b); molecular graphics: SHELXTL (Sheldrick, 2008) and Mercury (Macrae et al., 2020); software used to prepare material for publication: PLATON (Spek, 2020) and publCIF (Westrip, 2010).

Bis(2-[(diisopropylphosphanyl)methyl]quinoline-8-thiolato)palladium(II) bis(hexafluoroantimonate) dichloromethane monosolvate

Crystal data

\[\text{[Pd}_2\text{C}_{32}\text{H}_{42}\text{N}_2\text{P}_2\text{S}_2]\text{SbF}_6\cdot\text{CH}_2\text{Cl}_2\]

\[M_r = 1349.96\]

Orthorhombic, Pbc\(a\)

\[a = 23.5167\ (19) \text{ Å}\]

\[b = 16.1492\ (14) \text{ Å}\]

\[c = 24.0414\ (18) \text{ Å}\]

\[V = 9130.3\ (13) \text{ Å}^3\]

\[Z = 8\]

\[F(000) = 5232\]

Data collection

Bruker Kappa APEXII CCD Quazar diffractometer

Radiation source: Incoatec microfocus sealed tube

Phi and \(\omega\) scans

Absorption correction: multi-scan (SADABS; Bruker, 2014)

\[T_{\text{min}} = 0.677, T_{\text{max}} = 0.728\]

Refinement

Refinement on \(F^2\)

Least-squares matrix: full

\[R[F^2 > 2\sigma(F^2)] = 0.046\]

\[wR(F^2) = 0.113\]

\[S = 1.01\]

9812 reflections

577 parameters

213 restraints

Primary atom site location: dual

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

\[D_{\text{c}} = 1.964 \text{ Mg m}^{-3}\]

Mo \(K\alpha\) radiation, \(\lambda = 0.71073\ \text{Å}\)

Cell parameters from 9991 reflections

\[\theta = 3.0–22.0^\circ\]

\[\mu = 2.30\ \text{mm}^{-1}\]

\[T = 193 \text{ K}\]

Plate, yellow

0.10 \times 0.08 \times 0.04 \text{ mm}

152552 measured reflections

9812 independent reflections

6263 reflections with \(I > 2\sigma(I)\)

\[R_{\text{int}} = 0.122\]

\[\theta_{\text{max}} = 26.9^\circ, \theta_{\text{min}} = 1.9^\circ\]

\[h = -29\rightarrow29\]

\[k = -20\rightarrow20\]

\[l = -30\rightarrow30\]
\[ w = \frac{1}{\sigma^2(F_o^2) + (0.0384P)^2 + 45.7164P} \]

where \( P = (F_o^2 + 2F_c^2)/3 \)
\[ (\Delta/\sigma)_{\max} = 0.002 \]
\[ \Delta \rho_{\max} = 1.50 \text{ e } \AA^{-3} \]
\[ \Delta \rho_{\min} = -1.07 \text{ e } \AA^{-3} \]

**Special details**

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

|     | x    | y    | z    | U_{iso}/U_{eq} | Occ. (<1) |
|-----|------|------|------|----------------|-----------|
| Pd1 | 0.57179 (2) | 0.75620 (3) | 0.64839 (2) | 0.02433 (12) |
| Pd2 | 0.45502 (2) | 0.74339 (3) | 0.67769 (2) | 0.02348 (12) |
| P  | 0.61946 (7) | 0.69467 (10) | 0.57882 (7) | 0.0291 (4) |
| P2 | 0.37442 (7) | 0.81155 (10) | 0.65817 (7) | 0.0268 (4) |
| S1  | 0.51907 (7) | 0.84184 (10) | 0.70934 (6) | 0.0284 (4) |
| S2  | 0.52977 (7) | 0.65162 (10) | 0.69984 (7) | 0.0304 (4) |
| N1  | 0.5978 (2) | 0.8622 (3) | 0.6110 (2) | 0.0248 (11) |
| N2  | 0.4144 (2) | 0.6430 (3) | 0.6462 (2) | 0.0243 (11) |
| C1  | 0.6648 (3) | 0.7812 (4) | 0.5584 (3) | 0.0311 (15) |
| H1A | 0.701799 | 0.776732 | 0.577766 | 0.037* |
| H1B | 0.671982 | 0.778550 | 0.517885 | 0.037* |
| C2  | 0.6380 (3) | 0.8623 (4) | 0.5723 (3) | 0.0270 (14) |
| C3  | 0.5708 (3) | 0.9343 (4) | 0.6262 (3) | 0.0285 (14) |
| C4  | 0.5282 (3) | 0.9334 (4) | 0.6688 (2) | 0.0274 (14) |
| C5  | 0.5009 (3) | 1.0053 (4) | 0.6821 (3) | 0.0355 (16) |
| H5  | 0.472562 | 1.005157 | 0.710333 | 0.043* |
| C6  | 0.5141 (3) | 1.0796 (4) | 0.6546 (3) | 0.046 (2) |
| H6  | 0.493775 | 1.128646 | 0.663638 | 0.056* |
| C7  | 0.5560 (3) | 1.0825 (4) | 0.6149 (3) | 0.0418 (18) |
| H7  | 0.565065 | 1.133373 | 0.597251 | 0.050* |
| C8  | 0.5854 (3) | 1.0096 (4) | 0.6005 (3) | 0.0328 (16) |
| C9  | 0.6293 (3) | 1.0089 (4) | 0.5603 (3) | 0.0352 (16) |
| H9  | 0.640761 | 1.058936 | 0.542901 | 0.042* |
| C10 | 0.6549 (3) | 0.9363 (4) | 0.5467 (3) | 0.0360 (16) |
| H10 | 0.684390 | 0.935601 | 0.519667 | 0.043* |
| C11 | 0.6661 (3) | 0.6081 (4) | 0.5938 (3) | 0.0432 (19) |
| H11 | 0.641178 | 0.558737 | 0.599777 | 0.052* |
| C12 | 0.6989 (4) | 0.6226 (5) | 0.6488 (3) | 0.059 (2) |
| H12A | 0.722728 | 0.574233 | 0.656806 | 0.089* |
| H12B | 0.671824 | 0.630923 | 0.679202 | 0.089* |
| H12C | 0.723057 | 0.671770 | 0.645046 | 0.089* |
| C13 | 0.7053 (4) | 0.5874 (5) | 0.5455 (4) | 0.067 (3) |
| H13A | 0.731357 | 0.633794 | 0.538993 | 0.101* |
| H13B | 0.682578 | 0.577628 | 0.511957 | 0.101* |
| H13C | 0.727221 | 0.537571 | 0.554384 | 0.101* |
| C14 | 0.5769 (3) | 0.6701 (4) | 0.5169 (3) | 0.0381 (17) |
supporting information

H14  0.603766  0.662319  0.485083  0.046*
C15  0.5379 (3)  0.7421 (5)  0.5027 (3)  0.055 (2)
H15A  0.515430  0.728286  0.469620  0.082*
H15B  0.560770  0.791607  0.495211  0.082*
H15C  0.512291  0.752911  0.534025  0.082*
C16  0.5430 (4)  0.5895 (5)  0.5238 (3)  0.055 (2)
H16A  0.515351  0.596008  0.553935  0.083*
H16B  0.569058  0.544039  0.532664  0.083*
H16C  0.522942  0.577044  0.489023  0.083*
C17  0.3362 (3)  0.7327 (4)  0.6178 (3)  0.0331 (16)
H17A  0.295987  0.731432  0.629853  0.040*
H17B  0.336994  0.748252  0.577947  0.040*
C18  0.3612 (3)  0.6488 (4)  0.6244 (3)  0.0311 (15)
C19  0.3333 (3)  0.5775 (4)  0.6056 (3)  0.0341 (16)
H19  0.295630  0.581288  0.591709  0.041*
C20  0.3598 (3)  0.5032 (4)  0.6072 (3)  0.0351 (17)
H20  0.340085  0.455065  0.595184  0.042*
C21  0.4163 (3)  0.4960 (4)  0.6265 (3)  0.0308 (15)
C22  0.4467 (3)  0.4207 (4)  0.6265 (3)  0.0385 (18)
H22  0.428883  0.371171  0.614199  0.046*
C23  0.5014 (4)  0.4194 (4)  0.6440 (3)  0.0446 (19)
H23  0.522041  0.368879  0.643264  0.053*
C24  0.5279 (3)  0.4912 (4)  0.6632 (3)  0.0383 (17)
H24  0.566472  0.488814  0.675010  0.046*
C25  0.4995 (3)  0.5650 (4)  0.6654 (2)  0.0283 (15)
C26  0.4427 (3)  0.5686 (4)  0.6464 (2)  0.0257 (14)
C27  0.3749 (3)  0.9063 (4)  0.6176 (3)  0.0360 (16)
H27  0.388653  0.951774  0.642469  0.043*
C28  0.4167 (3)  0.8992 (5)  0.5693 (3)  0.0457 (19)
H28A  0.402839  0.857879  0.542684  0.069*
H28B  0.454011  0.882220  0.583404  0.069*
H28C  0.420108  0.952991  0.550674  0.069*
C29  0.3144 (3)  0.9306 (5)  0.5971 (4)  0.058 (2)
H29A  0.315917  0.984838  0.578951  0.086*
H29B  0.288394  0.933056  0.628914  0.086*
H29C  0.300799  0.889035  0.570524  0.086*
C30  0.3325 (3)  0.8286 (4)  0.7209 (3)  0.0330 (16)
H30  0.293211  0.845049  0.709329  0.040*
C31  0.3281 (3)  0.7487 (5)  0.7547 (3)  0.0458 (19)
H31A  0.366266  0.730653  0.765698  0.069*
H31B  0.310159  0.705558  0.732012  0.069*
H31C  0.305098  0.758646  0.788001  0.069*
C32  0.3579 (3)  0.8998 (5)  0.7557 (3)  0.051 (2)
H32A  0.337543  0.903830  0.791199  0.077*
H32B  0.354032  0.951989  0.735303  0.077*
H32C  0.398210  0.888704  0.762806  0.077*
Sb1  0.34706 (2)  0.68208 (3)  0.44208 (2)  0.03304 (12)
F1  0.4044 (2)  0.7271 (3)  0.3981 (2)  0.0681 (14)
### Atomic displacement parameters (Å²)

|     | U₁₁    | U₂₂    | U₃₃    | U₁₂    | U₁₃    | U₂₃    |
|-----|--------|--------|--------|--------|--------|--------|
| Pd1 | 0.0225 (2) | 0.0220 (2) | 0.0285 (2) | −0.0019 (2) | −0.0001 (2) | 0.0012 (2) |
| Pd2 | 0.0227 (2) | 0.0216 (2) | 0.0262 (2) | −0.0024 (2) | 0.0003 (2) | −0.0004 (2) |
| P1  | 0.0255 (9) | 0.0231 (9) | 0.0385 (9) | −0.0015 (7) | 0.0033 (8) | −0.0045 (7) |
| P2  | 0.0244 (9) | 0.0243 (8) | 0.0318 (9) | −0.0001 (7) | 0.0001 (7) | −0.0035 (7) |
| S1  | 0.0293 (9) | 0.0279 (9) | 0.0279 (8) | −0.0046 (7) | 0.0004 (7) | −0.0035 (7) |
| S2  | 0.0302 (9) | 0.0280 (9) | 0.0329 (8) | −0.0021 (7) | −0.0019 (7) | 0.0081 (7) |
| N1  | 0.024 (3) | 0.021 (3) | 0.029 (3) | 0.000 (2) | −0.001 (2) | 0.000 (2) |
| N2  | 0.021 (3) | 0.024 (3) | 0.028 (3) | −0.001 (2) | 0.001 (2) | −0.001 (2) |
| C1  | 0.027 (4) | 0.029 (3) | 0.038 (4) | 0.000 (3) | 0.006 (3) | 0.000 (3) |
| C2  | 0.019 (3) | 0.028 (3) | 0.034 (3) | −0.005 (3) | 0.002 (3) | 0.000 (3) |
| C3  | 0.023 (3) | 0.029 (4) | 0.034 (3) | −0.007 (3) | −0.007 (3) | 0.001 (3) |
| C4  | 0.025 (4) | 0.026 (3) | 0.031 (3) | −0.002 (3) | −0.003 (3) | −0.005 (3) |
| C5  | 0.032 (4) | 0.028 (4) | 0.047 (4) | −0.005 (3) | 0.002 (3) | −0.010 (3) |
| C6  | 0.047 (5) | 0.022 (4) | 0.070 (5) | 0.007 (3) | −0.005 (4) | −0.010 (4) |
| C7  | 0.041 (5) | 0.022 (4) | 0.062 (5) | 0.002 (3) | 0.000 (4) | 0.009 (3) |
| C8  | 0.031 (4) | 0.027 (4) | 0.041 (4) | −0.002 (3) | −0.005 (3) | −0.004 (3) |
| C9  | 0.036 (4) | 0.030 (4) | 0.039 (4) | −0.012 (3) | −0.004 (3) | 0.011 (3) |
| C10 | 0.037 (4) | 0.034 (4) | 0.037 (4) | −0.010 (3) | 0.007 (3) | 0.005 (3) |
| C11 | 0.035 (4) | 0.024 (4) | 0.071 (5) | 0.007 (3) | 0.012 (4) | 0.001 (3) |
| C12 | 0.047 (5) | 0.054 (5) | 0.077 (6) | 0.018 (4) | −0.015 (5) | 0.015 (5) |
| C13 | 0.045 (5) | 0.054 (5) | 0.103 (7) | 0.015 (4) | 0.021 (5) | −0.009 (5) |
Geometric parameters (Å, °)

|          |        |          |          |          |
|----------|--------|----------|----------|----------|
| Pd1—N1  | 2.027  | C17—H17A| 0.9900   |
| Pd1—P1  | 2.2455 | C17—H17B| 0.9900   |
| Pd1—S2  | 2.3149 | C18—C19 | 1.401 (9)|

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| Bond                  | Distance (Å)    | Bond                  | Distance (Å)    |
|----------------------|-----------------|----------------------|-----------------|
| Pd1—S1               | 2.3657 (17)     | C19—C20              | 1.352 (9)       |
| Pd1—Pd2              | 2.8425 (7)      | C19—H19              | 0.9500          |
| Pd2—N2               | 2.027 (5)       | C20—C21              | 1.411 (9)       |
| Pd2—P2               | 2.2417 (18)     | C20—H20              | 0.9500          |
| Pd2—S1               | 2.3184 (16)     | C21—C26              | 1.410 (9)       |
| Pd2—S2               | 2.3602 (17)     | C21—C22              | 1.411 (9)       |
| P1—C11               | 1.812 (7)       | C22—C23              | 1.355 (10)      |
| P1—C1                | 1.825 (6)       | C22—H22              | 0.9500          |
| P1—C14               | 1.836 (7)       | C23—C24              | 1.395 (10)      |
| P2—C27               | 1.814 (7)       | C23—H23              | 0.9500          |
| P2—C30               | 1.822 (6)       | C24—C25              | 1.366 (9)       |
| P2—C17               | 1.836 (6)       | C24—H24              | 0.9500          |
| S1—C4                | 1.784 (6)       | C25—C26              | 1.414 (9)       |
| S2—C25               | 1.774 (7)       | C27—C28              | 1.528 (10)      |
| N1—C2                | 1.327 (7)       | C27—C29              | 1.556 (10)      |
| N1—C3                | 1.376 (8)       | C27—H27              | 1.0000          |
| N2—C18               | 1.360 (8)       | C28—H28A             | 0.9800          |
| N2—C26               | 1.373 (7)       | C28—H28B             | 0.9800          |
| C1—C2                | 1.491 (9)       | C28—H28C             | 0.9800          |
| C1—H1A               | 0.9900          | C29—H29A             | 0.9800          |
| C1—H1B               | 0.9900          | C29—H29B             | 0.9800          |
| C2—C10               | 1.401 (9)       | C29—H29C             | 0.9800          |
| C3—C8                | 1.407 (9)       | C30—C31              | 1.528 (9)       |
| C3—C4                | 1.433 (9)       | C30—C32              | 1.543 (9)       |
| C4—C5                | 1.366 (9)       | C30—H30              | 1.0000          |
| C5—C6                | 1.405 (10)      | C31—H31A             | 0.9800          |
| C5—H5                | 0.9500          | C31—H31B             | 0.9800          |
| C6—C7                | 1.371 (10)      | C31—H31C             | 0.9800          |
| C6—H6                | 0.9500          | C32—H32A             | 0.9800          |
| C7—C8                | 1.409 (9)       | C32—H32B             | 0.9800          |
| C7—H7                | 0.9500          | C32—H32C             | 0.9800          |
| C8—C9                | 1.413 (9)       | Sb1—F3               | 1.830 (5)       |
| C9—C10               | 1.359 (9)       | Sb1—F2               | 1.832 (5)       |
| C9—H9                | 0.9500          | Sb1—F6               | 1.845 (5)       |
| C10—H10              | 0.9500          | Sb1—F5               | 1.852 (5)       |
| C11—C13              | 1.520 (10)      | Sb1—F4               | 1.856 (4)       |
| C11—C12              | 1.549 (11)      | Sb1—F1               | 1.861 (4)       |
| C11—H11              | 1.0000          | Sb2—F11              | 1.721 (13)      |
| C12—H12A             | 0.9800          | Sb2—F7               | 1.783 (8)       |
| C12—H12B             | 0.9800          | Sb2—F7′              | 1.784 (13)      |
| C12—H12C             | 0.9800          | Sb2—F8               | 1.796 (8)       |
| C13—H13A             | 0.9800          | Sb2—F12              | 1.800 (13)      |
| C13—H13B             | 0.9800          | Sb2—F11              | 1.849 (7)       |
| C13—H13C             | 0.9800          | Sb2—F12              | 1.862 (6)       |
| C14—C15              | 1.522 (10)      | Sb2—F9               | 1.874 (6)       |
| C14—C16              | 1.535 (10)      | Sb2—F8′              | 1.879 (14)      |
| C14—H14              | 1.0000          | Sb2—F10              | 1.888 (8)       |
| C15—H15A             | 0.9800          | Sb2—F10′             | 1.907 (13)      |
| Bond                  | Length (Å) | Angle (°) |
|----------------------|------------|-----------|
| C15—H15B            | 0.9800     |           |
| C15—H15C            | 0.9800     |           |
| C16—H16A            | 0.9800     |           |
| C16—H16B            | 0.9800     |           |
| C16—H16C            | 0.9800     |           |
| C17—C18             | 1.486 (9)  |           |
| C11—P1—C1           |           | 106.9 (3) |
| C11—P1—C14          |           | 108.9 (3) |
| C1—P1—Pd1           |           | 119.7 (3) |
| C14—P1—Pd1          |           | 98.8 (2)  |
| C14—P1—C1           |           | 105.4 (3) |
| C1—P1—Pd1           |           | 119.7 (3) |
| C11—P1—C14          |           | 106.9 (3) |
| C11—P1—C14          |           | 108.9 (3) |
| C1—P1—Pd1           |           | 119.7 (3) |
| C14—P1—Pd1          |           | 98.8 (2)  |
| C27—P2—C30          |           | 108.7 (3) |
| C27—P2—C17          |           | 107.7 (3) |
| C30—P2—C17          |           | 106.1 (3) |
| C27—P2—Pd2          |           | 121.4 (2) |
| C30—P2—Pd2          |           | 111.0 (2) |
| C17—P2—Pd2          |           | 100.6 (2) |
| C4—S1—Pd2           |           | 117.9 (2) |
| C4—S1—Pd1           |           | 94.8 (2)  |
| C25—S2—Pd1          |           | 119.8 (2) |
| C25—S2—Pd2          |           | 95.2 (2)  |
| Pd1—S2—Pd2          |           | 74.88 (5) |
| C2—N1—C3            |           | 120.8 (5) |
| C2—N1—Pd1           |           | 121.8 (4) |
| C3—N1—Pd1           |           | 117.3 (4) |
| Bond          | Angle (°) | Bond          | Angle (°) |
|--------------|-----------|--------------|-----------|
| C18—N2—C26  | 120.4 (5) | C27—C29—H29A | 109.5     |
| C18—N2—Pd2  | 121.4 (4) | C27—C29—H29B | 109.5     |
| C26—N2—Pd2  | 118.1 (4) | H29A—C29—H29B | 109.5     |
| C2—C1—P1    | 111.5 (4) | C27—C29—H29C | 109.5     |
| C2—C1—H1A   | 109.3     | H29A—C29—H29C | 109.5     |
| P1—C1—H1A   | 109.3     | C2—C1—H1B    | 109.3     |
| C2—C1—H1B   | 109.3     | C27—C29—H29A | 109.5     |
| H1A—C1—H1B  | 108.0     | C27—C29—P2   | 110.6 (5) |
| N1—C2—C10   | 120.9 (6) | C32—C30—H30  | 108.1     |
| N1—C2—C1    | 117.1 (5) | C32—C30—H30  | 108.1     |
| C10—C2—C1   | 122.0 (6) | P2—C30—H30   | 108.1     |
| N1—C3—C8    | 120.2 (6) | C30—C31—H31A | 109.5     |
| N1—C3—C4    | 120.2 (6) | C30—C31—H31B | 109.5     |
| C8—C3—C4    | 119.6 (6) | H31A—C31—H31B | 109.5     |
| C5—C4—C3    | 119.2 (6) | C32—C31—H31A | 109.5     |
| C5—C4—S1    | 121.4 (5) | C32—C31—H31C | 109.5     |
| C3—C4—S1    | 118.9 (5) | H31B—C31—H31C | 109.5     |
| C4—C5—C6    | 120.8 (7) | C30—C32—H32A | 109.5     |
| C4—C5—H5    | 119.6     | C30—C32—H32B | 109.5     |
| C6—C5—H5    | 119.6     | H32A—C32—H32B | 109.5     |
| C7—C6—C5    | 121.0 (7) | C30—C32—H32C | 109.5     |
| C7—C6—H6    | 119.5     | H32B—C32—H32C | 109.5     |
| C5—C6—H6    | 119.5     | F3—Sb1—F2    | 91.0 (4)  |
| C6—C7—C8    | 119.7 (7) | F3—Sb1—F6    | 177.3 (3) |
| C6—C7—H7    | 120.1     | F2—Sb1—F6    | 91.4 (4)  |
| C8—C7—H7    | 120.1     | F3—Sb1—F5    | 89.5 (3)  |
| C3—C8—C7    | 119.6 (6) | F2—Sb1—F5    | 179.2 (3) |
| C3—C8—C9    | 118.1 (6) | F6—Sb1—F5    | 88.1 (3)  |
| C7—C8—C9    | 122.3 (6) | F3—Sb1—F4    | 89.0 (2)  |
| C10—C9—C8   | 119.8 (6) | F2—Sb1—F4    | 92.3 (2)  |
| C10—C9—H9   | 120.1     | F6—Sb1—F4    | 89.5 (2)  |
| C8—C9—H9    | 120.1     | F3—Sb1—F4    | 88.3 (3)  |
| C9—C10—C2   | 120.2 (6) | F5—Sb1—F4    | 90.9 (2)  |
| C9—C10—H10  | 119.9     | F3—Sb1—F1    | 88.5 (2)  |
| C2—C10—H10  | 119.9     | F2—Sb1—F1    | 90.5 (3)  |
| C13—C11—C12 | 112.5 (7) | F5—Sb1—F1    | 90.8 (2)  |
| C13—C11—P1  | 112.6 (6) | F4—Sb1—F1    | 179.2 (2) |
| C12—C11—P1  | 110.8 (5) | F11′—Sb2—F7′ | 98.4 (10) |
| C13—C11—H11 | 106.8     | F7—Sb2—F8    | 93.9 (6)  |
| C12—C11—H11 | 106.8     | F11′—Sb2—F12′ | 85.3 (10) |
| P1—C11—H11  | 106.8     | C11—C12—H12A | 109.5     |
| C11—C12—H12A| 109.5     | C11—C12—H12B | 95.1 (9)  |
| C11—C12—H12B| 95.1      | C7—Sb2—F11   | 87.1 (5)  |
| H12A—C12—H12B| 109.5    | F8—Sb2—F11   | 179.0 (5) |
| C11—C12—H12C| 109.5     | F7—Sb2—F12   | 93.6 (4)  |
| H12A—C12—H12C| 93.7      | F8—Sb2—F12   | 93.7 (4)  |
| H12B—C12—H12C| 109.5    | F11—Sb2—F12  | 85.9 (3)  |
| Bond | Bond | Bond | Value (°) |
|------|------|------|----------|
| C11—C13—H13A | 109.5 | F7—Sb2—F9 | 91.0 (4) |
| C11—C13—H13B | 109.5 | F8—Sb2—F9 | 87.7 (4) |
| H13A—C13—H13B | 109.5 | F11—Sb2—F9 | 92.5 (4) |
| C11—C13—H13C | 109.5 | F12—Sb2—F9 | 175.0 (4) |
| H13A—C13—H13C | 109.5 | F11′—Sb2—F8′ | 105.2 (10) |
| H13B—C13—H13C | 109.5 | F7—Sb2—F8′ | 89.5 (8) |
| C15—C14—C16 | 111.0 (6) | F12—Sb2—F8′ | 167.8 (10) |
| C15—C14—P1 | 110.2 (5) | F7—Sb2—F10 | 175.7 (5) |
| C16—C14—P1 | 112.3 (5) | F8—Sb2—F10 | 89.5 (5) |
| C15—C14—H14 | 107.7 | F11—Sb2—F10 | 89.5 (5) |
| C16—C14—H14 | 107.7 | F12—Sb2—F10 | 88.8 (4) |
| P1—C14—H14 | 107.7 | F9—Sb2—F10 | 86.4 (4) |
| C14—C15—H15A | 109.5 | F11′—Sb2—F10′ | 94.0 (10) |
| C14—C15—H15B | 109.5 | F7′—Sb2—F10′ | 166.5 (11) |
| H15A—C15—H15B | 109.5 | F12′—Sb2—F10′ | 91.3 (10) |
| C14—C15—H15C | 109.5 | F8′—Sb2—F10′ | 82.0 (8) |
| H15A—C15—H15C | 109.5 | F11′—Sb2—F9′ | 171.8 (10) |
| H15B—C15—H15C | 109.5 | F7′—Sb2—F9′ | 89.5 (9) |
| C14—C16—H16A | 109.5 | F12′—Sb2—F9′ | 96.4 (9) |
| C14—C16—H16B | 109.5 | F8′—Sb2—F9′ | 72.3 (9) |
| H16A—C16—H16B | 109.5 | F10′—Sb2—F9′ | 78.0 (9) |
| C14—C16—H16C | 109.5 | C12—C33—C11 | 112.8 (5) |
| H16A—C16—H16C | 109.5 | C12—C33—H33A | 109.0 |
| H16B—C16—H16C | 109.5 | C11—C33—H33A | 109.0 |
| C18—C17—P2 | 112.4 (4) | C12—C33—H33B | 109.0 |
| C18—C17—H17A | 109.1 | C11—C33—H33B | 109.0 |
| P2—C17—H17A | 109.1 | H33A—C33—H33B | 107.8 |
| C18—C17—H17B | 109.1 | | |

| Bond | Bond | Bond | Value (°) |
|------|------|------|----------|
| C11—P1—C1—C2 | −151.4 (5) | C27—P2—C17—C18 | 143.6 (5) |
| C14—P1—C1—C2 | 92.8 (5) | C30—P2—C17—C18 | −100.2 (5) |
| Pd1—P1—C1—C2 | −26.6 (5) | Pd2—P2—C17—C18 | 15.5 (5) |
| C3—N1—C1—C2 | 1.4 (9) | C26—N2—C18—C19 | 4.7 (9) |
| Pd1—N1—C1—C2 | 179.4 (5) | Pd2—N2—C18—C19 | −176.8 (5) |
| C3—N1—C1—C2 | −179.9 (5) | C26—N2—C18—C17 | −171.1 (5) |
| Pd1—N1—C2—C1 | −1.8 (8) | Pd2—N2—C18—C17 | 7.4 (8) |
| P1—C1—C2—N1 | 21.0 (7) | P2—C17—C18—N2 | −15.9 (8) |
| P1—C1—C2—C10 | −160.3 (5) | P2—C17—C18—C19 | 168.4 (5) |
| C2—N1—C3—C8 | 0.3 (9) | N2—C18—C19—C20 | −2.4 (10) |
| Pd1—N1—C3—C8 | −177.8 (5) | C17—C18—C19—C20 | 173.2 (6) |
| C2—N1—C3—C4 | −178.9 (6) | C18—C19—C20—C21 | −1.5 (10) |
| Pd1—N1—C3—C4 | 3.0 (7) | C19—C20—C21—C26 | 3.0 (9) |
| N1—C3—C4—C5 | −178.2 (6) | C19—C20—C21—C22 | −176.8 (7) |
| C8—C3—C4—C5 | 2.6 (9) | C26—C21—C22—C23 | −1.9 (10) |
| N1—C3—C4—S1 | 10.2 (8) | C20—C21—C22—C23 | 177.9 (6) |
| C8—C3—C4—S1 | −169.0 (5) | C21—C22—C23—C24 | 1.3 (10) |
| Pd2—S1—C4—C5 | 98.5 (5) | C22—C23—C24—C25 | 0.6 (11) |
| Pd1—S1—C4—C5 | 173.7 (5) | C23—C24—C25—C26 | −1.8 (10) |
Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the C21–C26 ring.

| D—H···A | D—H | H···A | D···A | D—H···A |
|----------|------|-------|-------|---------|
| C1—H1A···F3i | 0.99 | 2.34 | 3.305 (9) | 166 |
| C7—H7···F1ii | 0.95 | 2.37 | 3.229 (8) | 151 |
| C11—H11···F2iii | 1.00 | 2.27 | 3.128 (9) | 143 |
| C17—H17A···F11iv | 0.99 | 2.41 | 3.279 (10) | 147 |
| C22—H22···F8v | 0.95 | 2.33 | 3.190 (11) | 150 |
| C23—H23···F11iii | 0.95 | 2.53 | 3.396 (9) | 152 |
| C27—H27···F12ii | 1.00 | 2.43 | 3.322 (10) | 148 |
| C31—H31C···F3iv | 0.98 | 2.50 | 3.399 (9) | 152 |
| C33—H33d···F10 | 0.99 | 2.54 | 3.172 (13) | 122 |
| C16—H16A···Cg1 | 0.98 | 2.93 | 3.701 (8) | 136 |

Symmetry codes: (i) x+1/2, −y+3/2, −z+1; (ii) −x+1, −y+2, −z+1; (iii) −x+1, −y+1, −z+1; (iv) x, −y+3/2, z+1/2; (v) −x+1/2, −y+1, z+1/2; (vi) −x+1/2, −y+2, z+1/2.
Selected geometric parameters (Å, °)

| Bond/Angle                        | Value      |
|----------------------------------|------------|
| Pd1-N1                           | 2.027 (5)  |
| Pd1-P1                           | 2.2455 (18)|
| Pd1-S2                           | 2.3149 (16)|
| Pd1-S1                           | 2.3657 (17)|
| P1-C1                            | 1.825 (6)  |
| S1-C4                            | 1.784 (6)  |
| Pd1-Pd2                          | 2.8425 (7) |
| Pd2-N2                           | 2.027 (5)  |
| Pd2-P2                           | 2.2417 (18)|
| Pd2-S1                           | 2.3184 (16)|
| Pd2-S2                           | 2.3602 (17)|
| P2-C17                           | 1.836 (6)  |
| S2-C25                           | 1.774 (7)  |
| N1-Pd1-P1                        | 83.86 (15) |
| N1-Pd1-S2                        | 168.93 (15)|
| P1-Pd1-S2                        | 106.75 (6) |
| N1-Pd1-S1                        | 86.49 (15) |
| P1-Pd1-S1                        | 169.03 (6) |
| S2-Pd1-S1                        | 82.64 (6)  |
| N1-Pd1-Pd2                       | 117.54 (14)|
| P1-Pd1-Pd2                       | 129.40 (5) |
| S2-Pd1-Pd2                       | 53.28 (4)  |
| S1-Pd1-Pd2                       | 51.89 (4)  |
| Pd2-S1-Pd1                       | 74.71 (5)  |
| Pd1-S2-Pd2                       | 74.88 (5)  |