



Structure of a diorganotelluroxonium(IV) cation, $\{[2,6-(\text{CH}_2\text{NMe}_2)_2\text{C}_6\text{H}_3\text{Te}(\mu\text{-O})]_2\}^{2+}$, with the trichlorido(dimethyl sulfoxide)platinum(II) anion

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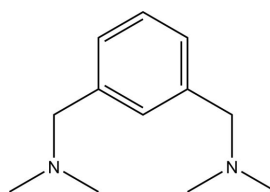
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Keywords: crystal structure; heteroleptic diorganotelluride; diorganotelluroxonium(IV) cation.**CCDC reference:** 1563166**Supporting information:** this article has supporting information at journals.iucr.org/e

In the title salt, di- μ -oxido-bis[2,6-bis[(dimethylamino)methyl]phenyl- κC^1]-tellurium(IV) bis[trichlorido(dimethyl sulfoxide- κS)platinate(II)], $(\text{C}_{24}\text{H}_{38}\text{N}_4\text{O}_2\text{Te}_2)[\text{PdCl}_3(\text{C}_2\text{H}_6\text{OS})]_2$, which crystallizes in the triclinic space group $P\bar{1}$, each Te atom is in a distorted five-coordinated $\text{TeO}_2\text{N}_2\text{C}$ square-pyramidal geometry (τ values of 0.026 and 0.001) with the C atoms of the phenyl rings occupying the apical positions. The phenyl rings in the $[\text{C}_{24}\text{H}_{38}\text{N}_4\text{O}_2\text{Te}_2]^{2+}$ cation are in a *cis* arrangement to enable this species to participate in $\text{Te}\cdots\text{Cl}$ cation–anion interactions. There are also $\text{C}-\text{H}\cdots\text{O}$ interactions involving the dimethyl sulfoxide ligands and numerous cation–anion and anion–anion $\text{C}-\text{H}\cdots\text{Cl}$ interactions, which link the ions into a complex three-dimensional array.

1. Chemical context

After the initial discovery (Moulton & Shaw, 1976) and seminal contributions from various research groups, the coordination chemistry of pincer ligands has become an important field in coordination chemistry (Peris & Crabtree, 2018). One pincer ligand scaffold that has recently attracted considerable attention with respect to its interesting structural features and reactivity, is the NCN pincer ligand, [2,6-(Me_2NCH_2) $_2\text{C}_6\text{H}_3$] (**HL**).



HL

Of particular interest are the group 16 derivatives of these ligands where, due to the presence of intramolecular $\text{N}\rightarrow\text{M}$ interactions from the two coordinating auxiliary arms, their compounds show interesting reactivity and have been used in the formation of selenium cations (Fujihara *et al.*, 1995; Poleschner & Seppelt, 2004, 2013; Gupta *et al.*, 2017; Pop *et al.*, 2014; Varga *et al.*, 2010; Rani *et al.*, 2018). It is worth noting that, compared to the selenium cation of ligand **L**, studies on their higher congener *i.e.*, tellurenum cations, are relatively scarce in the literature and this was the initial impetus for this work. Furukawa and co-workers reported the synthesis of a tellurenum cation by the reaction of heteroleptic diorganotelluride LTeR (where $R = n$ -butyl) with $\text{Br}_2/\text{K}[\text{PF}_6]$ (Fujihara

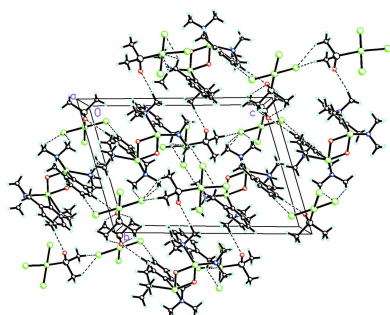
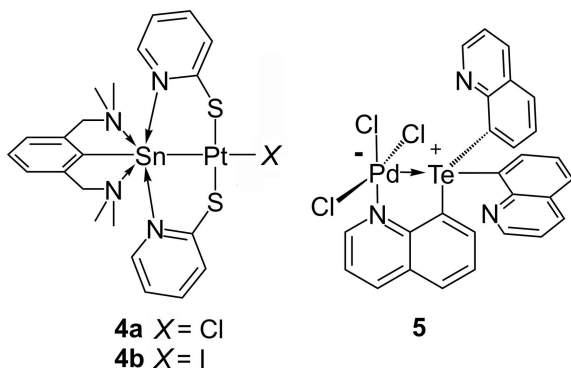


Table 1
Selected geometric parameters (Å, °).

Te1—O1	1.9836 (19)	Te2—O1	2.0071 (19)
Te1—O2	1.9871 (19)	Te2—O2	1.9844 (18)
Te1—C1	2.089 (3)	Te2—N1A	2.477 (2)
Te1—N2	2.450 (2)	Te2—N2A	2.459 (2)
Te1—N1	2.495 (2)	Te2—C1A	2.107 (3)
O1—Te1—O2	76.92 (8)	O2—Te2—O1	76.44 (8)
O1—Te1—C1	96.99 (10)	O2—Te2—C1A	95.66 (10)
O2—Te1—C1	93.43 (10)	O1—Te2—C1A	94.79 (10)
O1—Te1—N2	150.20 (8)	O2—Te2—N2A	76.19 (8)
O2—Te1—N2	75.53 (8)	O1—Te2—N2A	148.65 (8)
C1—Te1—N2	73.66 (10)	C1A—Te2—N2A	73.06 (10)
O1—Te1—N1	77.12 (8)	O2—Te2—N1A	148.72 (7)
O2—Te1—N1	148.63 (8)	O1—Te2—N1A	75.46 (8)
C1—Te1—N1	72.64 (10)	C1A—Te2—N1A	73.37 (10)
N2—Te1—N1	124.18 (8)	N2A—Te2—N1A	125.35 (9)

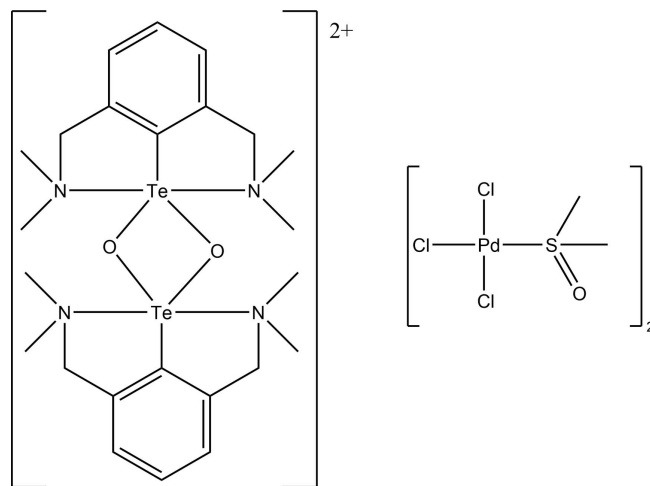
et al., 1995). However, the structural elucidation of the tellurenum cation of the ligand **L** remained elusive until Silvestru and co-workers reported the first structural characterization of a tellurenum cation (Beleaga *et al.*, 2011).

It is interesting to note that the related tin(II) cations of ligand **L**, containing one lone pair of electrons, have been used as ligands to isolate heterobimetallic complexes **4a,b** (Martincová *et al.*, 2011, 2012). However, no such coordination chemistry has been explored for the selenium(II) and tellurenum(II) cations of ligand **L**, which have two such pairs of electrons. A notable work is that by Lin & Gabbaï (2013) where they used Te^{IV} cations having one lone pair of electrons as ligands for isolating complex **5** where the Te^{IV} center acted as a σ -acceptor (Z-type) ligand.



Recently, we investigated the reactivity of the homoleptic diorganotelluride [2,6-(Me₂NCH₂)₂C₆H₃]₂Te, **1** with SO₂Cl₂:K₂PdCl₄ (Gupta *et al.*, 2019). We observed that the diorganotelluride underwent intramolecular chalcogen bonding (IChB) mediated Te-dearylation to afford the first example of a Pd^{II} complex [2,6-(Me₂NCH₂)₂C₆H₃]₂TePdCl₃, with any organotellurenum(II) cation as a ligand. This might be due to the formation of the highly stable tellurenum(II) cation where the Te is T-shaped and involved in a three-centered, four-electron bond. While checking the reproducibility of the reaction, in one instance, because of the adventitious uptake of oxygen, the reaction unexpectedly resulted in the isolation of the title compound, which contains the ditelluroxonium(IV) cation **2**, [2,6-(CH₂NMe₂)₂C₆H₃Te(μ -O)]₂

with the PdCl₃(DMSO) anion. It is worth noting that Furu-kawa and coworkers have reported a similar diorganotelluroxonium(IV) cation namely, [2,6-(CH₂NMe₂)₂C₆H₃Te(μ -O)]₂·PF₆, by the reaction of the diorganotelluride [2,6-(Me₂NCH₂)₂C₆H₃]₂Te with the oxidizing agent NOPF₆ (Kobayashi *et al.*, 2000).



2. Structural commentary

The title structure represents a rare example of a structurally characterized diorganotelluroxonium(IV) cation and key geometrical data are listed in Table 1. The salt [C₂₄H₃₈N₄O₂Te₂]²⁺·[PdCl₃(DMSO)]⁻², **3**, crystallizes in the triclinic space group *P* $\bar{1}$. In the structure of the cation **2** there is a *cis* arrangement of the aryl rings of the attached 2,6-[(dimethylamino)methyl]phenyl substituents (Fig. 1). This

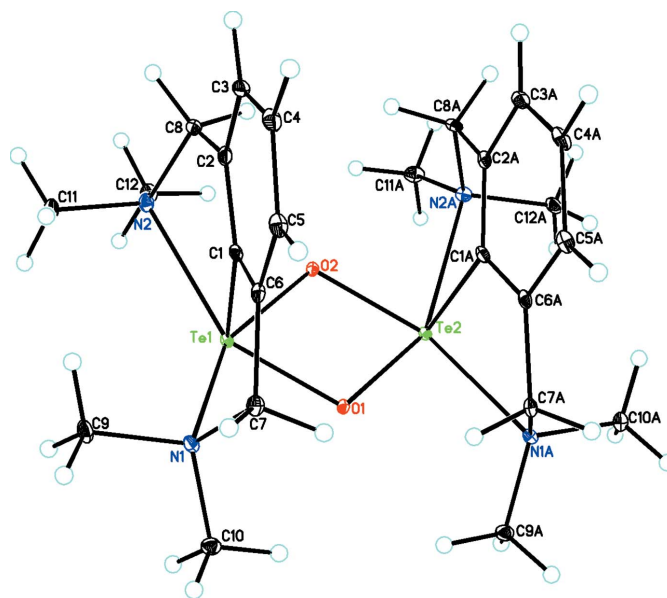


Figure 1
The molecular structure of the [C₂₄H₃₈N₄O₂Te₂]²⁺ cation, showing the *cis* arrangement of the phenyl rings with respect to the Te₂O₂ core. Atomic displacement parameters are drawn at the 30% probability level.

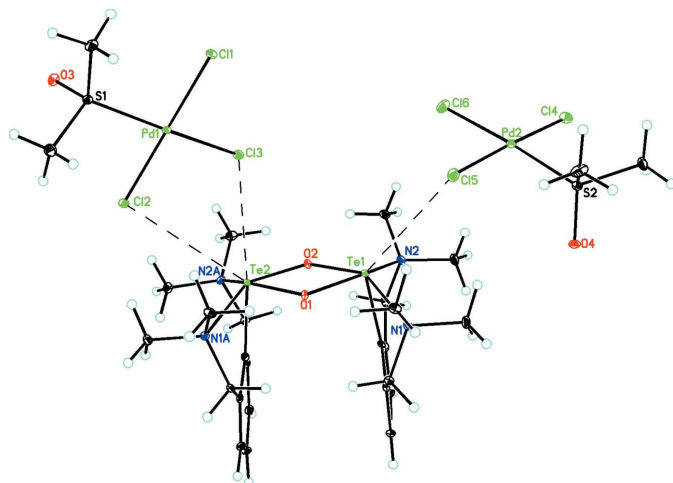


Figure 2
Diagram of the $[\text{C}_{24}\text{H}_{38}\text{N}_4\text{O}_2\text{Te}_2]^{2+}$ anion and the $[\text{PdCl}_3(\text{DMSO})]^-$ anions linked by $\text{Te}\cdots\text{Cl}$ interactions (shown as dashed lines).

is in contrast to that observed in the structure of $[\text{2,6-(CH}_2\text{NMe}_2)_2\text{C}_6\text{H}_3\text{Te}(\mu\text{-O})]_2^+\text{PF}_6^-$, wherein the cation lies on a center of inversion and thus the aryl groups are in a *trans* configuration (Kobayashi *et al.*, 2000). Each Te atom is in a five-coordinate geometry with the phenyl rings occupying the apical position. An analysis of this geometry using the continuous shape measurement (CSM) method (Cirera *et al.*, 2005; Llunell *et al.*, 2013) and using the four appropriate reference shapes [vacant octahedron, C_{4v} ; trigonal bipyramid, D_{3h} ; square pyramid, C_{4v} ; and Johnson trigonal bipyramid, D_{3h}] showed that the closest fit was the vacant octahedron. The Te–N bond distances, lying in the range from 2.450 (2)–2.495 (2) Å for **2**, are in good agreement with the

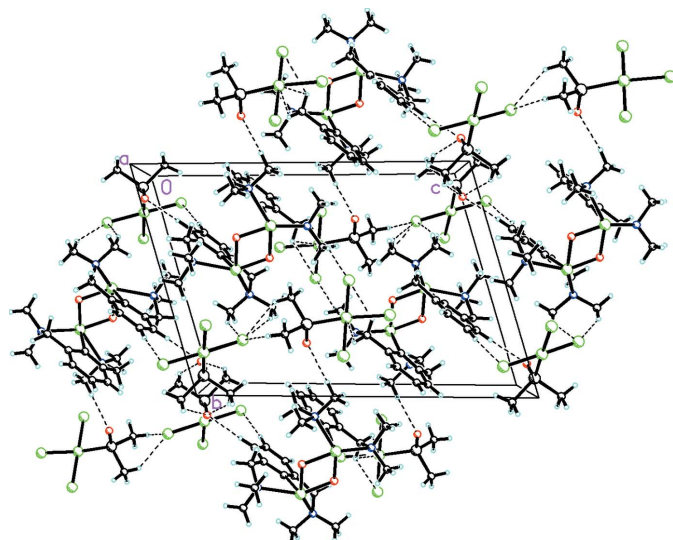


Figure 3
Packing diagram showing how the $\text{Te}\cdots\text{Cl}$ cation–anion interactions, $\text{C}\cdots\text{H}\cdots\text{O}$ interactions involving the DMSO ligands, and numerous cation–anion and anion–anion $\text{C}\cdots\text{H}\cdots\text{Cl}$ interactions linking these moieties into a complex three-dimensional array (all interactions shown as dashed lines).

Table 2
Hydrogen-bond geometry (Å, °).

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
C7–H7A \cdots Cl1	0.99	2.99	3.768 (3)	136
C7A–H7AB \cdots Cl1	0.99	2.90	3.663 (3)	135
C9A–H9AB \cdots Cl1 ⁱ	0.98	2.85	3.697 (4)	145
C9A–H9AC \cdots O1	0.98	2.49	3.000 (3)	112
C9–H9B \cdots O4 ⁱⁱ	0.98	2.64	3.355 (4)	130
C9–H9B \cdots Cl5 ⁱⁱ	0.98	2.87	3.741 (4)	149
C10A–H10C \cdots Cl2 ⁱⁱⁱ	0.98	2.80	3.706 (3)	154
C10–H10E \cdots O1	0.98	2.57	3.078 (4)	112
C10–H10F \cdots Cl5 ⁱⁱ	0.98	2.82	3.711 (4)	151
C11A–H11E \cdots O2	0.98	2.56	3.048 (4)	110
C11A–H11F \cdots Cl3 ⁱⁱⁱ	0.98	2.91	3.639 (4)	132
C12A–H12A \cdots O3 ^{iv}	0.98	2.42	3.316 (4)	151
C12A–H12A \cdots Cl2 ^{iv}	0.98	2.97	3.595 (3)	123
C12A–H12B \cdots Cl2 ⁱⁱⁱ	0.98	2.80	3.678 (4)	150
C12–H12D \cdots Cl6 ^v	0.98	2.92	3.825 (3)	155
C12–H12F \cdots O2	0.98	2.43	2.980 (4)	115
C21–H21A \cdots Cl5 ^{iv}	0.98	2.77	3.628 (3)	147
C21–H21C \cdots Cl3 ^{vi}	0.98	2.59	3.506 (3)	157
C22–H22B \cdots Cl5 ^{iv}	0.98	2.84	3.681 (4)	144
C22–H22C \cdots Cl1 ^{vi}	0.98	2.86	3.670 (4)	141
C22–H22D \cdots Cl2	0.98	2.77	3.308 (4)	115
C31–H31B \cdots O4 ^{vii}	0.98	2.53	3.389 (4)	147
C31–H31C \cdots Cl6 ^v	0.98	2.94	3.796 (4)	146
C32–H32B \cdots O4 ^{vii}	0.98	2.46	3.336 (4)	149
C32–H32C \cdots Cl5	0.98	2.73	3.275 (4)	115
C32–H32D \cdots Cl4 ^v	0.98	2.58	3.541 (4)	167

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

values observed in $[\text{2,6-(CH}_2\text{NMe}_2)_2\text{C}_6\text{H}_3\text{Te}(\mu\text{-O})]_2^+\text{PF}_6^-$ [2.475 (5)–2.486 (5) Å] (Kobayashi *et al.*, 2000). In **2**, the dihedral angle between the two aryl groups is 6.2 (2)° and those between the Te_2O_2 plane and the aryl rings are 88.77 (8) and 85.00 (8)°, indicating that the two aryl groups are not coplanar, and are too far apart to form π – π stacking interactions (the closest contact is between C1 and C1A at 3.672 Å). Thus, the driving force for the adoption of this sterically unfavorable *cis* conformation appears to be the formation of $\text{Te}\cdots\text{Cl}$ cation–anion interactions, which would not be possible if the *trans* conformation were adopted. In this case, there is a short $\text{Te2}\cdots\text{Cl3}$ contact of 3.386 (1) Å and longer contacts of 3.833 (1) Å ($\text{Te2}\cdots\text{Cl2}$) and 3.991 (1) Å ($\text{Te1}\cdots\text{Cl5}$) (see Fig. 2). In contrast, in the case of $[\text{2,6-(CH}_2\text{NMe}_2)_2\text{C}_6\text{H}_3\text{Te}(\mu\text{-O})]_2^+\text{PF}_6^-$, no such cation–anion interactions are present and hence the more sterically favorable *trans* conformation is adopted. In the other two related structures containing the $\text{Te}_2\text{O}_2^{2+}$ core dication, the same *cis* configuration is adopted to allow the formation of interionic $\text{Te}\cdots\text{O}$ interactions (Hupf *et al.*, 2017; Deka *et al.*, 2020).

3. Supramolecular features

In addition to the $\text{Te}\cdots\text{Cl}$ cation–anion interactions mentioned above, there are also $\text{C}\cdots\text{H}\cdots\text{O}$ interactions involving the DMSO ligands and numerous cation–anion and anion–anion $\text{C}\cdots\text{H}\cdots\text{Cl}$ interactions (Table 2), which link the ions into a complex three-dimensional array, as seen in Fig. 3.

Table 3
 Experimental details.

Crystal data	
Chemical formula	(C ₂₄ H ₃₈ N ₄ O ₂ Te ₂)[PdCl ₃ (C ₂ H ₆ OS)] ₂
<i>M</i> _r	1251.54
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.6333 (19), 12.770 (3), 17.956 (4)
α , β , γ (°)	73.82 (3), 83.55 (3), 88.86 (3)
<i>V</i> (Å ³)	2107.8 (8)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	2.73
Crystal size (mm)	0.39 × 0.20 × 0.14
Data collection	
Diffractometer	Rigaku Saturn 724 Dual Source CCD
Absorption correction	Numerical (<i>NUMABS</i> ; Rigaku, 1999)
<i>T</i> _{min} , <i>T</i> _{max}	0.417, 0.703
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	16345, 7532, 6351
<i>R</i> _{int}	0.028
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.602
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.022, 0.052, 0.99
No. of reflections	7532
No. of parameters	445
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.72, -0.95

Computer programs: *CrystalClear-SM Expert* (Rigaku, 2012), *SHELXT* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b) and *SHELXTL* (Sheldrick, 2008).

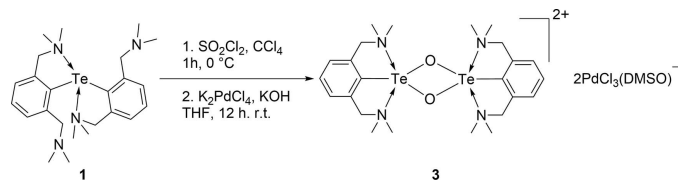
4. Database survey

There are only three reports available containing a cation with the Te₂O₂²⁺ core. The first report on the molecular structure of a diorganotelluroxonium(IV) cation was made by Furukawa and co-workers (Kobayashi *et al.*, 2000; Cambridge Structural Database refcode XAGGER), which contains a cation [2,6-(CH₂NMe₂)₂C₆H₃Te(μ -O)]₂⁺ charge-balanced as the PF₆⁻ salt. Beckmann and coworkers reported the molecular structure of [(6-Ph₂P(O)-Ace-5-) Te(μ -O)]₂·2OTf [Ace = acenaphthyl; Hupf *et al.*, 2017; refcode CAZCEO). Recently, we have reported the third example of a structurally characterized ditelluroxonium cation, namely [ppyTe(μ -O)]₂·2ClO₄ (ppy = phenylpyridine), stabilized by extensive IChB interactions (Deka *et al.*, 2020; refcode PUBWAN).

5. Synthesis and crystallization

To a solution of **1** (0.10 g, 0.20 mmol) in CCl₄ (3 ml), a solution of SO₂Cl₂ (0.03 g, 17.76 μ L, 0.22 mmol) in CCl₄ (2 ml) was added dropwise at 273 K under an N₂ atmosphere. After stirring the reaction mixture for 1 h, hexane (10 ml) was added, resulting in the formation of a white precipitate. The precipitate was washed with hexane (2 × 5 ml) and dissolved in THF (20 ml). To it, K₂PdCl₄ (0.06 g, 0.20 mmol) and KOH (0.01 g, 0.17 mmol) were added at ambient temperature. After stirring for 12 h, the solvent was removed under vacuum, resulting in the precipitation of a dark-purple solid. The solid

was washed with CH₂Cl₂ (3 × 5 ml) and Et₂O (2 × 10 ml), and dried under vacuum to afford the analytically pure solid of **2**. Dark-purple prisms of **2** suitable for single-crystal diffraction analysis were acquired by slow diffusion of Et₂O into a DMSO solution at room temperature.



Yield: 59%; m.p. 444–446 K; ¹H NMR: δ (ppm) 7.35–7.31 (*m*, 1H, Ar-H), 7.24–7.20 (*m*, 2H, Ar-H), 4.25 (*d*, 2H, ArCH₂), 3.55 (*d*, 2H, ArCH₂), 2.52 (*s*, 6H, NMe₂), 2.41 (*s*, 6H, NMe₂); ¹³C NMR: δ (ppm) 130.55, 125.22, 122.89, 120.44, 67.14, 45.70; ¹²⁵Te NMR: δ (ppm) 1500; ESI-MS (positive mode): *m/z* calculated for [C₁₂H₁₉N₂O₂Te]⁺: 336.0545, found: 336.0541.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. A riding model was used for the H atoms with atomic displacement parameters = 1.2U_{eq}(C) [1.5U_{eq}(CH₃)] and C–H distances ranging from 0.95 to 0.99 Å.

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References

- Beleaga, A., Bojan, V. R., Pöllnitz, A., Rač, C. I. & Silvestru, C. (2011). *Dalton Trans.* **40**, 8830–8838.
- Cirera, J., Ruiz, E. & Alvarez, S. (2005). *Organometallics*, **24**, 1556–1562.
- Deka, R., Sarkar, A., Butcher, R. J., Junk, P. C., Turner, D. R., Deacon, G. B. & Singh, H. B. (2020). *Organometallics*, **39**, 334–343.
- Fujihara, H., Mima, H. & Furukawa, N. (1995). *J. Am. Chem. Soc.* **117**, 10153–10154.
- Gupta, A., Singh, H. B. & Butcher, R. J. (2017). *IUCrData*, **2**, x171634.
- Gupta, A. K., Deka, R., Singh, H. B. & Butcher, R. J. (2019). *New J. Chem.* **43**, 13225–13233.
- Hupf, E., Do, T. G., Nordheider, A., Wehrhahn, M., Sanz Camacho, P., Ashbrook, S. E., Lork, E., Slawin, A. M. Z., Mebs, S., Woollins, J. D. & Beckmann, J. (2017). *Organometallics*, **36**, 1566–1579.
- Kobayashi, K., Sato, S., Horn, E. & Furukawa, N. (2000). *Z. Kristallogr.* **215**, 21–24.
- Lin, T.-P. & Gabbai, F. P. (2013). *Angew. Chem. Int. Ed.* **52**, 3864–3868.
- Llunell, M., Casanova, D., Cirera, P. A. & Alvarez, J. (2013). *Shape*. University of Barcelona.
- Martincová, J., Dostál, L., Herres-Pawlis, S., Růžička, A. & Jambor, R. (2011). *Chem. Eur. J.* **17**, 7423–7427.
- Martincová, J., Dostál, L., Růžička, A., Herres-Pawlis, S. & Jambor, R. (2012). *Z. Anorg. Allg. Chem.* **638**, 1672–1675.
- Moulton, C. J. & Shaw, B. L. (1976). *J. Chem. Soc. Dalton Trans.* pp. 1020–1024.

- Peris, E. & Crabtree, R. H. (2018). *Chem. Soc. Rev.* **47**, 1959–1968.
- Poleschner, H. & Seppelt, K. (2004). *Chem. Eur. J.* **10**, 6565–6574.
- Poleschner, H. & Seppelt, K. (2013). *Angew. Chem. Int. Ed.* **52**, 12838–12842.
- Pop, A., Silvestru, A., Juárez-Pérez, E. J., Arca, M., Lippolis, V. & Silvestru, C. (2014). *Dalton Trans.* **43**, 2221–2233.
- Rani, V., Boda, M., Raju, S., Naresh Patwari, G., Singh, H. B. & Butcher, R. J. (2018). *Dalton Trans.* **47**, 9114–9127.
- Rigaku (1999). *NUMABS*. Rigaku Corporation, Tokyo, Japan.
- Rigaku (2012). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Sheldrick, G. M. (2015a). *Acta Cryst. A* **71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst. C* **71**, 3–8.
- Varga, R. A., Kulcsar, M. & Silvestru, A. (2010). *Acta Cryst. E* **66**, o771.

supporting information

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Computing details

Data collection: *CrystalClear-SM Expert* (Rigaku, 2012); cell refinement: *CrystalClear-SM Expert* (Rigaku, 2012); data reduction: *CrystalClear-SM Expert* (Rigaku, 2012); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Di- μ -oxido-bis[2,6-bis[(dimethylamino)methyl]phenyl- κC^1]tellurium(IV) bis[trichlorido(dimethyl sulfoxide- κS)platinate(II)]

Crystal data

$(\text{C}_{24}\text{H}_{38}\text{N}_4\text{O}_2\text{Te}_2)[\text{PdCl}_3(\text{C}_2\text{H}_6\text{OS})]_2$
 $M_r = 1251.54$
 Triclinic, $P\bar{1}$
 $a = 9.6333$ (19) Å
 $b = 12.770$ (3) Å
 $c = 17.956$ (4) Å
 $\alpha = 73.82$ (3)°
 $\beta = 83.55$ (3)°
 $\gamma = 88.86$ (3)°
 $V = 2107.8$ (8) Å³

$Z = 2$
 $F(000) = 1216$
 $D_x = 1.972$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 4389 reflections
 $\theta = 3.0\text{--}25.3^\circ$
 $\mu = 2.73$ mm⁻¹
 $T = 100$ K
 Prism, dark purple
 $0.39 \times 0.20 \times 0.14$ mm

Data collection

Rigaku Saturn 724 Dual Source CCD
 diffractometer
 Detector resolution: 28.5714 pixels mm⁻¹
 ω scans
 Absorption correction: numerical
 (NUMABS; Rigaku, 1999)
 $T_{\min} = 0.417$, $T_{\max} = 0.703$
 16345 measured reflections

7532 independent reflections
 6351 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$
 $\theta_{\text{max}} = 25.4^\circ$, $\theta_{\text{min}} = 3.0^\circ$
 $h = -10 \rightarrow 11$
 $k = -15 \rightarrow 15$
 $l = -18 \rightarrow 21$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.052$
 $S = 0.99$
 7532 reflections
 445 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

$$w = 1/[\sigma^2(F_o^2) + (0.0225P)^2]$$

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

$$\Delta\rho_{\max} = 0.72 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.95 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Te1	0.33401 (2)	0.04241 (2)	0.28514 (2)	0.01035 (6)
Pd1	0.94231 (2)	0.16499 (2)	0.01042 (2)	0.01127 (6)
Cl1	0.81302 (7)	0.00483 (6)	0.05078 (4)	0.01552 (17)
S1	0.89105 (8)	0.19555 (6)	-0.11264 (4)	0.01283 (17)
N1A	0.4790 (2)	0.2407 (2)	0.02780 (13)	0.0115 (6)
C1A	0.4649 (3)	0.3347 (2)	0.14904 (16)	0.0127 (7)
O1	0.40044 (19)	0.09584 (16)	0.17231 (10)	0.0107 (5)
N1	0.5460 (2)	-0.0692 (2)	0.27189 (14)	0.0133 (6)
C1	0.4960 (3)	0.1100 (2)	0.32559 (16)	0.0112 (6)
Te2	0.29877 (2)	0.23691 (2)	0.13837 (2)	0.00938 (5)
Pd2	0.10998 (2)	0.68021 (2)	0.44760 (2)	0.01459 (6)
S2	0.29029 (8)	0.56851 (7)	0.47852 (4)	0.01472 (17)
N2	0.2358 (2)	0.0782 (2)	0.40747 (13)	0.0144 (6)
O2	0.23723 (19)	0.18393 (17)	0.25186 (10)	0.0114 (5)
N2A	0.1943 (2)	0.3983 (2)	0.17064 (14)	0.0129 (6)
C2A	0.4399 (3)	0.4105 (2)	0.19095 (16)	0.0115 (7)
C2	0.4621 (3)	0.1733 (3)	0.37634 (16)	0.0147 (7)
Cl3	0.96704 (8)	0.15286 (7)	0.14002 (4)	0.01622 (17)
O3	0.7830 (2)	0.27971 (18)	-0.13078 (11)	0.0175 (5)
C3A	0.5517 (3)	0.4697 (3)	0.20169 (17)	0.0158 (7)
H3AA	0.537194	0.519754	0.232222	0.019*
C3	0.5686 (3)	0.2270 (3)	0.39672 (17)	0.0176 (7)
H3A	0.548200	0.269940	0.432012	0.021*
Cl2	1.07137 (8)	0.32486 (6)	-0.02994 (4)	0.01833 (17)
Cl4	0.00771 (8)	0.63088 (7)	0.57463 (4)	0.02292 (19)
O4	0.4201 (2)	0.62606 (18)	0.48098 (12)	0.0172 (5)
C4A	0.6855 (3)	0.4554 (3)	0.16736 (17)	0.0173 (7)
H4AA	0.762485	0.494414	0.175776	0.021*
C4	0.7059 (3)	0.2181 (3)	0.36546 (17)	0.0187 (7)
H4A	0.777779	0.259323	0.376730	0.022*
Cl5	0.21996 (8)	0.73154 (8)	0.32293 (4)	0.0282 (2)
C5	0.7392 (3)	0.1501 (3)	0.31822 (17)	0.0160 (7)
H5A	0.833870	0.142102	0.299431	0.019*
C5A	0.7069 (3)	0.3844 (3)	0.12092 (17)	0.0149 (7)
H5AA	0.797667	0.377838	0.095907	0.018*
Cl6	-0.06703 (9)	0.80252 (8)	0.40930 (5)	0.0279 (2)

C6A	0.5978 (3)	0.3236 (3)	0.11093 (16)	0.0125 (7)
C6	0.6342 (3)	0.0934 (3)	0.29826 (16)	0.0132 (7)
C7	0.6628 (3)	0.0113 (3)	0.25245 (17)	0.0147 (7)
H7A	0.672555	0.048960	0.195871	0.018*
H7B	0.751358	-0.026580	0.265278	0.018*
C7A	0.6129 (3)	0.2492 (3)	0.05866 (16)	0.0125 (7)
H7AA	0.686396	0.278106	0.014850	0.015*
H7AB	0.641317	0.175920	0.088484	0.015*
C8A	0.2900 (3)	0.4297 (3)	0.21981 (16)	0.0132 (7)
H8AA	0.268099	0.386007	0.274743	0.016*
H8AB	0.277568	0.507681	0.217519	0.016*
C8	0.3110 (3)	0.1770 (3)	0.40978 (17)	0.0156 (7)
H8A	0.306764	0.180806	0.464321	0.019*
H8B	0.266195	0.242929	0.379013	0.019*
C9A	0.4723 (3)	0.1439 (3)	-0.00092 (17)	0.0166 (7)
H9AA	0.542769	0.150699	-0.045863	0.025*
H9AB	0.379207	0.138039	-0.016649	0.025*
H9AC	0.490338	0.078522	0.040633	0.025*
C9	0.5562 (3)	-0.1486 (3)	0.34914 (17)	0.0191 (8)
H9A	0.639146	-0.193593	0.346083	0.029*
H9B	0.472556	-0.195482	0.364070	0.029*
H9C	0.563665	-0.109263	0.388236	0.029*
C10A	0.4566 (3)	0.3395 (3)	-0.03633 (16)	0.0160 (7)
H10A	0.527925	0.343701	-0.080528	0.024*
H10B	0.463240	0.404439	-0.017966	0.024*
H10C	0.363715	0.335566	-0.052866	0.024*
C10	0.5437 (3)	-0.1274 (3)	0.21195 (17)	0.0168 (7)
H10D	0.629019	-0.170147	0.210198	0.025*
H10E	0.538531	-0.074539	0.160977	0.025*
H10F	0.462038	-0.176280	0.224740	0.025*
C11	0.2664 (3)	-0.0165 (3)	0.47220 (17)	0.0203 (8)
H11A	0.229057	-0.003978	0.522014	0.030*
H11B	0.367714	-0.026302	0.470967	0.030*
H11C	0.222739	-0.082175	0.466593	0.030*
C11A	0.0504 (3)	0.3825 (3)	0.21053 (18)	0.0187 (8)
H11D	0.016516	0.451347	0.219420	0.028*
H11E	0.049883	0.326727	0.260701	0.028*
H11F	-0.010523	0.358949	0.177925	0.028*
C12A	0.1962 (3)	0.4811 (3)	0.09374 (17)	0.0172 (7)
H12A	0.167029	0.551598	0.101602	0.026*
H12B	0.131865	0.458418	0.062439	0.026*
H12C	0.290992	0.488054	0.066435	0.026*
C12	0.0820 (3)	0.0938 (3)	0.40960 (17)	0.0185 (8)
H12D	0.046264	0.111991	0.457722	0.028*
H12E	0.036883	0.026492	0.408038	0.028*
H12F	0.061573	0.153370	0.364434	0.028*
C21	0.8346 (3)	0.0792 (3)	-0.13645 (18)	0.0201 (7)
H21A	0.814868	0.099776	-0.190980	0.030*

H21B	0.749658	0.049098	-0.102401	0.030*
H21C	0.908035	0.024203	-0.129171	0.030*
C22	1.0399 (3)	0.2339 (3)	-0.18270 (17)	0.0236 (8)
H22B	1.012324	0.243964	-0.235132	0.035*
H22C	1.110033	0.176508	-0.172427	0.035*
H22D	1.079343	0.302250	-0.179196	0.035*
C31	0.2581 (3)	0.4638 (3)	0.56735 (19)	0.0268 (9)
H31B	0.340628	0.417616	0.575523	0.040*
H31C	0.177774	0.419428	0.564930	0.040*
H31D	0.238166	0.496447	0.610681	0.040*
C32	0.3259 (3)	0.4885 (3)	0.4126 (2)	0.0272 (9)
H32B	0.401809	0.438141	0.429211	0.041*
H32C	0.353752	0.536234	0.360159	0.041*
H32D	0.241933	0.446834	0.411990	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Te1	0.01126 (11)	0.00795 (11)	0.01136 (10)	-0.00191 (8)	-0.00056 (8)	-0.00204 (8)
Pd1	0.01032 (13)	0.00973 (13)	0.01451 (12)	-0.00091 (10)	-0.00135 (9)	-0.00456 (9)
Cl1	0.0150 (4)	0.0123 (4)	0.0193 (4)	-0.0034 (3)	-0.0003 (3)	-0.0048 (3)
S1	0.0130 (4)	0.0111 (4)	0.0155 (4)	0.0003 (3)	-0.0023 (3)	-0.0051 (3)
N1A	0.0113 (13)	0.0091 (14)	0.0141 (13)	0.0003 (11)	-0.0016 (10)	-0.0029 (10)
C1A	0.0155 (16)	0.0078 (16)	0.0141 (15)	-0.0024 (13)	-0.0049 (12)	-0.0005 (12)
O1	0.0134 (11)	0.0092 (11)	0.0084 (10)	0.0014 (9)	-0.0012 (8)	-0.0010 (8)
N1	0.0150 (14)	0.0093 (14)	0.0148 (13)	-0.0005 (11)	-0.0013 (10)	-0.0022 (11)
C1	0.0120 (16)	0.0085 (16)	0.0118 (15)	-0.0052 (13)	-0.0027 (12)	-0.0001 (12)
Te2	0.00944 (11)	0.00794 (11)	0.01094 (10)	-0.00101 (8)	-0.00156 (7)	-0.00269 (8)
Pd2	0.01263 (13)	0.01427 (14)	0.01753 (13)	-0.00153 (10)	-0.00298 (10)	-0.00488 (10)
S2	0.0148 (4)	0.0131 (4)	0.0168 (4)	-0.0020 (3)	-0.0023 (3)	-0.0045 (3)
N2	0.0128 (13)	0.0132 (15)	0.0145 (13)	0.0004 (12)	0.0020 (10)	-0.0006 (11)
O2	0.0143 (11)	0.0096 (12)	0.0093 (10)	0.0006 (9)	0.0004 (8)	-0.0015 (8)
N2A	0.0111 (13)	0.0137 (15)	0.0150 (13)	0.0021 (11)	-0.0043 (10)	-0.0048 (11)
C2A	0.0118 (16)	0.0097 (16)	0.0114 (15)	0.0010 (13)	-0.0060 (12)	0.0014 (12)
C2	0.0173 (17)	0.0128 (17)	0.0117 (15)	-0.0006 (14)	-0.0030 (12)	0.0007 (13)
Cl3	0.0163 (4)	0.0178 (4)	0.0163 (4)	-0.0028 (3)	-0.0007 (3)	-0.0077 (3)
O3	0.0186 (12)	0.0151 (13)	0.0205 (11)	0.0072 (10)	-0.0058 (9)	-0.0070 (9)
C3A	0.0197 (17)	0.0130 (18)	0.0162 (16)	-0.0029 (14)	-0.0094 (13)	-0.0033 (13)
C3	0.0284 (19)	0.0117 (17)	0.0137 (16)	-0.0002 (15)	-0.0073 (14)	-0.0035 (13)
Cl2	0.0188 (4)	0.0124 (4)	0.0234 (4)	-0.0047 (3)	-0.0064 (3)	-0.0025 (3)
Cl4	0.0210 (4)	0.0270 (5)	0.0217 (4)	-0.0029 (4)	0.0031 (3)	-0.0102 (4)
O4	0.0134 (11)	0.0158 (13)	0.0242 (12)	-0.0039 (10)	-0.0038 (9)	-0.0077 (10)
C4A	0.0141 (17)	0.0125 (18)	0.0245 (17)	-0.0067 (14)	-0.0114 (13)	0.0000 (14)
C4	0.0202 (18)	0.0156 (19)	0.0197 (17)	-0.0065 (14)	-0.0090 (14)	-0.0007 (14)
Cl5	0.0225 (5)	0.0388 (6)	0.0175 (4)	-0.0002 (4)	-0.0016 (3)	0.0015 (4)
C5	0.0111 (16)	0.0161 (18)	0.0188 (16)	-0.0045 (14)	-0.0037 (13)	-0.0002 (13)
C5A	0.0105 (16)	0.0129 (18)	0.0195 (16)	0.0009 (13)	-0.0055 (13)	0.0001 (13)
Cl6	0.0236 (5)	0.0292 (5)	0.0349 (5)	0.0099 (4)	-0.0122 (4)	-0.0126 (4)

C6A	0.0148 (16)	0.0090 (16)	0.0117 (15)	0.0000 (13)	-0.0053 (12)	0.0020 (12)
C6	0.0151 (17)	0.0118 (17)	0.0104 (15)	0.0000 (13)	-0.0021 (12)	0.0009 (12)
C7	0.0118 (16)	0.0155 (18)	0.0151 (16)	-0.0018 (14)	0.0000 (12)	-0.0019 (13)
C7A	0.0113 (16)	0.0111 (17)	0.0127 (15)	-0.0020 (13)	-0.0004 (12)	0.0006 (12)
C8A	0.0152 (16)	0.0101 (17)	0.0167 (16)	-0.0003 (13)	-0.0041 (13)	-0.0065 (13)
C8	0.0219 (18)	0.0112 (17)	0.0131 (15)	0.0023 (14)	0.0007 (13)	-0.0035 (13)
C9A	0.0168 (17)	0.0155 (18)	0.0188 (16)	-0.0036 (14)	0.0013 (13)	-0.0080 (14)
C9	0.0214 (18)	0.0132 (18)	0.0189 (17)	0.0041 (15)	-0.0033 (13)	0.0020 (13)
C10A	0.0162 (17)	0.0148 (18)	0.0147 (16)	-0.0010 (14)	-0.0005 (13)	-0.0004 (13)
C10	0.0157 (17)	0.0166 (18)	0.0188 (16)	-0.0011 (14)	0.0026 (13)	-0.0075 (14)
C11	0.0222 (18)	0.0190 (19)	0.0149 (16)	-0.0012 (15)	0.0013 (13)	0.0021 (14)
C11A	0.0130 (17)	0.021 (2)	0.0243 (17)	0.0042 (15)	-0.0003 (13)	-0.0117 (15)
C12A	0.0222 (18)	0.0097 (17)	0.0197 (17)	0.0032 (14)	-0.0062 (13)	-0.0029 (13)
C12	0.0132 (16)	0.0193 (19)	0.0200 (17)	-0.0016 (14)	0.0029 (13)	-0.0025 (14)
C21	0.0275 (19)	0.0146 (18)	0.0232 (18)	-0.0016 (15)	-0.0103 (14)	-0.0106 (14)
C22	0.0209 (18)	0.031 (2)	0.0174 (17)	-0.0031 (16)	0.0018 (14)	-0.0058 (15)
C31	0.0218 (19)	0.019 (2)	0.0300 (19)	-0.0012 (16)	-0.0004 (15)	0.0081 (15)
C32	0.024 (2)	0.028 (2)	0.042 (2)	0.0050 (17)	-0.0120 (16)	-0.0271 (18)

Geometric parameters (Å, °)

Te1—O1	1.9836 (19)	C4—H4A	0.9500
Te1—O2	1.9871 (19)	C5—C6	1.389 (4)
Te1—C1	2.089 (3)	C5—H5A	0.9500
Te1—N2	2.450 (2)	C5A—C6A	1.375 (4)
Te1—N1	2.495 (2)	C5A—H5AA	0.9500
Te1—Te2	3.1222 (12)	C6A—C7A	1.506 (4)
Pd1—S1	2.2440 (9)	C6—C7	1.507 (4)
Pd1—Cl2	2.3049 (12)	C7—H7A	0.9900
Pd1—Cl1	2.3091 (11)	C7—H7B	0.9900
Pd1—Cl3	2.3278 (9)	C7A—H7AA	0.9900
S1—O3	1.477 (2)	C7A—H7AB	0.9900
S1—C21	1.768 (3)	C8A—H8AA	0.9900
S1—C22	1.777 (3)	C8A—H8AB	0.9900
N1A—C9A	1.471 (4)	C8—H8A	0.9900
N1A—C7A	1.477 (4)	C8—H8B	0.9900
N1A—C10A	1.483 (4)	C9A—H9AA	0.9800
C1A—C2A	1.384 (4)	C9A—H9AB	0.9800
C1A—C6A	1.407 (4)	C9A—H9AC	0.9800
Te2—O1	2.0071 (19)	C9—H9A	0.9800
Te2—O2	1.9844 (18)	C9—H9B	0.9800
Te2—N1A	2.477 (2)	C9—H9C	0.9800
Te2—N2A	2.459 (2)	C10A—H10A	0.9800
Te2—C1A	2.107 (3)	C10A—H10B	0.9800
N1—C10	1.471 (4)	C10A—H10C	0.9800
N1—C7	1.484 (4)	C10—H10D	0.9800
N1—C9	1.485 (4)	C10—H10E	0.9800
C1—C2	1.387 (4)	C10—H10F	0.9800

C1—C6	1.400 (4)	C11—H11A	0.9800
Pd2—S2	2.2444 (10)	C11—H11B	0.9800
Pd2—Cl5	2.2891 (11)	C11—H11C	0.9800
Pd2—Cl4	2.2997 (11)	C11A—H11D	0.9800
Pd2—Cl6	2.3194 (11)	C11A—H11E	0.9800
S2—O4	1.474 (2)	C11A—H11F	0.9800
S2—C32	1.769 (3)	C12A—H12A	0.9800
S2—C31	1.773 (3)	C12A—H12B	0.9800
N2—C11	1.476 (4)	C12A—H12C	0.9800
N2—C8	1.481 (4)	C12—H12D	0.9800
N2—C12	1.489 (4)	C12—H12E	0.9800
N2A—C11A	1.477 (4)	C12—H12F	0.9800
N2A—C8A	1.479 (4)	C21—H21A	0.9800
N2A—C12A	1.486 (4)	C21—H21B	0.9800
C2A—C3A	1.389 (4)	C21—H21C	0.9800
C2A—C8A	1.518 (4)	C22—H22B	0.9800
C2—C3	1.382 (5)	C22—H22C	0.9800
C2—C8	1.516 (4)	C22—H22D	0.9800
C3A—C4A	1.397 (4)	C31—H31B	0.9800
C3A—H3AA	0.9500	C31—H31C	0.9800
C3—C4	1.393 (4)	C31—H31D	0.9800
C3—H3A	0.9500	C32—H32B	0.9800
C4A—C5A	1.391 (4)	C32—H32C	0.9800
C4A—H4AA	0.9500	C32—H32D	0.9800
C4—C5	1.384 (4)		
O1—Te1—O2	76.92 (8)	C6—C5—H5A	120.0
O1—Te1—C1	96.99 (10)	C6A—C5A—C4A	120.5 (3)
O2—Te1—C1	93.43 (10)	C6A—C5A—H5AA	119.7
O1—Te1—N2	150.20 (8)	C4A—C5A—H5AA	119.7
O2—Te1—N2	75.53 (8)	C5A—C6A—C1A	118.4 (3)
C1—Te1—N2	73.66 (10)	C5A—C6A—C7A	123.1 (3)
O1—Te1—N1	77.12 (8)	C1A—C6A—C7A	118.5 (3)
O2—Te1—N1	148.63 (8)	C5—C6—C1	117.9 (3)
C1—Te1—N1	72.64 (10)	C5—C6—C7	123.2 (3)
N2—Te1—N1	124.18 (8)	C1—C6—C7	118.8 (3)
O1—Te1—Te2	38.79 (5)	N1—C7—C6	109.5 (2)
O2—Te1—Te2	38.14 (5)	N1—C7—H7A	109.8
C1—Te1—Te2	97.50 (8)	C6—C7—H7A	109.8
N2—Te1—Te2	113.10 (6)	N1—C7—H7B	109.8
N1—Te1—Te2	114.34 (6)	C6—C7—H7B	109.8
S1—Pd1—Cl2	88.13 (4)	H7A—C7—H7B	108.2
S1—Pd1—Cl1	91.84 (4)	N1A—C7A—C6A	110.0 (2)
Cl2—Pd1—Cl1	179.97 (3)	N1A—C7A—H7AA	109.7
S1—Pd1—Cl3	170.82 (3)	C6A—C7A—H7AA	109.7
Cl2—Pd1—Cl3	90.42 (4)	N1A—C7A—H7AB	109.7
Cl1—Pd1—Cl3	89.61 (4)	C6A—C7A—H7AB	109.7
O3—S1—C21	107.75 (14)	H7AA—C7A—H7AB	108.2

O3—S1—C22	109.19 (14)	N2A—C8A—C2A	109.6 (2)
C21—S1—C22	100.00 (17)	N2A—C8A—H8AA	109.7
O3—S1—Pd1	111.49 (9)	C2A—C8A—H8AA	109.7
C21—S1—Pd1	114.91 (11)	N2A—C8A—H8AB	109.7
C22—S1—Pd1	112.80 (12)	C2A—C8A—H8AB	109.7
C9A—N1A—C7A	112.2 (2)	H8AA—C8A—H8AB	108.2
C9A—N1A—C10A	109.0 (2)	N2—C8—C2	109.5 (2)
C7A—N1A—C10A	110.5 (2)	N2—C8—H8A	109.8
C9A—N1A—Te2	112.60 (18)	C2—C8—H8A	109.8
C7A—N1A—Te2	104.52 (16)	N2—C8—H8B	109.8
C10A—N1A—Te2	107.85 (16)	C2—C8—H8B	109.8
C2A—C1A—C6A	121.7 (3)	H8A—C8—H8B	108.2
C2A—C1A—Te2	119.5 (2)	N1A—C9A—H9AA	109.5
C6A—C1A—Te2	118.8 (2)	N1A—C9A—H9AB	109.5
Te1—O1—Te2	102.96 (8)	H9AA—C9A—H9AB	109.5
C10—N1—C7	111.5 (2)	N1A—C9A—H9AC	109.5
C10—N1—C9	109.8 (2)	H9AA—C9A—H9AC	109.5
C7—N1—C9	110.4 (2)	H9AB—C9A—H9AC	109.5
C10—N1—Te1	113.63 (17)	N1—C9—H9A	109.5
C7—N1—Te1	103.85 (17)	N1—C9—H9B	109.5
C9—N1—Te1	107.35 (16)	H9A—C9—H9B	109.5
C2—C1—C6	122.4 (3)	N1—C9—H9C	109.5
C2—C1—Te1	118.6 (2)	H9A—C9—H9C	109.5
C6—C1—Te1	119.0 (2)	H9B—C9—H9C	109.5
O2—Te2—O1	76.44 (8)	N1A—C10A—H10A	109.5
O2—Te2—C1A	95.66 (10)	N1A—C10A—H10B	109.5
O1—Te2—C1A	94.79 (10)	H10A—C10A—H10B	109.5
O2—Te2—N2A	76.19 (8)	N1A—C10A—H10C	109.5
O1—Te2—N2A	148.65 (8)	H10A—C10A—H10C	109.5
C1A—Te2—N2A	73.06 (10)	H10B—C10A—H10C	109.5
O2—Te2—N1A	148.72 (7)	N1—C10—H10D	109.5
O1—Te2—N1A	75.46 (8)	N1—C10—H10E	109.5
C1A—Te2—N1A	73.37 (10)	H10D—C10—H10E	109.5
N2A—Te2—N1A	125.35 (9)	N1—C10—H10F	109.5
O2—Te2—Te1	38.20 (6)	H10D—C10—H10F	109.5
O1—Te2—Te1	38.25 (5)	H10E—C10—H10F	109.5
C1A—Te2—Te1	97.51 (8)	N2—C11—H11A	109.5
N2A—Te2—Te1	113.27 (6)	N2—C11—H11B	109.5
N1A—Te2—Te1	112.83 (6)	H11A—C11—H11B	109.5
S2—Pd2—Cl5	86.92 (4)	N2—C11—H11C	109.5
S2—Pd2—Cl4	91.79 (4)	H11A—C11—H11C	109.5
Cl5—Pd2—Cl4	177.60 (3)	H11B—C11—H11C	109.5
S2—Pd2—Cl6	176.40 (3)	N2A—C11A—H11D	109.5
Cl5—Pd2—Cl6	89.84 (4)	N2A—C11A—H11E	109.5
Cl4—Pd2—Cl6	91.39 (4)	H11D—C11A—H11E	109.5
O4—S2—C32	108.18 (15)	N2A—C11A—H11F	109.5
O4—S2—C31	107.93 (15)	H11D—C11A—H11F	109.5
C32—S2—C31	99.92 (18)	H11E—C11A—H11F	109.5

O4—S2—Pd2	113.54 (9)	N2A—C12A—H12A	109.5
C32—S2—Pd2	111.49 (11)	N2A—C12A—H12B	109.5
C31—S2—Pd2	114.78 (11)	H12A—C12A—H12B	109.5
C11—N2—C8	111.0 (2)	N2A—C12A—H12C	109.5
C11—N2—C12	109.6 (2)	H12A—C12A—H12C	109.5
C8—N2—C12	112.5 (2)	H12B—C12A—H12C	109.5
C11—N2—Te1	107.77 (17)	N2—C12—H12D	109.5
C8—N2—Te1	104.65 (16)	N2—C12—H12E	109.5
C12—N2—Te1	111.16 (18)	H12D—C12—H12E	109.5
Te2—O2—Te1	103.65 (8)	N2—C12—H12F	109.5
C11A—N2A—C8A	110.7 (2)	H12D—C12—H12F	109.5
C11A—N2A—C12A	110.0 (2)	H12E—C12—H12F	109.5
C8A—N2A—C12A	111.2 (3)	S1—C21—H21A	109.5
C11A—N2A—Te2	115.2 (2)	S1—C21—H21B	109.5
C8A—N2A—Te2	105.52 (15)	H21A—C21—H21B	109.5
C12A—N2A—Te2	103.88 (17)	S1—C21—H21C	109.5
C1A—C2A—C3A	119.0 (3)	H21A—C21—H21C	109.5
C1A—C2A—C8A	118.5 (3)	H21B—C21—H21C	109.5
C3A—C2A—C8A	122.5 (3)	S1—C22—H22B	109.5
C3—C2—C1	118.5 (3)	S1—C22—H22C	109.5
C3—C2—C8	122.6 (3)	H22B—C22—H22C	109.5
C1—C2—C8	118.8 (3)	S1—C22—H22D	109.5
C2A—C3A—C4A	119.6 (3)	H22B—C22—H22D	109.5
C2A—C3A—H3AA	120.2	H22C—C22—H22D	109.5
C4A—C3A—H3AA	120.2	S2—C31—H31B	109.5
C2—C3—C4	119.9 (3)	S2—C31—H31C	109.5
C2—C3—H3A	120.0	H31B—C31—H31C	109.5
C4—C3—H3A	120.0	S2—C31—H31D	109.5
C5A—C4A—C3A	120.5 (3)	H31B—C31—H31D	109.5
C5A—C4A—H4AA	119.8	H31C—C31—H31D	109.5
C3A—C4A—H4AA	119.8	S2—C32—H32B	109.5
C5—C4—C3	120.9 (3)	S2—C32—H32C	109.5
C5—C4—H4A	119.5	H32B—C32—H32C	109.5
C3—C4—H4A	119.5	S2—C32—H32D	109.5
C4—C5—C6	120.0 (3)	H32B—C32—H32D	109.5
C4—C5—H5A	120.0	H32C—C32—H32D	109.5
C6A—C1A—C2A—C3A	-6.1 (4)	C2—C1—C6—C5	-5.3 (4)
Te2—C1A—C2A—C3A	176.0 (2)	Te1—C1—C6—C5	172.1 (2)
C6A—C1A—C2A—C8A	170.7 (3)	C2—C1—C6—C7	171.6 (3)
Te2—C1A—C2A—C8A	-7.1 (3)	Te1—C1—C6—C7	-11.0 (4)
C6—C1—C2—C3	4.0 (4)	C10—N1—C7—C6	161.0 (2)
Te1—C1—C2—C3	-173.4 (2)	C9—N1—C7—C6	-76.6 (3)
C6—C1—C2—C8	-173.5 (3)	Te1—N1—C7—C6	38.2 (2)
Te1—C1—C2—C8	9.1 (4)	C5—C6—C7—N1	153.4 (3)
C1A—C2A—C3A—C4A	2.8 (4)	C1—C6—C7—N1	-23.3 (4)
C8A—C2A—C3A—C4A	-173.9 (3)	C9A—N1A—C7A—C6A	-160.8 (2)
C1—C2—C3—C4	1.0 (4)	C10A—N1A—C7A—C6A	77.3 (3)

C8—C2—C3—C4	178.4 (3)	Te2—N1A—C7A—C6A	-38.5 (3)
C2A—C3A—C4A—C5A	1.7 (4)	C5A—C6A—C7A—N1A	-150.9 (3)
C2—C3—C4—C5	-4.5 (4)	C1A—C6A—C7A—N1A	26.6 (4)
C3—C4—C5—C6	3.1 (4)	C11A—N2A—C8A—C2A	162.0 (2)
C3A—C4A—C5A—C6A	-2.9 (5)	C12A—N2A—C8A—C2A	-75.3 (3)
C4A—C5A—C6A—C1A	-0.3 (4)	Te2—N2A—C8A—C2A	36.7 (3)
C4A—C5A—C6A—C7A	177.2 (3)	C1A—C2A—C8A—N2A	-23.8 (4)
C2A—C1A—C6A—C5A	4.9 (4)	C3A—C2A—C8A—N2A	153.0 (3)
Te2—C1A—C6A—C5A	-177.2 (2)	C11—N2—C8—C2	78.9 (3)
C2A—C1A—C6A—C7A	-172.8 (3)	C12—N2—C8—C2	-157.9 (2)
Te2—C1A—C6A—C7A	5.1 (3)	Te1—N2—C8—C2	-37.1 (2)
C4—C5—C6—C1	1.7 (4)	C3—C2—C8—N2	-154.2 (3)
C4—C5—C6—C7	-175.0 (3)	C1—C2—C8—N2	23.1 (4)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C7—H7A...C11	0.99	2.99	3.768 (3)	136
C7A—H7AB...C11	0.99	2.90	3.663 (3)	135
C9A—H9AB...C11 ⁱ	0.98	2.85	3.697 (4)	145
C9A—H9AC...O1	0.98	2.49	3.000 (3)	112
C9—H9B...O4 ⁱⁱ	0.98	2.64	3.355 (4)	130
C9—H9B...C15 ⁱⁱ	0.98	2.87	3.741 (4)	149
C10A—H10C...C12 ⁱⁱⁱ	0.98	2.80	3.706 (3)	154
C10—H10E...O1	0.98	2.57	3.078 (4)	112
C10—H10F...C15 ⁱⁱ	0.98	2.82	3.711 (4)	151
C11A—H11E...O2	0.98	2.56	3.048 (4)	110
C11A—H11F...C13 ⁱⁱⁱ	0.98	2.91	3.639 (4)	132
C12A—H12A...O3 ^{iv}	0.98	2.42	3.316 (4)	151
C12A—H12A...C12 ^{iv}	0.98	2.97	3.595 (3)	123
C12A—H12B...C12 ⁱⁱⁱ	0.98	2.80	3.678 (4)	150
C12—H12D...C16 ^v	0.98	2.92	3.825 (3)	155
C12—H12F...O2	0.98	2.43	2.980 (4)	115
C21—H21A...C15 ^{iv}	0.98	2.77	3.628 (3)	147
C21—H21C...C13 ^{vi}	0.98	2.59	3.506 (3)	157
C22—H22B...C15 ^{iv}	0.98	2.84	3.681 (4)	144
C22—H22C...C11 ^{vi}	0.98	2.86	3.670 (4)	141
C22—H22D...C12	0.98	2.77	3.308 (4)	115
C31—H31B...O4 ^{vii}	0.98	2.53	3.389 (4)	147
C31—H31C...C16 ^v	0.98	2.94	3.796 (4)	146
C32—H32B...O4 ^{vii}	0.98	2.46	3.336 (4)	149
C32—H32C...C15	0.98	2.73	3.275 (4)	115
C32—H32D...C14 ^v	0.98	2.58	3.541 (4)	167

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