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Crystal structure of *rac*-(3a*R**,9a*S**)-4,4,4-trichloro-1,2,3,3a,4,9a-hexahydro-4λ^5,9λ^4-cyclopenta[4,5][1,3]tellurazolo-[3,2-*a*]pyridine

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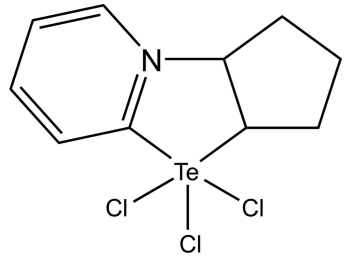
The title compound, $C_{10}H_{12}Cl_3NTe$, crystallizes with two crystallographically independent molecules (*A* and *B*) in the asymmetric unit. In each case, the coordination around the Te atom is distorted square-pyramidal, with the equatorial plane composed of the three Cl atoms and the C atom of the pyridinium ring. The Te atom is displaced from the mean-square plane by 0.1926 (7) and 0.1981 (8) Å, in molecules *A* and *B*, respectivly, away from the apical C atom. The bond lengths from the Te atom to the two Cl atoms arranged *trans* to each other [2.5009 (7)/2.5145 (7) and 2.5184 (7)/2.5220 (8) Å in molecules *A* and *B*, respectivly] are substantially shorter than the third Te—Cl distance [2.8786 (7) and 2.8763 (7) Å in molecules *A* and *B*, respectivly]. The 1,3-tellurazole ring is almost planar (r.m.s. deviations of 0.042 and 0.045 Å in molecules *A* and *B*, respectivly). The cyclopentane rings in both molecules *A* and *B* adopt envelope conformations with the carbon atom opposed to the (Te)C—C(N) bond as the flap. In the crystal, molecules form centrosymmetric 2 + 2 associates *via* Te···Cl interactions [3.3993 (7) and 3.2030 (7) Å]. As a result of these secondary interactions, the Te atom attains a strongly distorted 5 + 1 octahedral environment. Further, the 2 + 2 associates are bound by weak C—H···Cl hydrogen bonds into a three–dimensional framework.

Keywords: crystal structure; arenetellurium trihalide; Te···Cl interactions; C—H···Cl hydrogen bonding.

CCDC reference: 1409052

1. Related literature

For general background and synthesis, see: Petragnani & Stefani (2007); Borisov *et al.* (2013). For related compounds, see: Singh *et al.* (1990); Sundberg *et al.* (1994); Zukerman-Schpector *et al.* (2000); Kandasamy *et al.* (2003); Raghavendra *et al.* (2006); Dutton *et al.* (2009); Lee *et al.* (2010); Rakesh *et al.* (2012).



2. Experimental

2.1. Crystal data

$C_{10}H_{12}Cl_3NTe$
M_r = 380.16
Monoclinic, $P2_1/c$
a = 14.3279 (6) Å
b = 11.2539 (5) Å
c = 16.2967 (7) Å
β = 94.546 (1)°
V = 2619.5 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.85 mm^{-1}
T = 120 K
0.20 × 0.15 × 0.15 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.595, T_{max} = 0.666
32448 measured reflections
7642 independent reflections
6535 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.059
S = 1.08
7642 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···Cl3^{i}	0.95	2.78	3.533 (3)	137
C7—H7···Cl3^{ii}	0.95	2.78	3.340 (3)	119
C9*A*—H9*A*···Cl6	1.00	2.57	3.465 (3)	149
C15—H15···Cl3^{ii}	0.95	2.63	3.384 (3)	136
C17—H17···Cl6^{iii}	0.95	2.74	3.558 (3)	145
C18—H18···Cl6^{iv}	0.95	2.73	3.539 (3)	144
C19*A*—H19*A*···Cl6^{iv}	1.00	2.69	3.544 (3)	144

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (iii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iv) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine

structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: RK2431).

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supporting information

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Crystal structure of *rac*-(3a*R**,9a*S**)-4,4,4-trichloro-1,2,3,3a,4,9a-hexahydro-4λ^5,9λ^4-cyclopenta[4,5][1,3]tellurazolo[3,2-*a*]pyridine

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S1. Structural commentary

It is known that the reaction of arenetellurium trihalides *Ar*Te*Hal*$_3$ with alkenes and acetylenes usually gives the products of 1,2–addition at the multiple bonds, *β*–haloalkyl(vinyl)tellurium dihalides or the products of transannular cyclization with the ring closure by the electron–donating center of the functional group containing in the molecule of the unsaturated substrate, lactones, ordinary cyclic ethers, pyrrolidine and piperidine derivatives (Petragnani & Stefani, 2007).

This work reports the structural characterization of a product of reaction of 2–pyridinetellurium trichloride - the first representative of hetarenetellurium trihalides containing a nitrogen base as the hetaryl substituent (Borisov *et al.*, 2013) with cyclopentene (Figure 1).

Compound (**I**), $C_{10}H_{12}Cl_3NTe$, crystallizes with two crystallographically independent molecules in the asymmetric unit (Figure 2). These crystallographically independent molecules are geometrically very similar. The coordination around the tellurium atom is a distorted square–pyramidal. The equatorial plane is composed of the three chlorine atoms and the carbon atom of pyridinium ring. The tellurium atom is displaced from the mean square plane by 0.1926 (7) and 0.1981 (8) Å for the two crystallographically independent molecules, respectively, away from the apical carbon atom. The bond lengths from the tellurium atom to the two chlorine atoms arranged *trans* to each other [2.5009 (7)/2.5145 (7) and 2.5184 (7)/2.5220 (8) Å for the two crystallographically independent molecules, respectively] are close to those in related complexes (Singh *et al.*, 1990; Sundberg *et al.*, 1994; Zukerman–Schpector *et al.*, 2000; Kandasamy *et al.*, 2003; Raghavendra *et al.*, 2006; Dutton *et al.*, 2009; Lee *et al.*, 2010; Rakesh *et al.*, 2012). The third Te—Cl distance (2.8786 (7) and 2.8763 (7) Å for the two crystallographically independent molecules, respectively) is substantially longer than the other two Te—Cl distances. This geometry is apparently determined by the zwitterionic nature of the complex and the hypervalent configuration of the tellurium atom. The analogous geometry was observed previously for trichloro-(ethane–1,2-diolato–*O*,*O*′)tellurate(IV) (Sundberg *et al.*, 1994). The Te—C distances are in good agreement with typical values found in tellurium(IV) complexes, which range from 2.11 to 2.16 Å. The 1,3–tellurazole ring in (**I**) is almost planar (r.m.s. deviation is 0.042 and 0.045 Å for the two crystallographically independent molecules, respectively). The cyclopentane ring adopts the usual *envelope* conformation.

In the crystal, the molecules of (**I**) form centrosymmetrical 2+2–associates *via* additional non–valent attractive Te···Cl interactions (Te4···Cl3 [-*x*, 2-*y*, 1-*z*] 3.3993 (7) Å, Te14···Cl3 [*x*, 1.5-*y*, -0.5+*z*] 3.2030 (7) Å), in which the Cl3 chlorine atom is μ^3–bridging, while the Cl6 chlorine atom is terminal (Figure 3). Due to these additional secondary interactions, the tellurium atom attains the strongly distorted 5+1–octahedral environment. Further, the 2+2–associates of (**I**) are bound by weak intermolecular C—H···Cl hydrogen bonds into a 3–dimensional framework (Table 1, Figure 4). There are

no intermolecular Cl···Cl interactions.

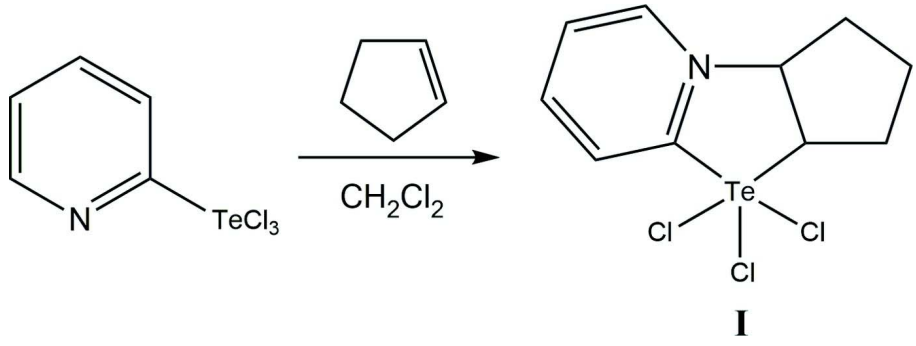
The molecule of (**I**) possesses two asymmetric centers at the C3A and C9A carbon atoms and can have potentially four diastereomers. The crystal of (**I**) is racemic and consists of enantiomeric pairs with the following relative configuration of the centers: ***rac***-3A***R****,9A***S****.

S2. Synthesis and crystallization

Complex (**I**) was prepared according to the procedure described by us earlier (Borisov *et al.*, 2013). The single crystals of (**I**) suitable for an X–ray diffraction analysis were obtained after recrystallization of the crude product from methylene chloride.

S3. Refinement

All hydrogen atoms were placed in calculated positions with C—H = 0.95 Å (for aryl–H), 0.99 Å (for methylene–H) and 1.00 Å (for methine–H) and refined in the riding model with fixed isotropic displacement parameters [U_{iso}(H) = 1.2U_{eq}(C)].



I

Figure 1

The reaction of 2–pyridinetellurium trichloride with cyclopentene.

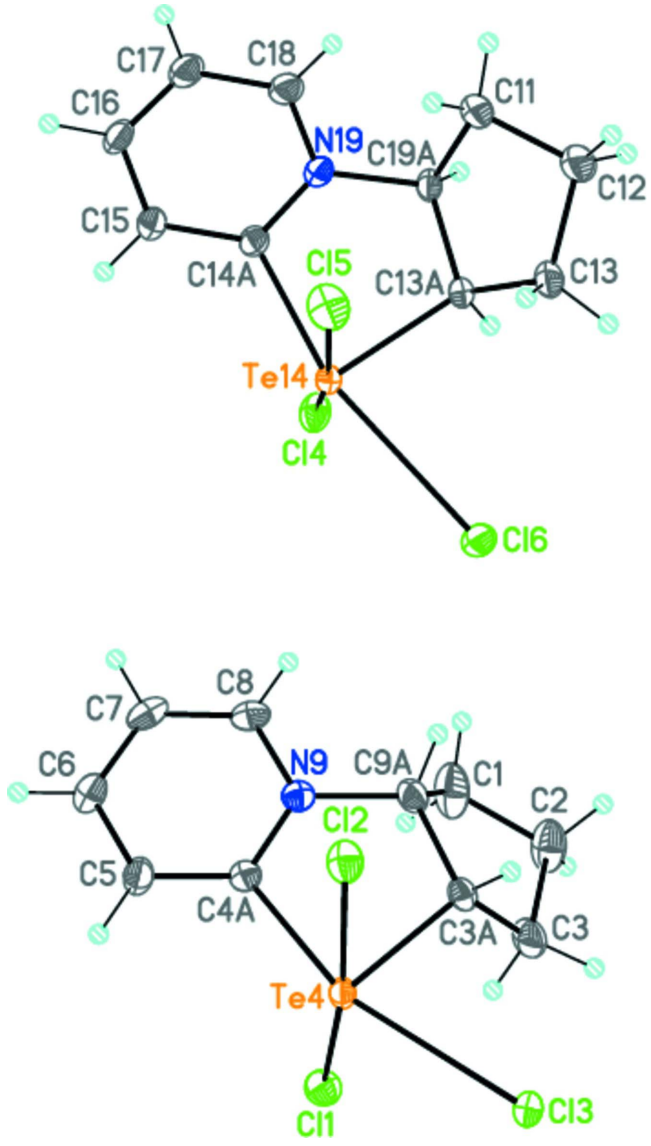


Figure 2

Molecular structure of (**I**) (the two crystallographically independent molecules are depicted). Displacement ellipsoids are shown at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

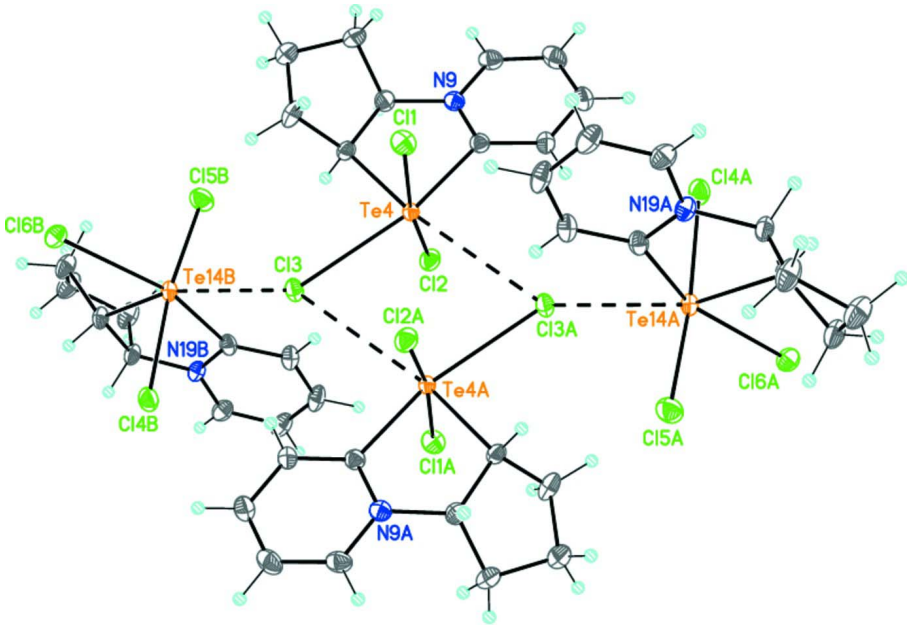


Figure 3

The centrosymmetrical 2+2–associates of (**I**). Dashed lines indicate the intermolecular non–valent attractive Te···Cl interactions.

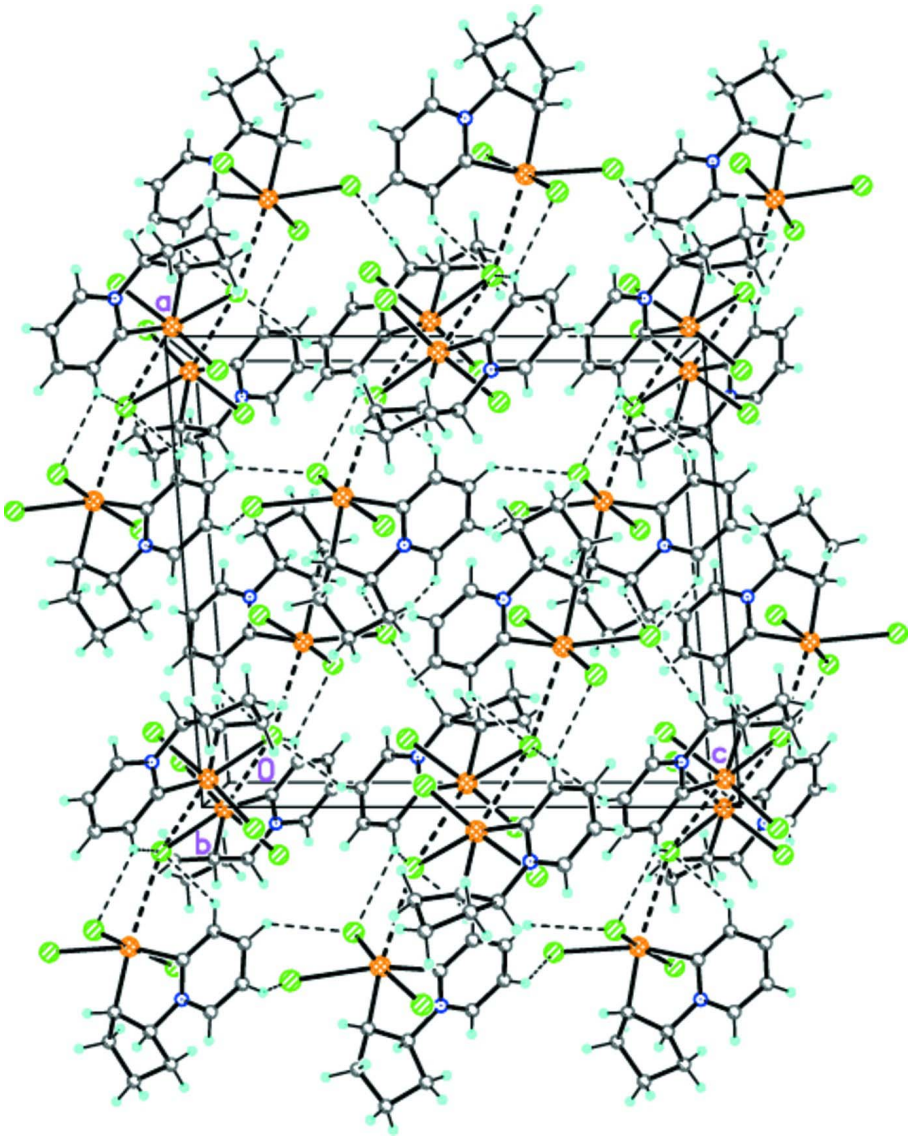


Figure 4

Crystal packing of (**I**). The thick dashed lines indicate the intermolecular non–valent attractive Te···Cl interactions, and the thin dashed lines indicate the intermolecular C—H···Cl hydrogen bonds.

rac-(3a*R**,9a*S**)-4,4,4-Trichloro-1,2,3,3a,4,9a-hexahydro-4λ^5,9λ^4-cyclopenta[4,5][1,3]tellurazolo[3,2-*a*]pyridine

Crystal data

$C_{10}H_{12}Cl_3NTe$
M_r = 380.16
Monoclinic, $P2_1/c$
a = 14.3279 (6) Å
b = 11.2539 (5) Å
c = 16.2967 (7) Å
β = 94.546 (1)°
V = 2619.5 (2) Å^3
Z = 8

$F(000)$ = 1456
D_x = 1.928 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9992 reflections
θ = 2.2–32.5°
μ = 2.85 mm^{-1}
T = 120 K
Prism, yellow
0.20 × 0.15 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine–focus sealed tube
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.595, T_{max} = 0.666
32448 measured reflections
7642 independent reflections
6535 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 30.0°, θ_{min} = 1.4°
h = −20→20
k = −15→15
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.059
S = 1.08
7642 reflections
271 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
$w = 1/[\sigma^2(F_o^2) + (0.0215P)^2 + 1.2054P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	−0.05985 (5)	0.72835 (7)	0.58167 (5)	0.02922 (15)
Cl2	0.14184 (5)	0.93448 (6)	0.38971 (4)	0.02747 (15)
Cl3	0.12938 (5)	1.00286 (6)	0.61789 (4)	0.02427 (14)
C1	0.1831 (3)	0.5277 (3)	0.5165 (2)	0.0453 (9)
H1A	0.1220	0.4886	0.5215	0.054*
H1B	0.2254	0.4714	0.4911	0.054*
C2	0.2250 (3)	0.5689 (3)	0.5989 (2)	0.0422 (9)
H2A	0.2929	0.5843	0.5976	0.051*
H2B	0.2155	0.5091	0.6420	0.051*
C3	0.1724 (2)	0.6828 (3)	0.61445 (19)	0.0329 (7)
H3A	0.2083	0.7337	0.6552	0.040*
H3B	0.1101	0.6658	0.6341	0.040*
C3A	0.16345 (18)	0.7410 (2)	0.52939 (17)	0.0214 (5)
H3C	0.2194	0.7934	0.5259	0.026*
Te4	0.04220 (2)	0.84673 (2)	0.49461 (2)	0.01829 (5)
C4A	0.01838 (19)	0.7106 (2)	0.40406 (17)	0.0213 (5)
C5	−0.0573 (2)	0.7027 (3)	0.34626 (18)	0.0275 (6)
H5	−0.1078	0.7574	0.3471	0.033*
C6	−0.0589 (2)	0.6143 (3)	0.28727 (18)	0.0311 (7)
H6	−0.1106	0.6076	0.2473	0.037*

C7	0.0154 (2)	0.5356 (3)	0.28687 (18)	0.0313 (7)
H7	0.0149	0.4743	0.2468	0.038*
C8	0.0895 (2)	0.5471 (3)	0.34498 (18)	0.0272 (6)
H8	0.1413	0.4945	0.3444	0.033*
N9	0.08939 (16)	0.6327 (2)	0.40306 (14)	0.0219 (5)
C9A	0.1713 (2)	0.6402 (3)	0.46615 (19)	0.0265 (6)
H9A	0.2293	0.6531	0.4370	0.032*
Cl4	0.28653 (5)	0.27629 (7)	0.24383 (4)	0.02950 (16)
Cl5	0.40398 (6)	0.64964 (7)	0.11901 (5)	0.03456 (17)
Cl6	0.36234 (5)	0.56379 (6)	0.35946 (4)	0.02687 (15)
C11	0.5970 (2)	0.4070 (3)	0.1259 (2)	0.0338 (7)
H11A	0.6415	0.3549	0.0995	0.041*
H11B	0.5744	0.4696	0.0865	0.041*
C12	0.6412 (2)	0.4601 (3)	0.2044 (2)	0.0369 (8)
H12A	0.6820	0.5280	0.1927	0.044*
H12B	0.6787	0.4001	0.2369	0.044*
C13	0.55749 (19)	0.5014 (3)	0.2505 (2)	0.0306 (7)
H13A	0.5737	0.5025	0.3107	0.037*
H13B	0.5368	0.5818	0.2325	0.037*
C13A	0.48125 (18)	0.4089 (3)	0.22756 (17)	0.0220 (6)
H13C	0.4777	0.3543	0.2756	0.026*
Te14	0.34174 (2)	0.47397 (2)	0.19378 (2)	0.01873 (5)
C14A	0.36030 (19)	0.3737 (3)	0.08412 (16)	0.0217 (6)
C15	0.2958 (2)	0.3570 (3)	0.01782 (17)	0.0262 (6)
H15	0.2388	0.4004	0.0138	0.031*
C16	0.3149 (2)	0.2764 (3)	−0.04306 (17)	0.0307 (7)
H16	0.2713	0.2653	−0.0894	0.037*
C17	0.3974 (2)	0.2124 (3)	−0.03626 (19)	0.0319 (7)
H17	0.4099	0.1551	−0.0768	0.038*
C18	0.4612 (2)	0.2323 (3)	0.02985 (18)	0.0276 (6)
H18	0.5186	0.1898	0.0347	0.033*
N19	0.44226 (16)	0.3125 (2)	0.08791 (14)	0.0222 (5)
C19A	0.51593 (18)	0.3360 (3)	0.15587 (17)	0.0234 (6)
H19A	0.5405	0.2582	0.1779	0.028*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0258 (3)	0.0311 (4)	0.0313 (4)	−0.0041 (3)	0.0053 (3)	−0.0004 (3)
Cl2	0.0271 (3)	0.0286 (4)	0.0263 (4)	−0.0033 (3)	−0.0006 (3)	0.0069 (3)
Cl3	0.0208 (3)	0.0290 (4)	0.0222 (3)	−0.0004 (3)	−0.0029 (2)	−0.0050 (3)
C1	0.051 (2)	0.0229 (16)	0.057 (2)	0.0052 (15)	−0.0242 (18)	0.0049 (16)
C2	0.048 (2)	0.0284 (17)	0.047 (2)	0.0007 (15)	−0.0177 (17)	0.0069 (15)
C3	0.0283 (16)	0.0419 (19)	0.0277 (16)	0.0102 (14)	−0.0034 (12)	0.0090 (14)
C3A	0.0181 (12)	0.0208 (13)	0.0247 (14)	0.0035 (10)	−0.0017 (10)	0.0023 (11)
Te4	0.01718 (8)	0.01745 (8)	0.01955 (9)	0.00076 (6)	−0.00290 (6)	−0.00165 (7)
C4A	0.0222 (13)	0.0208 (13)	0.0209 (13)	0.0001 (11)	0.0021 (10)	−0.0005 (11)
C5	0.0299 (15)	0.0264 (15)	0.0248 (15)	0.0027 (12)	−0.0067 (12)	−0.0029 (12)

C6	0.0371 (17)	0.0318 (16)	0.0233 (15)	−0.0023 (13)	−0.0037 (13)	−0.0031 (13)
C7	0.0435 (18)	0.0300 (16)	0.0212 (15)	−0.0057 (14)	0.0084 (13)	−0.0071 (13)
C8	0.0335 (16)	0.0227 (14)	0.0263 (15)	0.0031 (12)	0.0084 (12)	−0.0029 (12)
N9	0.0224 (11)	0.0212 (12)	0.0223 (12)	−0.0008 (9)	0.0032 (9)	−0.0002 (9)
C9A	0.0214 (14)	0.0258 (15)	0.0317 (16)	0.0061 (11)	−0.0027 (12)	−0.0038 (12)
Cl4	0.0306 (4)	0.0338 (4)	0.0233 (3)	−0.0059 (3)	−0.0024 (3)	0.0080 (3)
Cl5	0.0336 (4)	0.0306 (4)	0.0393 (4)	−0.0030 (3)	0.0012 (3)	0.0096 (3)
Cl6	0.0283 (4)	0.0286 (4)	0.0239 (3)	−0.0009 (3)	0.0033 (3)	−0.0047 (3)
C11	0.0202 (14)	0.050 (2)	0.0319 (17)	−0.0041 (14)	0.0028 (12)	−0.0112 (15)
C12	0.0240 (15)	0.048 (2)	0.0391 (19)	−0.0058 (14)	0.0030 (13)	−0.0151 (16)
C13	0.0201 (14)	0.0386 (18)	0.0321 (17)	0.0015 (12)	−0.0044 (12)	−0.0116 (14)
C13A	0.0165 (12)	0.0299 (15)	0.0190 (13)	0.0028 (11)	−0.0023 (10)	−0.0020 (11)
Te14	0.01635 (8)	0.02350 (9)	0.01601 (8)	0.00111 (7)	−0.00087 (6)	0.00012 (7)
C14A	0.0215 (13)	0.0270 (15)	0.0165 (13)	−0.0005 (11)	0.0016 (10)	0.0042 (11)
C15	0.0227 (14)	0.0365 (17)	0.0189 (14)	−0.0001 (12)	−0.0007 (11)	0.0016 (12)
C16	0.0292 (15)	0.047 (2)	0.0154 (13)	−0.0090 (14)	−0.0004 (11)	−0.0029 (13)
C17	0.0330 (16)	0.0387 (18)	0.0241 (15)	−0.0061 (14)	0.0030 (12)	−0.0100 (13)
C18	0.0284 (15)	0.0295 (16)	0.0254 (15)	−0.0015 (12)	0.0047 (12)	−0.0066 (12)
N19	0.0227 (12)	0.0262 (12)	0.0175 (11)	−0.0017 (9)	0.0004 (9)	−0.0030 (9)
C19A	0.0186 (13)	0.0282 (15)	0.0222 (14)	0.0027 (11)	−0.0045 (10)	−0.0062 (12)

Geometric parameters (Å, º)

Cl1—Te4	2.5009 (7)	Cl4—Te14	2.5184 (7)
Cl2—Te4	2.5145 (7)	Cl5—Te14	2.5220 (8)
Cl3—Te4	2.8786 (7)	Cl6—Te14	2.8763 (7)
C1—C2	1.501 (5)	C11—C12	1.506 (4)
C1—C9A	1.510 (4)	C11—C19A	1.521 (4)
C1—H1A	0.9900	C11—H11A	0.9900
C1—H1B	0.9900	C11—H11B	0.9900
C2—C3	1.518 (5)	C12—C13	1.536 (4)
C2—H2A	0.9900	C12—H12A	0.9900
C2—H2B	0.9900	C12—H12B	0.9900
C3—C3A	1.529 (4)	C13—C13A	1.533 (4)
C3—H3A	0.9900	C13—H13A	0.9900
C3—H3B	0.9900	C13—H13B	0.9900
C3A—C9A	1.543 (4)	C13A—C19A	1.542 (4)
C3A—Te4	2.144 (3)	C13A—Te14	2.159 (3)
C3A—H3C	1.0000	C13A—H13C	1.0000
Te4—C4A	2.136 (3)	Te14—C14A	2.148 (3)
C4A—N9	1.344 (3)	C14A—N19	1.359 (3)
C4A—C5	1.382 (4)	C14A—C15	1.377 (4)
C5—C6	1.382 (4)	C15—C16	1.388 (4)
C5—H5	0.9500	C15—H15	0.9500
C6—C7	1.385 (4)	C16—C17	1.381 (4)
C6—H6	0.9500	C16—H16	0.9500
C7—C8	1.372 (4)	C17—C18	1.375 (4)
C7—H7	0.9500	C17—H17	0.9500

C8—N9	1.351 (4)	C18—N19	1.350 (4)
C8—H8	0.9500	C18—H18	0.9500
N9—C9A	1.500 (4)	N19—C19A	1.492 (3)
C9A—H9A	1.0000	C19A—H19A	1.0000
C2—C1—C9A	104.3 (3)	C12—C11—C19A	102.5 (2)
C2—C1—H1A	110.9	C12—C11—H11A	111.3
C9A—C1—H1A	110.9	C19A—C11—H11A	111.3
C2—C1—H1B	110.9	C12—C11—H11B	111.3
C9A—C1—H1B	110.9	C19A—C11—H11B	111.3
H1A—C1—H1B	108.9	H11A—C11—H11B	109.2
C1—C2—C3	104.0 (3)	C11—C12—C13	104.1 (2)
C1—C2—H2A	111.0	C11—C12—H12A	110.9
C3—C2—H2A	111.0	C13—C12—H12A	110.9
C1—C2—H2B	111.0	C11—C12—H12B	110.9
C3—C2—H2B	111.0	C13—C12—H12B	110.9
H2A—C2—H2B	109.0	H12A—C12—H12B	109.0
C2—C3—C3A	102.6 (3)	C13A—C13—C12	104.1 (2)
C2—C3—H3A	111.3	C13A—C13—H13A	110.9
C3A—C3—H3A	111.3	C12—C13—H13A	110.9
C2—C3—H3B	111.3	C13A—C13—H13B	110.9
C3A—C3—H3B	111.3	C12—C13—H13B	110.9
H3A—C3—H3B	109.2	H13A—C13—H13B	109.0
C3—C3A—C9A	106.6 (2)	C13—C13A—C19A	106.3 (2)
C3—C3A—Te4	119.02 (19)	C13—C13A—Te14	117.36 (19)
C9A—C3A—Te4	109.39 (17)	C19A—C13A—Te14	109.55 (17)
C3—C3A—H3C	107.1	C13—C13A—H13C	107.8
C9A—C3A—H3C	107.1	C19A—C13A—H13C	107.8
Te4—C3A—H3C	107.1	Te14—C13A—H13C	107.8
C4A—Te4—C3A	82.32 (10)	C14A—Te14—C13A	82.00 (10)
C4A—Te4—Cl1	86.64 (8)	C14A—Te14—Cl4	82.42 (7)
C3A—Te4—Cl1	93.00 (8)	C13A—Te14—Cl4	85.77 (8)
C4A—Te4—Cl2	83.11 (8)	C14A—Te14—Cl5	86.45 (8)
C3A—Te4—Cl2	84.59 (8)	C13A—Te14—Cl5	91.91 (8)
Cl1—Te4—Cl2	169.70 (3)	Cl4—Te14—Cl5	168.84 (3)
N9—C4A—C5	120.2 (3)	N19—C14A—C15	119.4 (3)
N9—C4A—Te4	113.36 (19)	N19—C14A—Te14	113.09 (18)
C5—C4A—Te4	126.2 (2)	C15—C14A—Te14	127.2 (2)
C4A—C5—C6	119.3 (3)	C14A—C15—C16	119.4 (3)
C4A—C5—H5	120.4	C14A—C15—H15	120.3
C6—C5—H5	120.4	C16—C15—H15	120.3
C5—C6—C7	119.6 (3)	C17—C16—C15	120.0 (3)
C5—C6—H6	120.2	C17—C16—H16	120.0
C7—C6—H6	120.2	C15—C16—H16	120.0
C8—C7—C6	119.3 (3)	C18—C17—C16	119.3 (3)
C8—C7—H7	120.3	C18—C17—H17	120.4
C6—C7—H7	120.3	C16—C17—H17	120.4
N9—C8—C7	120.4 (3)	N19—C18—C17	120.0 (3)

N9—C8—H8	119.8	N19—C18—H18	120.0
C7—C8—H8	119.8	C17—C18—H18	120.0
C4A—N9—C8	121.1 (2)	C18—N19—C14A	121.8 (2)
C4A—N9—C9A	120.5 (2)	C18—N19—C19A	118.0 (2)
C8—N9—C9A	118.4 (2)	C14A—N19—C19A	120.1 (2)
N9—C9A—C1	111.9 (2)	N19—C19A—C11	111.6 (2)
N9—C9A—C3A	113.9 (2)	N19—C19A—C13A	113.9 (2)
C1—C9A—C3A	105.3 (3)	C11—C19A—C13A	105.3 (2)
N9—C9A—H9A	108.5	N19—C19A—H19A	108.6
C1—C9A—H9A	108.5	C11—C19A—H19A	108.6
C3A—C9A—H9A	108.5	C13A—C19A—H19A	108.6
C9A—C1—C2—C3	40.7 (4)	C19A—C11—C12—C13	−42.7 (3)
C1—C2—C3—C3A	−39.5 (4)	C11—C12—C13—C13A	34.0 (3)
C2—C3—C3A—C9A	23.5 (3)	C12—C13—C13A—C19A	−12.0 (3)
C2—C3—C3A—Te4	147.7 (2)	C12—C13—C13A—Te14	−134.9 (2)
N9—C4A—C5—C6	−0.4 (4)	N19—C14A—C15—C16	1.2 (4)
Te4—C4A—C5—C6	174.7 (2)	Te14—C14A—C15—C16	−171.3 (2)
C4A—C5—C6—C7	−0.2 (5)	C14A—C15—C16—C17	1.0 (5)
C5—C6—C7—C8	−0.3 (5)	C15—C16—C17—C18	−2.1 (5)
C6—C7—C8—N9	1.3 (5)	C16—C17—C18—N19	1.1 (5)
C5—C4A—N9—C8	1.5 (4)	C17—C18—N19—C14A	1.2 (4)
Te4—C4A—N9—C8	−174.2 (2)	C17—C18—N19—C19A	−176.6 (3)
C5—C4A—N9—C9A	−179.4 (3)	C15—C14A—N19—C18	−2.4 (4)
Te4—C4A—N9—C9A	4.9 (3)	Te14—C14A—N19—C18	171.2 (2)
C7—C8—N9—C4A	−2.0 (4)	C15—C14A—N19—C19A	175.4 (3)
C7—C8—N9—C9A	178.9 (3)	Te14—C14A—N19—C19A	−11.1 (3)
C4A—N9—C9A—C1	120.3 (3)	C18—N19—C19A—C11	72.4 (3)
C8—N9—C9A—C1	−60.6 (4)	C14A—N19—C19A—C11	−105.4 (3)
C4A—N9—C9A—C3A	1.0 (4)	C18—N19—C19A—C13A	−168.5 (3)
C8—N9—C9A—C3A	−179.9 (2)	C14A—N19—C19A—C13A	13.7 (4)
C2—C1—C9A—N9	−149.5 (3)	C12—C11—C19A—N19	158.9 (2)
C2—C1—C9A—C3A	−25.2 (4)	C12—C11—C19A—C13A	34.8 (3)
C3—C3A—C9A—N9	123.7 (3)	C13—C13A—C19A—N19	−136.5 (2)
Te4—C3A—C9A—N9	−6.2 (3)	Te14—C13A—C19A—N19	−8.8 (3)
C3—C3A—C9A—C1	0.8 (3)	C13—C13A—C19A—C11	−13.9 (3)
Te4—C3A—C9A—C1	−129.1 (2)	Te14—C13A—C19A—C11	113.8 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···Cl3^{i}	0.95	2.78	3.533 (3)	137
C7—H7···Cl3^{ii}	0.95	2.78	3.340 (3)	119
C9*A*—H9*A*···Cl6	1.00	2.57	3.465 (3)	149
C15—H15···Cl3^{ii}	0.95	2.63	3.384 (3)	136
C17—H17···Cl6^{iii}	0.95	2.74	3.558 (3)	145

C18—H18···Cl6^{iv}	0.95	2.73	3.539 (3)	144
C19*A*—H19*A*···Cl6^{iv}	1.00	2.69	3.544 (3)	144

Symmetry codes: (i) −*x*, −*y*+2, −*z*+1; (ii) *x*, −*y*+3/2, *z*−1/2; (iii) *x*, −*y*+1/2, *z*−1/2; (iv) −*x*+1, *y*−1/2, −*z*+1/2.