## Structure Reports

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## Dibromidochlorido\{2-[(dimethylamino)-methyl]phenyl- $\left.\kappa^{2} N, C^{1}\right\}$ tellurium(IV)

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Key indicators: single-crystal X-ray study; $T=123 \mathrm{~K}$; mean $\sigma(\mathrm{C}-\mathrm{C})=0.005 \AA$; disorder in main residue; $R$ factor $=0.038 ; w R$ factor $=0.056$; data-to-parameter ratio $=30.1$.

The title compound, $\mathrm{C}_{9} \mathrm{H}_{13} \mathrm{Br}_{2} \mathrm{ClNTe}$, was synthesized by reacting [2-(dimethylaminomethyl)phenyl]tellurium(II) chloride with $\mathrm{Br}_{2}$. As a consequence, the Cl and Br atoms are not well ordered but distributed over the three possible positions such that the overall stiochiometry is two Br atoms and one Cl atom. The scrambling of the Br and Cl atoms indicates a small energy barrier for the exchange process between the apical and equatorial positions. Overall, the Te atom geometry is slightly distorted square pyramidal ( $\tau=0.052$ for the major component). However, there is a weak secondary interaction between the Te atoms and the disordered $\mathrm{Br} / \mathrm{Cl}$ atoms of a nearby molecule. The $\mathrm{Te}-\mathrm{Br}$ and $\mathrm{Te}-\mathrm{Cl}$ distances in both disorder components fall into two groups; a longer distance for the $\mathrm{Br} / \mathrm{Cl}$ involved in this secondary interaction [2.6945 (17) $\AA$ for Br and 2.601 (9) $\AA$ for Cl ] and shorter bond distances to the remaining halogen atoms, indicating that this interaction has slightly weakened the $\mathrm{Te}-X$ bond, as is the case in the previously reported tribromido structure [Singh et al. (1990). J. Chem. Soc. Dalton Trans. pp. 907-913]. Otherwise, the metrical parameters in the two structures are not significantly different. An intermolecular $\mathrm{C}-\mathrm{H} \cdot \cdot \mathrm{Br}$ interaction occurs.

## Related literature

For related structures, see: Panda et al. (1999); Singh \& McWhinnie (1985); Singh et al. (1992); Singh et al. (1990). For the synthesis of similar dibromidochlorido derivatives of tellurium, see: Rivkin et al. (1991); Cobbledick et al. (1979). For the asymmetry parameter, see: Addison et al. (1984). For the preparation of bis[2-(dimethylaminomethyl)phenyl]ditelluride, see: Kaur et al. (1995).


## Experimental

Crystal data
$\mathrm{C}_{9} \mathrm{H}_{12} \mathrm{Br}_{2} \mathrm{ClNTe}$
$V=1296.61(9) \AA^{3}$
$M_{r}=457.07$
Monoclinic, $P 2_{1} / c$
$a=7.2854$ (3) A
$b=12.4785$ (5) $\AA$
$c=14.4098$ (6) $\AA$
$\beta=98.200(4)^{\circ}$

## Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Absorption correction: analytical [CrysAlis PRO (Oxford Diffraction, 2007), based on expressions derived by Clark \&

## Reid (1995)]

$T_{\text {min }}=0.042, T_{\text {max }}=0.409$
8229 measured reflections
4241 independent reflections
2981 reflections with $I>2 \sigma(I)$
$R_{\text {int }}=0.044$

## Refinement

$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.038 \quad 1$ restraint
$w R\left(F^{2}\right)=0.056$
H -atom parameters constrained
$S=0.96$
$\Delta \rho_{\text {max }}=0.91 \mathrm{e}^{-3}{ }^{-3}$
4241 reflections
$\Delta \rho_{\text {min }}=-0.92 \mathrm{e}^{\AA^{-3}}$

141 parameters

Table 1
Hydrogen-bond geometry $\left(\AA^{\circ},^{\circ}\right)$.

| $D-\mathrm{H} \cdots A$ | $D-\mathrm{H}$ | $\mathrm{H} \cdots A$ | $D \cdots A$ | $D-\mathrm{H} \cdots A$ |
| :--- | :--- | :--- | :--- | :--- |
| $\mathrm{C} 7-\mathrm{H} 7 A \cdots \mathrm{Br}^{2}$ | 0.99 | 2.96 | $3.839(4)$ | 149 |
| Symmetry code: (i) $x-1, y, z$. |  |  |  |  |

Data collection: CrysAlis PRO (Oxford Diffraction, 2007); cell refinement: CrysAlis PRO; data reduction: CrysAlis PRO; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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[^0]IUCr electronic archives (Reference: JJ2114).

## References

Addison, A. W., Rao, T. N., Reedijk, J., van Rijn, J. \& Verschoor, G. C. (1984). J. Chem. Soc. Dalton Trans. pp. 1349-1356.

Clark, R. C. \& Reid, J. S. (1995). Acta Cryst. A51, 887-897.
Cobbledick, R. E., Einstein, F. W. B., McWhinnie, W. R. \& Musa, F. H. (1979). J. Chem. Res. (S), p. 145.

Kaur, R., Singh, H. B. \& Butcher, R. J. (1995). Organometallics, 14, 4755-4763.
Oxford Diffraction (2007). CrysAlis PRO, CrysAlis RED and CrysAlis CCD. Oxford Diffraction Ltd, Abingdon, England.

## organic compounds

Panda, A., Mugesh, G., Singh, H. B. \& Butcher, R. J. (1999). Organometallics, 18, 1986-1993.
Rivkin, B. B., Maksimenko, A. A. \& Sadekov, I. D. (1991). Zh. Obshch. Khim. 61, 1154-1162.
Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

Singh, H. B. \& McWhinnie, W. R. (1985). J. Chem. Soc. Dalton Trans. pp. 821825.

Singh, H. B., Sudha, N. \& Butcher, R. J. (1992). Inorg. Chem. 31, 1431-1435. Singh, H. B., Sudha, N., West, A. A. \& Hamor, T. A. (1990). J. Chem. Soc. Dalton Trans. pp. 907-913.

## supporting information

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## Dibromidochlorido\{2-[(dimethylamino)methyl]phenyl $\left.-\kappa^{2} N, C^{1}\right\}$ tellurium(IV)

Prakul Rakesh, Harkesh B. Singh and Ray J. Butcher

## S1. Comment

Unlike their selenium analogues, simple aryltellurenyl halides are thermally unstable and polymeric in nature. However, it has been shown that they can be stabilized by intramolecular coordination and thus be isolated and structurally characterized (Singh \& McWhinnie, 1985; Singh et al., 1990; Singh et al., 1992; Panda et al., 1999). Previously the structures $\{2-[(S)-1$-(dimethylamino)ethyl]phenyl $\}$ tellurium(IV) trichloride (Singh et al. 1992) and 2-(dimethylaminomethyl)phenyl]tellurium(IV) tribromide (Singh et al. 1990) have been published. In this report the structure of 2-(dimethylaminomethyl)phenyl]tellurium(IV)dibromide chloride is presented in which the 2 Br 's and Cl are distributed over the three possible sites. The scrambling of the $\mathrm{Br} / \mathrm{Cl}$ position indicates a small energy barrier for the exchange process between the axial and equatorial positions. The synthesis of similar dibromochloro derivatives of Te have been reported previously although no crystal structures were completed (Cobbledick et al., 1979; Rivkin et al., 1991).
Overall the molecule is slightly distorted square pyramidal [ $\tau=0.052$ for the major component (Addison et al., 1984]. However there is a weak secondary interaction between the Te and $\mathrm{Br} / \mathrm{Cl}$ of an adjoining molecule. $\mathrm{The} \mathrm{Te}-\mathrm{Br}$ and $\mathrm{Te}-$ Cl distances in both molecules fall into two groups; a longer distance for the $\mathrm{Br} / \mathrm{Cl}$ involved in this secondary interaction (2.6945 (17) $\AA$ for Br and 2.601 (9) $\AA$ for Cl ) and shorter bond distances to the remaining halogens, indicating that this interaction has slightly weakened the $\mathrm{Te}-X$ bond, as is the case in the previously reported polymorph. Otherwise, the metrical parameters in both polymorphs are not significantly different.

## S2. Experimental

As shown in the reaction scheme (scheme 2), a stirred solution of bis[2-(dimethylaminomethyl)phenyl]ditelluride, $\mathbf{1}$, (Kaur et al., 1995) ( $0.5 \mathrm{~g}, 0.94 \mathrm{mmol})$ in diethylether ( 10 ml ) was treated with $\mathrm{HCl}(3 \mathrm{ml}$ in 20 ml distilled water). The reaction mixture was further stirred for 10 min . The resulting reaction mixture was evaporated to one third of its original volume and ethanol ( 5 ml ) was added to get a yellow solid. It was redissolved in ethanol and stored in the refrigerator to get yellow needles of the monochloride, 2.
A stirred solution of $2(0.2 \mathrm{~g}, 0.66 \mathrm{mmol})$ in dry $\mathrm{CHCl}_{3}(10 \mathrm{ml})$ was treated with $\mathrm{Br}_{2}(0.37 \mathrm{ml}, 2.34 \mathrm{mmol})$ under $\mathrm{N}_{2}$ at $0^{\circ} \mathrm{C}$. The reaction mixture was further stirred for 2 h and then reduced to half volume and kept in freezer to give a yellow crystalline solid, 3 , which contained crystals of two morphologies. This is the structure of one of these.

## S3. Refinement

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with $\mathrm{C}-\mathrm{H}$ distances of $0.95-0.97 \AA\left[U_{\text {iso }}(\mathrm{H})=1.2 U_{\mathrm{eq}}\left(\mathrm{OH}, \mathrm{CH}, \mathrm{CH}_{2}\right)\left[U_{\mathrm{iso}}(\mathrm{H})=1.5 U_{\mathrm{eq}}\left(\mathrm{CH}_{3}\right)\right]\right.$. As is discussed above, the 2 Br's and Cl are distributed over the three possible positions. Initially the $\mathrm{Br} / \mathrm{Cl}$ occupancy in each position was refined as a free variable. These Br and Cl occupancies summed to $\mathrm{Br}_{2.03}$ and $\mathrm{Cl}_{0.98}$. The three free variables were then constrained to match a stoichiometry of $\mathrm{Br}_{2}$ and Cl .


Figure 1
Diagram of the major component of $\mathrm{C}_{9} \mathrm{H}_{12} \mathrm{Br}_{2} \mathrm{ClNTe}$, showing atom labeling. Atomic displacement parameters are at the $30 \%$ level.


Figure 2
Diagram showing the formation of a dimer through weak $\mathrm{Te} \cdots \mathrm{Br}$ interactions. These interactions are shown as dashed lines


Figure 3
The molecular packing for $\mathrm{C}_{9} \mathrm{H}_{12} \mathrm{Br}_{2} \mathrm{ClNTe}$ viewed along the $a$ axis. $\mathrm{Te}-\mathrm{Br}$ secondary interactions are shown by dashed lines.


Figure 4
The formation of the title compound.
Dibromidochlorido\{2-[(dimethylamino)methyl]phenyl- $\left.\kappa^{2} N, C^{1}\right\}$ tellurium(IV)

## Crystal data

$\mathrm{C}_{9} \mathrm{H}_{12} \mathrm{Br}_{2} \mathrm{ClNTe}$
$M_{r}=457.07$
Monoclinic, $P 2_{1} / c$

$$
\begin{aligned}
& \text { Hall symbol: -P } 2 \mathrm{ybc} \\
& a=7.2854(3) \AA \\
& b=12.4785(5) \AA
\end{aligned}
$$

$c=14.4098(6) \AA$
$\beta=98.200(4)^{\circ}$
$V=1296.61(9) \AA^{3}$
$Z=4$
$F(000)=848$
$D_{\mathrm{x}}=2.341 \mathrm{Mg} \mathrm{m}^{-3}$
Mo $K \alpha$ radiation, $\lambda=0.71073 \AA$

## Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels $\mathrm{mm}^{-1}$
$\omega$ scans
Absorption correction: analytical
[CrysAlis PRO (Oxford Diffraction, 2007), based on expressions derived by Clark \& Reid (1995)]

## Refinement

Refinement on $F^{2}$
Least-squares matrix: full
$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.038$
$w R\left(F^{2}\right)=0.056$
$S=0.96$
4241 reflections
141 parameters
1 restraint
Primary atom site location: structure-invariant direct methods

Cell parameters from 3585 reflections
$\theta=5.1-32.5^{\circ}$
$\mu=8.63 \mathrm{~mm}^{-1}$
$T=123 \mathrm{~K}$
Plate, yellow
$0.63 \times 0.50 \times 0.10 \mathrm{~mm}$

$$
\begin{aligned}
& T_{\min }=0.042, T_{\max }=0.409 \\
& 8229 \text { measured reflections } \\
& \text { 4241 independent reflections } \\
& 2981 \text { reflections with } I>2 \sigma(I) \\
& R_{\text {int }}=0.044 \\
& \theta_{\max }=32.6^{\circ}, \theta_{\min }=5.4^{\circ} \\
& h=-9 \rightarrow 11 \\
& k=-18 \rightarrow 13 \\
& l=-16 \rightarrow 20
\end{aligned}
$$

```
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H -atom parameters constrained
\(w=1 /\left[\sigma^{2}\left(F_{0}^{2}\right)+(0.0084 P)^{2}\right]\)
where \(P=\left(F_{0}^{2}+2 F_{\mathrm{c}}^{2}\right) / 3\)
\((\Delta / \sigma)_{\max }=0.001\)
\(\Delta \rho_{\text {max }}=0.91 \mathrm{e}_{\AA^{-3}}\)
\(\Delta \rho_{\text {min }}=-0.92\) e \(\AA^{-3}\)
```


## Special details

Experimental. CrysAlisPro (Oxford Diffraction, 2007) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark \& J.S. Reid. (Clark, R. C. \& Reid, J. S. (1995). Acta Cryst. A51, 887-897)
Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two 1.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.
Refinement. Refinement of $F^{2}$ against ALL reflections. The weighted $R$-factor $w R$ and goodness of fit $S$ are based on $F^{2}$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^{2}$. The threshold expression of $F^{2}>\sigma\left(F^{2}\right)$ is used only for calculating $R$-factors $(\mathrm{gt})$ etc. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^{2}$ are statistically about twice as large as those based on $F$, and $R$ - factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\AA^{2}$ )

|  | $x$ | $y$ | $z$ | $U_{\text {iso }} * / U_{\mathrm{eq}}$ | Occ. $(<1)$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| Te | $0.51999(3)$ | $0.349798(17)$ | $0.583822(16)$ | $0.01724(6)$ |  |
| Br 1 | $0.2864(3)$ | $0.39052(12)$ | $0.42535(11)$ | $0.0262(2)$ | $0.6585(4)$ |
| Br 2 | $0.7403(2)$ | $0.28626(15)$ | $0.73580(13)$ | $0.0228(2)$ | $0.6374(13)$ |
| Br 3 | $0.7448(2)$ | $0.26391(13)$ | $0.47988(10)$ | $0.0291(2)$ | $0.7041(13)$ |
| Cl 1 | $0.2892(15)$ | $0.4029(7)$ | $0.4363(6)$ | $0.0262(2)$ | $0.3415(4)$ |
| Cl 2 | $0.7179(11)$ | $0.2938(7)$ | $0.7271(6)$ | $0.0228(2)$ | $0.3626(13)$ |


|  |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- |
| C13 | $0.7337(15)$ | $0.2589(9)$ | $0.4931(7)$ | $0.0291(2)$ |
| N1 | $0.3019(4)$ | $0.4005(2)$ | $0.6881(2)$ | $0.0190(6)$ |
| C1 | $0.3619(4)$ | $0.2094(2)$ | $0.5943(2)$ | $0.0153(7)$ |
| C2 | $0.3578(5)$ | $0.1257(3)$ | $0.5303(3)$ | $0.0212(8)$ |
| H2A | 0.4292 | 0.1294 | 0.4801 | $0.025^{*}$ |
| C3 | $0.2486(5)$ | $0.0371(3)$ | $0.5405(3)$ | $0.0266(9)$ |
| H3A | 0.2463 | -0.0212 | 0.4980 | $0.032^{*}$ |
| C4 | $0.1421(5)$ | $0.0337(3)$ | $0.6134(3)$ | $0.0253(9)$ |
| H4A | 0.0673 | -0.0273 | 0.6203 | $0.030^{*}$ |
| C5 | $0.1438(5)$ | $0.1179(3)$ | $0.6758(3)$ | $0.0238(8)$ |
| H5A | 0.0695 | 0.1148 | 0.7249 | $0.029^{*}$ |
| C6 | $0.2551(4)$ | $0.2077(3)$ | $0.6667(2)$ | $0.0180(7)$ |
| C7 | $0.2670(5)$ | $0.2987(3)$ | $0.7364(3)$ | $0.0210(8)$ |
| H7A | 0.1495 | 0.3041 | 0.7632 | $0.025^{*}$ |
| H7B | 0.3689 | 0.2852 | 0.7883 | $0.025^{*}$ |
| C8 | $0.3833(5)$ | $0.4816(3)$ | $0.7561(3)$ | $0.0258(8)$ |
| H8A | 0.2979 | 0.4958 | 0.8014 | $0.039^{*}$ |
| H8B | 0.4049 | 0.5479 | 0.7229 | $0.039^{*}$ |
| H8C | 0.5014 | 0.4549 | 0.7892 | $0.039^{*}$ |
| C9 | $0.1283(5)$ | $0.4418(3)$ | $0.6349(3)$ | $0.0268(9)$ |
| H9A | 0.0422 | 0.4613 | $0.040^{*}$ |  |
| H9B | 0.0719 | 0.3864 | $0.040^{*}$ |  |
| H9C | 0.1554 | 0.5052 | $0.040^{*}$ |  |
|  |  | 0.59918 |  |  |

Atomic displacement parameters $\left(\hat{A}^{2}\right)$

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Te | $0.02085(12)$ | $0.01446(11)$ | $0.01669(11)$ | $-0.00383(10)$ | $0.00360(9)$ | $-0.00064(9)$ |
| Br 1 | $0.0431(3)$ | $0.0156(5)$ | $0.0177(5)$ | $-0.0027(3)$ | $-0.0030(3)$ | $-0.0001(3)$ |
| Br 2 | $0.0143(5)$ | $0.0283(4)$ | $0.0240(5)$ | $0.0002(3)$ | $-0.0033(3)$ | $0.0020(3)$ |
| Br 3 | $0.0366(4)$ | $0.0252(3)$ | $0.0299(6)$ | $-0.0057(3)$ | $0.0193(3)$ | $-0.0062(3)$ |
| C 11 | $0.0431(3)$ | $0.0156(5)$ | $0.0177(5)$ | $-0.0027(3)$ | $-0.0030(3)$ | $-0.0001(3)$ |
| C 2 | $0.0143(5)$ | $0.0283(4)$ | $0.0240(5)$ | $0.0002(3)$ | $-0.0033(3)$ | $0.0020(3)$ |
| C 3 | $0.0366(4)$ | $0.0252(3)$ | $0.0299(6)$ | $-0.0057(3)$ | $0.0193(3)$ | $-0.0062(3)$ |
| N 1 | $0.0209(16)$ | $0.0156(14)$ | $0.0207(16)$ | $-0.0032(12)$ | $0.0037(13)$ | $0.0001(11)$ |
| C 1 | $0.0146(17)$ | $0.0139(16)$ | $0.0159(17)$ | $-0.0063(14)$ | $-0.0032(14)$ | $0.0001(12)$ |
| C 2 | $0.0176(18)$ | $0.0156(18)$ | $0.028(2)$ | $0.0011(14)$ | $-0.0056(15)$ | $-0.0009(14)$ |
| C 3 | $0.027(2)$ | $0.0149(18)$ | $0.034(2)$ | $0.0026(16)$ | $-0.0091(17)$ | $0.0010(15)$ |
| C 4 | $0.0190(19)$ | $0.0184(18)$ | $0.035(2)$ | $-0.0076(16)$ | $-0.0087(17)$ | $0.0080(15)$ |
| C 5 | $0.0184(19)$ | $0.025(2)$ | $0.026(2)$ | $-0.0041(16)$ | $-0.0018(16)$ | $0.0085(15)$ |
| C 6 | $0.0157(18)$ | $0.0150(17)$ | $0.0209(19)$ | $-0.0015(14)$ | $-0.0055(14)$ | $0.0028(13)$ |
| C 7 | $0.0185(19)$ | $0.0224(19)$ | $0.023(2)$ | $0.0002(15)$ | $0.0047(15)$ | $0.0055(14)$ |
| C 8 | $0.025(2)$ | $0.026(2)$ | $0.027(2)$ | $-0.0069(16)$ | $0.0057(17)$ | $-0.0086(15)$ |
| C 9 | $0.021(2)$ | $0.025(2)$ | $0.034(2)$ | $0.0042(16)$ | $0.0018(17)$ | $0.0005(16)$ |
|  |  |  |  |  |  |  |

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

| $\mathrm{Te}-\mathrm{C} 1$ | 2.114 (3) | C2-H2A | 0.9500 |
| :---: | :---: | :---: | :---: |
| $\mathrm{Te}-\mathrm{N} 1$ | 2.421 (3) | C3-C4 | 1.393 (5) |
| $\mathrm{Te}-\mathrm{Cl} 2$ | 2.446 (8) | C3-H3A | 0.9500 |
| $\mathrm{Te}-\mathrm{Cl} 3$ | 2.450 (11) | C4- 55 | 1.381 (5) |
| Te-Cl1 | 2.601 (9) | C4-H4A | 0.9500 |
| $\mathrm{Te}-\mathrm{Br} 3$ | 2.6027 (15) | C5-C6 | 1.400 (4) |
| $\mathrm{Te}-\mathrm{Br} 2$ | 2.6454 (15) | C5-H5A | 0.9500 |
| $\mathrm{Te}-\mathrm{Br} 1$ | 2.6945 (17) | C6-C7 | 1.511 (5) |
| $\mathrm{Te}-\mathrm{Cl1}^{\text {i }}$ | 3.414 (9) | C7-H7A | 0.9900 |
| $\mathrm{Te}-\mathrm{Br} 1^{\text {i }}$ | 3.5441 (17) | C7-H7B | 0.9900 |
| N1-C8 | 1.473 (4) | C8-H8A | 0.9800 |
| N1-C9 | 1.476 (4) | C8-H8B | 0.9800 |
| N1-C7 | 1.488 (4) | C8-H8C | 0.9800 |
| C1-C6 | 1.387 (4) | C9-H9A | 0.9800 |
| C1-C2 | 1.391 (4) | C9-H9B | 0.9800 |
| C2-C3 | 1.382 (5) | C9-H9C | 0.9800 |
| C1-Te-N1 | 76.09 (11) | C8-N1-C7 | 110.7 (3) |
| $\mathrm{C} 1-\mathrm{Te}-\mathrm{Cl} 2$ | 88.0 (2) | C9-N1-C7 | 110.5 (3) |
| $\mathrm{N} 1-\mathrm{Te}-\mathrm{Cl} 2$ | 84.9 (2) | C8-N1-Te | 110.8 (2) |
| $\mathrm{C} 1-\mathrm{Te}-\mathrm{Cl} 3$ | 92.8 (3) | C9-N1-Te | 111.0 (2) |
| $\mathrm{N} 1-\mathrm{Te}-\mathrm{Cl} 3$ | 167.3 (2) | C7-N1-Te | 103.81 (18) |
| $\mathrm{Cl2}-\mathrm{Te}-\mathrm{Cl} 3$ | 88.6 (3) | C6- $\mathrm{C} 1-\mathrm{C} 2$ | 121.7 (3) |
| $\mathrm{C} 1-\mathrm{Te}-\mathrm{Cl1}$ | 88.5 (2) | C6-C1-Te | 115.9 (2) |
| $\mathrm{N} 1-\mathrm{Te}-\mathrm{Cl1}$ | 92.0 (2) | $\mathrm{C} 2-\mathrm{C} 1-\mathrm{Te}$ | 122.3 (2) |
| $\mathrm{C} 2-\mathrm{Te}-\mathrm{Cl1}$ | 175.8 (3) | C3-C2-C1 | 119.2 (3) |
| $\mathrm{Cl} 3-\mathrm{Te}-\mathrm{Cl1}$ | 93.9 (3) | C3-C2-H2A | 120.4 |
| $\mathrm{C} 1-\mathrm{Te}-\mathrm{Br} 3$ | 95.40 (9) | $\mathrm{C} 1-\mathrm{C} 2-\mathrm{H} 2 \mathrm{~A}$ | 120.4 |
| $\mathrm{N} 1-\mathrm{Te}-\mathrm{Br} 3$ | 170.80 (7) | C2-C3-C4 | 119.7 (3) |
| $\mathrm{Cl2}-\mathrm{Te}-\mathrm{Br} 3$ | 91.4 (2) | C2-C3-H3A | 120.2 |
| $\mathrm{Cl1}-\mathrm{Te}-\mathrm{Br} 3$ | 91.2 (2) | $\mathrm{C} 4-\mathrm{C} 3-\mathrm{H} 3 \mathrm{~A}$ | 120.2 |
| $\mathrm{C} 1-\mathrm{Te}-\mathrm{Br} 2$ | 87.99 (10) | C5-C4-C3 | 120.9 (3) |
| $\mathrm{N} 1-\mathrm{Te}-\mathrm{Br} 2$ | 86.50 (8) | C5-C4-H4A | 119.5 |
| $\mathrm{Cl} 3-\mathrm{Te}-\mathrm{Br} 2$ | 86.9 (3) | C3-C4-H4A | 119.5 |
| $\mathrm{Cl1}-\mathrm{Te}-\mathrm{Br} 2$ | 176.5 (2) | C4-C5-C6 | 119.9 (3) |
| $\mathrm{Br} 3-\mathrm{Te}-\mathrm{Br} 2$ | 89.75 (6) | C4-C5-H5A | 120.0 |
| $\mathrm{C} 1-\mathrm{Te}-\mathrm{Br} 1$ | 86.11 (9) | C6-C5-H5A | 120.0 |
| $\mathrm{N} 1-\mathrm{Te}-\mathrm{Br} 1$ | 94.91 (8) | C1-C6-C5 | 118.5 (3) |
| $\mathrm{Cl2}-\mathrm{Te}-\mathrm{Br} 1$ | 173.9 (2) | C1-C6-C7 | 120.2 (3) |
| $\mathrm{Cl} 3-\mathrm{Te}-\mathrm{Br} 1$ | 90.4 (3) | C5-C6-C7 | 121.2 (3) |
| $\mathrm{Br} 3-\mathrm{Te}-\mathrm{Br} 1$ | 87.89 (5) | N1-C7-C6 | 109.1 (3) |
| $\mathrm{Br} 2-\mathrm{Te}-\mathrm{Br} 1$ | 173.41 (5) | N1-C7-H7A | 109.9 |
| $\mathrm{C} 1-\mathrm{Te}-\mathrm{Cl1}^{\text {i }}$ | 171.06 (19) | C6-C7- H 7 A | 109.9 |
| $\mathrm{N} 1-\mathrm{Te}-\mathrm{Cl1}{ }^{\text {i }}$ | 97.34 (17) | N1-C7- H 7 B | 109.9 |
| $\mathrm{Cl2-Te-Cl1}{ }^{\text {i }}$ | 97.6 (3) | C6-C7-H7B | 109.9 |
| $\mathrm{Cl} 3-\mathrm{Te}-\mathrm{Cl1}^{1}$ | 94.3 (3) | H7A-C7-H7B | 108.3 |


| $\mathrm{Cl1}-\mathrm{Te}-\mathrm{Cl1}^{\mathrm{i}}$ | 85.6 (3) |
| :---: | :---: |
| $\mathrm{Br} 3-\mathrm{Te}-\mathrm{Cl1}{ }^{\text {i }}$ | 91.49 (17) |
| $\mathrm{Br} 2-\mathrm{Te}-\mathrm{Cl1}^{\text {i }}$ | 97.76 (16) |
| $\mathrm{Br} 1-\mathrm{Te}-\mathrm{Cl1}^{\text {i }}$ | 88.46 (16) |
| $\mathrm{C} 1-\mathrm{Te}-\mathrm{Br} 1^{1}$ | 169.81 (9) |
| $\mathrm{N} 1-\mathrm{Te}-\mathrm{Br} 1^{1}$ | 94.83 (7) |
| $\mathrm{Cl2}-\mathrm{Te}-\mathrm{Br} 1^{\mathrm{i}}$ | 95.9 (2) |
| $\mathrm{Cl} 3-\mathrm{Te}-\mathrm{Br} 1^{\text {i }}$ | 96.7 (2) |
| $\mathrm{Cl} 1-\mathrm{Te}-\mathrm{Br} 1^{\text {i }}$ | 87.2 (2) |
| $\mathrm{Br} 3-\mathrm{Te}-\mathrm{Br} 1^{\mathrm{i}}$ | 93.93 (5) |
| $\mathrm{Br} 2-\mathrm{Te}-\mathrm{Br} 1^{\mathrm{i}}$ | 96.16 (5) |
| $\mathrm{Br} 1-\mathrm{Te}-\mathrm{Br} 1^{\text {i }}$ | 90.15 (4) |
| C8-N1-C9 | 109.9 (3) |
| $\mathrm{C} 1-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 8$ | 149.1 (2) |
| $\mathrm{Cl} 2-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 8$ | 59.9 (3) |
| $\mathrm{Cl3}-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 8$ | 119.3 (12) |
| $\mathrm{Cl1}-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 8$ | -123.0 (3) |
| $\mathrm{Br} 2-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 8$ | 60.3 (2) |
| $\mathrm{Br} 1-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 8$ | -126.2 (2) |
| Cl1 ${ }^{\text {i }}$ - $\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 8$ | -37.1 (3) |
| $\mathrm{Br} 1^{\mathrm{i}}-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 8$ | -35.6 (2) |
| $\mathrm{C} 1-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 9$ | -88.6 (2) |
| $\mathrm{Cl2}-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 9$ | -177.7 (3) |
| $\mathrm{Cl} 3-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 9$ | -118.4 (12) |
| $\mathrm{Cl1}-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 9$ | -0.6 (3) |
| $\mathrm{Br} 2-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 9$ | -177.4 (2) |
| $\mathrm{Br} 1-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 9$ | -3.8(2) |
| $\mathrm{Cl1}{ }^{\text {i }}-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 9$ | 85.2 (3) |
| $\mathrm{Br} 1^{\mathrm{i}}-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 9$ | 86.7 (2) |
| $\mathrm{C} 1-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 7$ | 30.2 (2) |
| $\mathrm{Cl} 2-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 7$ | -59.0 (3) |
| $\mathrm{Cl} 3-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 7$ | 0.4 (13) |
| $\mathrm{Cl} 1-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 7$ | 118.2 (3) |
| $\mathrm{Br} 2-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 7$ | -58.60 (19) |
| $\mathrm{Br} 1-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 7$ | 114.94 (19) |
| Cl1 ${ }^{\text {i }}$ - $\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 7$ | -156.0 (2) |
| $\mathrm{Br} 1^{\mathrm{i}}-\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 7$ | -154.50 (19) |
| $\mathrm{N} 1-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 6$ | -14.5 (2) |
| C12-Te-C1-C6 | 70.7 (3) |
| $\mathrm{Cl} 3-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 6$ | 159.2 (4) |
| $\mathrm{C} 11-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 6$ | -107.0 (3) |


| N1-C8-H8A | 109.5 |
| :--- | :--- |
| N1-C8-H8B | 109.5 |
| H8A-C8-H8B | 109.5 |
| N1-C8-H8C | 109.5 |
| H8A-C8-H8C | 109.5 |
| H8B-C8-H8C | 109.5 |
| N1-C9—H9A | 109.5 |
| N1-C9—H9B | 109.5 |
| H9A-C9-H9B | 109.5 |
| N1-C9—H9C | 109.5 |
| H9A-C9-H9C | 109.5 |
| H9B-C9-H9C | 109.5 |


| $\mathrm{Br} 3-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 6$ | $161.9(2)$ |
| :--- | :--- |
| $\mathrm{Br} 2-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 6$ | $72.3(2)$ |
| $\mathrm{Br} 1-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 6$ | $-110.6(2)$ |
| $\mathrm{Br} 1-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 6$ | $-41.9(7)$ |
| $\mathrm{N} 1-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 2$ | $162.6(3)$ |
| $\mathrm{C} 12-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 2$ | $-112.2(4)$ |
| $\mathrm{C} 13-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 2$ | $-23.7(4)$ |
| $\mathrm{C} 11-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 2$ | $-21.0(3)$ |
| $\mathrm{Br} 3-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 2$ | $-110.5(3)$ |
| $\mathrm{Br} 2-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 2$ | $66.5(3)$ |
| $\mathrm{Br} 1-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 2$ | $135.2(4)$ |
| $\mathrm{Br} 1-\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 2$ | $-1.9(5)$ |
| $\mathrm{C} 6-\mathrm{C} 1-\mathrm{C} 2-\mathrm{C} 3$ | $-178.8(2)$ |
| $\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 2-\mathrm{C} 3$ | $1.2(5)$ |
| $\mathrm{C} 1-\mathrm{C} 2-\mathrm{C} 3-\mathrm{C} 4$ | $0.0(5)$ |
| $\mathrm{C} 2-\mathrm{C} 3-\mathrm{C} 4-\mathrm{C} 5$ | $-0.6(5)$ |
| $\mathrm{C} 3-\mathrm{C} 4-\mathrm{C} 5-\mathrm{C} 6$ | $1.3(5)$ |
| $\mathrm{C} 2-\mathrm{C} 1-\mathrm{C} 6-\mathrm{C} 5$ | $178.4(2)$ |
| $\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 6-\mathrm{C} 5$ | $178.4(3)$ |
| $\mathrm{C} 2-\mathrm{C} 1-\mathrm{C} 6-\mathrm{C} 7$ | $-4.5(4)$ |
| $\mathrm{Te}-\mathrm{C} 1-\mathrm{C} 6-\mathrm{C} 7$ | $0.0(5)$ |
| $\mathrm{C} 4-\mathrm{C} 5-\mathrm{C} 6-\mathrm{C} 1$ | $-177.1(3)$ |
| $\mathrm{C} 4-\mathrm{C} 5-\mathrm{C} 6-\mathrm{C} 7$ | $-158.5(3)$ |
| $\mathrm{C} 8-\mathrm{N} 1-\mathrm{C} 7-\mathrm{C} 6$ | $79.5(3)$ |
| $\mathrm{C} 9-\mathrm{N} 1-\mathrm{C} 7-\mathrm{C} 6$ | $-39.6(3)$ |
| $\mathrm{Te}-\mathrm{N} 1-\mathrm{C} 7-\mathrm{C} 6$ | $33.4(4)$ |
| $\mathrm{C} 1-\mathrm{C} 6-\mathrm{C} 7-\mathrm{N} 1$ | $-149.6(3)$ |
| $\mathrm{C} 5-\mathrm{C} 6-\mathrm{C} 7-\mathrm{N} 1$ |  |

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

Hydrogen-bond geometry $\left(\AA,{ }^{\circ}\right)$

| $D — \mathrm{H} \cdots A$ | $D — \mathrm{H}$ | $\mathrm{H} \cdots A$ | $D \cdots A$ | $D-\mathrm{H} \cdots A$ |
| :--- | :--- | :--- | :--- | :--- |

## supporting information

| $\mathrm{C} 7 — \mathrm{H} 7 A \cdots \mathrm{Br}^{2 i}$ | 0.99 | 2.96 | $3.839(4)$ | 149 |
| :--- | :--- | :--- | :--- | :--- |

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


[^0]:    Supplementary data and figures for this paper are available from the

