

Dibromidochlorido[2-[(dimethylamino)-methyl]phenyl- κ^2N,C^1]tellurium(IV)

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

The title compound, $C_9H_{13}Br_2ClTe$, was synthesized by reacting [2-(dimethylaminomethyl)phenyl]tellurium(II) chloride with 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 stoichiometry 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 Br/Cl atoms of a nearby molecule. The Te—Br and Te—Cl distances in both disorder components fall into two groups; a longer distance for the Br/Cl involved in this secondary interaction [2.6945 (17) Å for Br and 2.601 (9) Å for Cl] and shorter bond distances to the remaining halogen atoms, indicating that this interaction has slightly weakened the 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 C—H...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); Cobbleddick *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

| | |
|-----------------------|-----------------------------------|
| $C_9H_{12}Br_2ClTe$ | $V = 1296.61$ (9) Å ³ |
| $M_r = 457.07$ | $Z = 4$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 7.2854$ (3) Å | $\mu = 8.63$ mm ⁻¹ |
| $b = 12.4785$ (5) Å | $T = 123$ K |
| $c = 14.4098$ (6) Å | $0.63 \times 0.50 \times 0.10$ mm |
| $\beta = 98.200$ (4)° | |

Data collection

| | |
|---|--|
| Oxford Diffraction Xcalibur Ruby Gemini diffractometer | Reid (1995)] |
| Absorption correction: analytical [<i>CrysAlis PRO</i> (Oxford Diffraction, 2007), based on expressions derived by Clark & | $T_{min} = 0.042$, $T_{max} = 0.409$ |
| | 8229 measured reflections |
| | 4241 independent reflections |
| | 2981 reflections with $I > 2\sigma(I)$ |
| | $R_{int} = 0.044$ |

Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | 1 restraint |
| $wR(F^2) = 0.056$ | H-atom parameters constrained |
| $S = 0.96$ | $\Delta\rho_{max} = 0.91$ e Å ⁻³ |
| 4241 reflections | $\Delta\rho_{min} = -0.92$ e Å ⁻³ |
| 141 parameters | |

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------|-------|-------------|-------------|---------------|
| $C7-H7A\cdots Br2^i$ | 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2114).

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Dibromidochlorido{2-[(dimethylamino)methyl]phenyl- κ^2N,C^1 }tellurium(IV)

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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 2Br's and Cl are distributed over the three possible sites. The scrambling of the Br/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 Br/Cl of an adjoining molecule. The Te—Br and Te—Cl distances in both molecules fall into two groups; a longer distance for the Br/Cl involved in this secondary interaction (2.6945 (17)Å for Br and 2.601 (9)Å for Cl) and shorter bond distances to the remaining halogens, indicating that this interaction has slightly weakened the Te—X bond, as is the case in the previously reported polymorph. Otherwise, the metrical parameters in both polymorphs are not significantly different.

Experimental

As shown in the reaction scheme (scheme 2), a stirred solution of bis[2-(dimethylaminomethyl)phenyl]ditelluride, **1**, (Kaur *et al.*, 1995) (0.5 g, 0.94 mmol) in diethylether (10 ml) was treated with HCl (3 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 g, 0.66 mmol) in dry CHCl₃ (10 ml) was treated with Br₂ (0.37 ml, 2.34 mmol) under N₂ at 0° 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.

Refinement

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.95 - 0.97 Å [$U_{iso}(H) = 1.2U_{eq}(OH, CH, CH_2)$ [$U_{iso}(H) = 1.5U_{eq}(CH_3)$]]. As is discussed above, the 2 Br's and Cl are distributed over the three possible positions. Initially the Br/Cl occupancy in each position was refined as a free variable.

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These Br and Cl occupancies summed to Br_{2.03} and Cl_{0.98}. The three free variables were then constrained to match a stoichiometry of Br₂ and Cl.

Figures

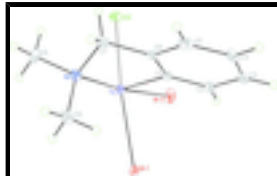


Fig. 1. Diagram of the major component of C₉H₁₂Br₂ClTe, showing atom labeling. Atomic displacement parameters are at the 30% level.

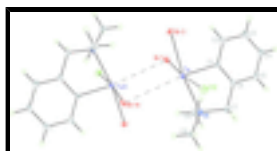


Fig. 2. Diagram showing the formation of a dimer through weak Te...Br interactions. These interactions are shown as dashed lines

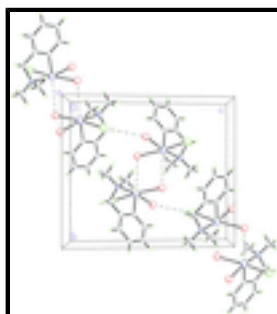


Fig. 3. The molecular packing for C₉H₁₂Br₂ClTe viewed along the *a* axis. Te—Br secondary interactions are shown by dashed lines.



Fig. 4. The formation of the title compound.

Dibromidochlorido{2-[(dimethylamino)methyl]phenyl-κ²N,C¹}tellurium(IV)

Crystal data

| | |
|---|---|
| C ₉ H ₁₂ Br ₂ ClTe | $F(000) = 848$ |
| $M_r = 457.07$ | $D_x = 2.341 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| Hall symbol: -P 2ybc | Cell parameters from 3585 reflections |
| $a = 7.2854 (3) \text{ \AA}$ | $\theta = 5.1\text{--}32.5^\circ$ |
| $b = 12.4785 (5) \text{ \AA}$ | $\mu = 8.63 \text{ mm}^{-1}$ |
| $c = 14.4098 (6) \text{ \AA}$ | $T = 123 \text{ K}$ |
| $\beta = 98.200 (4)^\circ$ | Plate, yellow |
| $V = 1296.61 (9) \text{ \AA}^3$ | $0.63 \times 0.50 \times 0.10 \text{ mm}$ |
| $Z = 4$ | |

Data collection

| | |
|--|--|
| Oxford Diffraction Xcalibur Ruby Gemini diffractometer | 4241 independent reflections |
| Radiation source: Enhance (Mo) X-ray Source | 2981 reflections with $I > 2\sigma(I)$ |

graphite $R_{\text{int}} = 0.044$
 Detector resolution: 10.5081 pixels mm^{-1} $\theta_{\text{max}} = 32.6^\circ$, $\theta_{\text{min}} = 5.4^\circ$
 ω scans $h = -9 \rightarrow 11$
 Absorption correction: analytical
 [CrysAlis PRO (Oxford Diffraction, 2007), based on $k = -18 \rightarrow 13$
 expressions derived by Clark & Reid (1995)]
 $T_{\text{min}} = 0.042$, $T_{\text{max}} = 0.409$ $l = -16 \rightarrow 20$
 8229 measured reflections

Refinement

Refinement on F^2 Primary atom site location: structure-invariant direct methods
 Least-squares matrix: full Secondary atom site location: difference Fourier map
 $R[F^2 > 2\sigma(F^2)] = 0.038$ Hydrogen site location: inferred from neighbouring sites
 $wR(F^2) = 0.056$ H-atom parameters constrained
 $S = 0.96$ $w = 1/[\sigma^2(F_o^2) + (0.0084P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 4241 reflections $(\Delta/\sigma)_{\text{max}} = 0.001$
 141 parameters $\Delta\rho_{\text{max}} = 0.91 \text{ e } \text{\AA}^{-3}$
 1 restraint $\Delta\rho_{\text{min}} = -0.92 \text{ e } \text{\AA}^{-3}$

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR 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 $F^2 > \sigma(F^2)$ is used only for calculating R -factors(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)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|-----|-------------|---------------|---------------|----------------------------------|-------------|
| Te | 0.51999 (3) | 0.349798 (17) | 0.583822 (16) | 0.01724 (6) | |
| Br1 | 0.2864 (3) | 0.39052 (12) | 0.42535 (11) | 0.0262 (2) | 0.6585 (4) |
| Br2 | 0.7403 (2) | 0.28626 (15) | 0.73580 (13) | 0.0228 (2) | 0.6374 (13) |
| Br3 | 0.7448 (2) | 0.26391 (13) | 0.47988 (10) | 0.0291 (2) | 0.7041 (13) |
| Cl1 | 0.2892 (15) | 0.4029 (7) | 0.4363 (6) | 0.0262 (2) | 0.3415 (4) |
| Cl2 | 0.7179 (11) | 0.2938 (7) | 0.7271 (6) | 0.0228 (2) | 0.3626 (13) |
| Cl3 | 0.7337 (15) | 0.2589 (9) | 0.4931 (7) | 0.0291 (2) | 0.2959 (13) |
| N1 | 0.3019 (4) | 0.4005 (2) | 0.6881 (2) | 0.0190 (6) | |

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|-----|------------|------------|------------|------------|
| 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 | 0.6785 | 0.040* |
| H9B | 0.0719 | 0.3864 | 0.5918 | 0.040* |
| H9C | 0.1554 | 0.5052 | 0.5991 | 0.040* |

Atomic displacement parameters (\AA^2)

| | 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) |
| Br1 | 0.0431 (3) | 0.0156 (5) | 0.0177 (5) | -0.0027 (3) | -0.0030 (3) | -0.0001 (3) |
| Br2 | 0.0143 (5) | 0.0283 (4) | 0.0240 (5) | 0.0002 (3) | -0.0033 (3) | 0.0020 (3) |
| Br3 | 0.0366 (4) | 0.0252 (3) | 0.0299 (6) | -0.0057 (3) | 0.0193 (3) | -0.0062 (3) |
| Cl1 | 0.0431 (3) | 0.0156 (5) | 0.0177 (5) | -0.0027 (3) | -0.0030 (3) | -0.0001 (3) |
| Cl2 | 0.0143 (5) | 0.0283 (4) | 0.0240 (5) | 0.0002 (3) | -0.0033 (3) | 0.0020 (3) |
| Cl3 | 0.0366 (4) | 0.0252 (3) | 0.0299 (6) | -0.0057 (3) | 0.0193 (3) | -0.0062 (3) |
| N1 | 0.0209 (16) | 0.0156 (14) | 0.0207 (16) | -0.0032 (12) | 0.0037 (13) | 0.0001 (11) |
| C1 | 0.0146 (17) | 0.0139 (16) | 0.0159 (17) | -0.0063 (14) | -0.0032 (14) | 0.0001 (12) |
| C2 | 0.0176 (18) | 0.0156 (18) | 0.028 (2) | 0.0011 (14) | -0.0056 (15) | -0.0009 (14) |
| C3 | 0.027 (2) | 0.0149 (18) | 0.034 (2) | 0.0026 (16) | -0.0091 (17) | 0.0010 (15) |
| C4 | 0.0190 (19) | 0.0184 (18) | 0.035 (2) | -0.0076 (16) | -0.0087 (17) | 0.0080 (15) |
| C5 | 0.0184 (19) | 0.025 (2) | 0.026 (2) | -0.0041 (16) | -0.0018 (16) | 0.0085 (15) |
| C6 | 0.0157 (18) | 0.0150 (17) | 0.0209 (19) | -0.0015 (14) | -0.0055 (14) | 0.0028 (13) |
| C7 | 0.0185 (19) | 0.0224 (19) | 0.023 (2) | 0.0002 (15) | 0.0047 (15) | 0.0055 (14) |
| C8 | 0.025 (2) | 0.026 (2) | 0.027 (2) | -0.0069 (16) | 0.0057 (17) | -0.0086 (15) |
| C9 | 0.021 (2) | 0.025 (2) | 0.034 (2) | 0.0042 (16) | 0.0018 (17) | 0.0005 (16) |

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

| | | | |
|--------|------------|--------|-----------|
| Te—C1 | 2.114 (3) | C2—H2A | 0.9500 |
| Te—N1 | 2.421 (3) | C3—C4 | 1.393 (5) |
| Te—Cl2 | 2.446 (8) | C3—H3A | 0.9500 |
| Te—Cl3 | 2.450 (11) | C4—C5 | 1.381 (5) |

| | | | |
|-------------------------|-------------|------------|-------------|
| Te—Cl1 | 2.601 (9) | C4—H4A | 0.9500 |
| Te—Br3 | 2.6027 (15) | C5—C6 | 1.400 (4) |
| Te—Br2 | 2.6454 (15) | C5—H5A | 0.9500 |
| Te—Br1 | 2.6945 (17) | C6—C7 | 1.511 (5) |
| Te—Cl1 ⁱ | 3.414 (9) | C7—H7A | 0.9900 |
| Te—Br1 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) |
| C1—Te—Cl2 | 88.0 (2) | C9—N1—C7 | 110.5 (3) |
| N1—Te—Cl2 | 84.9 (2) | C8—N1—Te | 110.8 (2) |
| C1—Te—Cl3 | 92.8 (3) | C9—N1—Te | 111.0 (2) |
| N1—Te—Cl3 | 167.3 (2) | C7—N1—Te | 103.81 (18) |
| Cl2—Te—Cl3 | 88.6 (3) | C6—C1—C2 | 121.7 (3) |
| C1—Te—Cl1 | 88.5 (2) | C6—C1—Te | 115.9 (2) |
| N1—Te—Cl1 | 92.0 (2) | C2—C1—Te | 122.3 (2) |
| Cl2—Te—Cl1 | 175.8 (3) | C3—C2—C1 | 119.2 (3) |
| Cl3—Te—Cl1 | 93.9 (3) | C3—C2—H2A | 120.4 |
| C1—Te—Br3 | 95.40 (9) | C1—C2—H2A | 120.4 |
| N1—Te—Br3 | 170.80 (7) | C2—C3—C4 | 119.7 (3) |
| Cl2—Te—Br3 | 91.4 (2) | C2—C3—H3A | 120.2 |
| Cl1—Te—Br3 | 91.2 (2) | C4—C3—H3A | 120.2 |
| C1—Te—Br2 | 87.99 (10) | C5—C4—C3 | 120.9 (3) |
| N1—Te—Br2 | 86.50 (8) | C5—C4—H4A | 119.5 |
| Cl3—Te—Br2 | 86.9 (3) | C3—C4—H4A | 119.5 |
| Cl1—Te—Br2 | 176.5 (2) | C4—C5—C6 | 119.9 (3) |
| Br3—Te—Br2 | 89.75 (6) | C4—C5—H5A | 120.0 |
| C1—Te—Br1 | 86.11 (9) | C6—C5—H5A | 120.0 |
| N1—Te—Br1 | 94.91 (8) | C1—C6—C5 | 118.5 (3) |
| Cl2—Te—Br1 | 173.9 (2) | C1—C6—C7 | 120.2 (3) |
| Cl3—Te—Br1 | 90.4 (3) | C5—C6—C7 | 121.2 (3) |
| Br3—Te—Br1 | 87.89 (5) | N1—C7—C6 | 109.1 (3) |
| Br2—Te—Br1 | 173.41 (5) | N1—C7—H7A | 109.9 |
| C1—Te—Cl1 ⁱ | 171.06 (19) | C6—C7—H7A | 109.9 |
| N1—Te—Cl1 ⁱ | 97.34 (17) | N1—C7—H7B | 109.9 |
| Cl2—Te—Cl1 ⁱ | 97.6 (3) | C6—C7—H7B | 109.9 |
| Cl3—Te—Cl1 ⁱ | 94.3 (3) | H7A—C7—H7B | 108.3 |
| Cl1—Te—Cl1 ⁱ | 85.6 (3) | N1—C8—H8A | 109.5 |
| Br3—Te—Cl1 ⁱ | 91.49 (17) | N1—C8—H8B | 109.5 |
| Br2—Te—Cl1 ⁱ | 97.76 (16) | H8A—C8—H8B | 109.5 |
| Br1—Te—Cl1 ⁱ | 88.46 (16) | N1—C8—H8C | 109.5 |
| C1—Te—Br1 ⁱ | 169.81 (9) | H8A—C8—H8C | 109.5 |

supplementary materials

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|----------------------------|--------------|----------------------------|------------|
| N1—Te—Br1 ⁱ | 94.83 (7) | H8B—C8—H8C | 109.5 |
| Cl2—Te—Br1 ⁱ | 95.9 (2) | N1—C9—H9A | 109.5 |
| Cl3—Te—Br1 ⁱ | 96.7 (2) | N1—C9—H9B | 109.5 |
| Cl1—Te—Br1 ⁱ | 87.2 (2) | H9A—C9—H9B | 109.5 |
| Br3—Te—Br1 ⁱ | 93.93 (5) | N1—C9—H9C | 109.5 |
| Br2—Te—Br1 ⁱ | 96.16 (5) | H9A—C9—H9C | 109.5 |
| Br1—Te—Br1 ⁱ | 90.15 (4) | H9B—C9—H9C | 109.5 |
| C8—N1—C9 | 109.9 (3) | | |
| C1—Te—N1—C8 | 149.1 (2) | Br3—Te—C1—C6 | 161.9 (2) |
| Cl2—Te—N1—C8 | 59.9 (3) | Br2—Te—C1—C6 | 72.3 (2) |
| Cl3—Te—N1—C8 | 119.3 (12) | Br1—Te—C1—C6 | -110.6 (2) |
| Cl1—Te—N1—C8 | -123.0 (3) | Br1 ⁱ —Te—C1—C6 | -41.9 (7) |
| Br2—Te—N1—C8 | 60.3 (2) | N1—Te—C1—C2 | 162.6 (3) |
| Br1—Te—N1—C8 | -126.2 (2) | Cl2—Te—C1—C2 | -112.2 (4) |
| Cl1 ⁱ —Te—N1—C8 | -37.1 (3) | Cl3—Te—C1—C2 | -23.7 (4) |
| Br1 ⁱ —Te—N1—C8 | -35.6 (2) | Cl1—Te—C1—C2 | 70.1 (3) |
| C1—Te—N1—C9 | -88.6 (2) | Br3—Te—C1—C2 | -21.0 (3) |
| Cl2—Te—N1—C9 | -177.7 (3) | Br2—Te—C1—C2 | -110.5 (3) |
| Cl3—Te—N1—C9 | -118.4 (12) | Br1—Te—C1—C2 | 66.5 (3) |
| Cl1—Te—N1—C9 | -0.6 (3) | Br1 ⁱ —Te—C1—C2 | 135.2 (4) |
| Br2—Te—N1—C9 | -177.4 (2) | C6—C1—C2—C3 | -1.9 (5) |
| Br1—Te—N1—C9 | -3.8 (2) | Te—C1—C2—C3 | -178.8 (2) |
| Cl1 ⁱ —Te—N1—C9 | 85.2 (3) | C1—C2—C3—C4 | 1.2 (5) |
| Br1 ⁱ —Te—N1—C9 | 86.7 (2) | C2—C3—C4—C5 | 0.0 (5) |
| C1—Te—N1—C7 | 30.2 (2) | C3—C4—C5—C6 | -0.6 (5) |
| Cl2—Te—N1—C7 | -59.0 (3) | C2—C1—C6—C5 | 1.3 (5) |
| Cl3—Te—N1—C7 | 0.4 (13) | Te—C1—C6—C5 | 178.4 (2) |
| Cl1—Te—N1—C7 | 118.2 (3) | C2—C1—C6—C7 | 178.4 (3) |
| Br2—Te—N1—C7 | -58.60 (19) | Te—C1—C6—C7 | -4.5 (4) |
| Br1—Te—N1—C7 | 114.94 (19) | C4—C5—C6—C1 | 0.0 (5) |
| Cl1 ⁱ —Te—N1—C7 | -156.0 (2) | C4—C5—C6—C7 | -177.1 (3) |
| Br1 ⁱ —Te—N1—C7 | -154.50 (19) | C8—N1—C7—C6 | -158.5 (3) |
| N1—Te—C1—C6 | -14.5 (2) | C9—N1—C7—C6 | 79.5 (3) |
| Cl2—Te—C1—C6 | 70.7 (3) | Te—N1—C7—C6 | -39.6 (3) |
| Cl3—Te—C1—C6 | 159.2 (4) | C1—C6—C7—N1 | 33.4 (4) |
| Cl1—Te—C1—C6 | -107.0 (3) | C5—C6—C7—N1 | -149.6 (3) |

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

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------------|-------|-------------|-------------|---------------|
| C7—H7A \cdots Br2 ⁱⁱ | 0.99 | 2.96 | 3.839 (4) | 149. |

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

Fig. 1

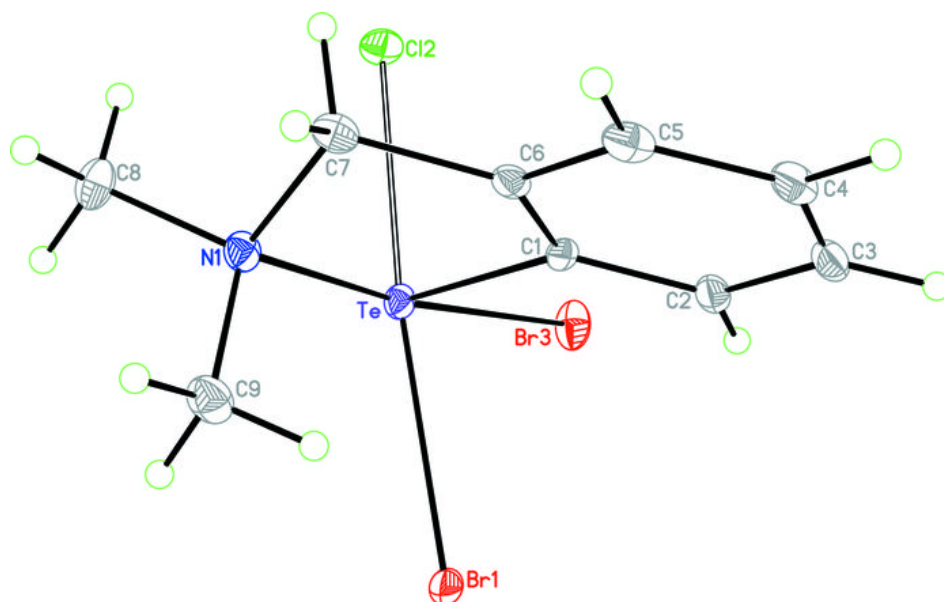


Fig. 2

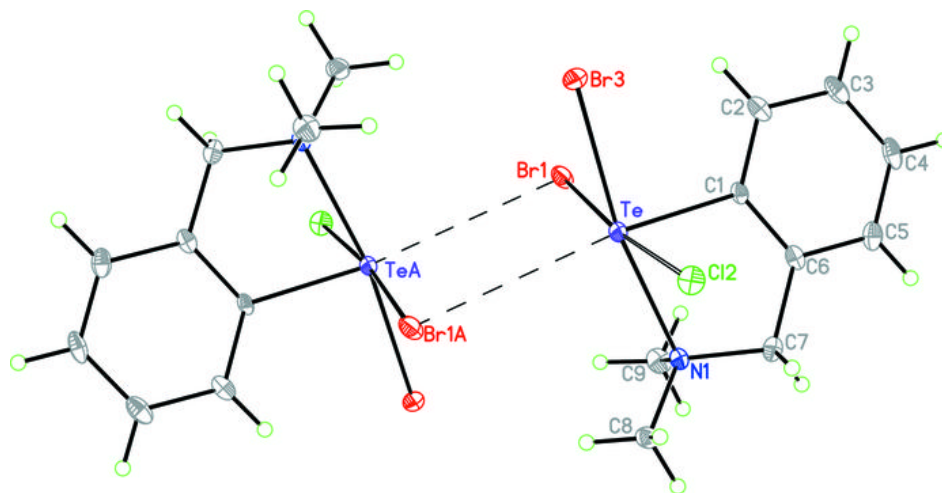


Fig. 3

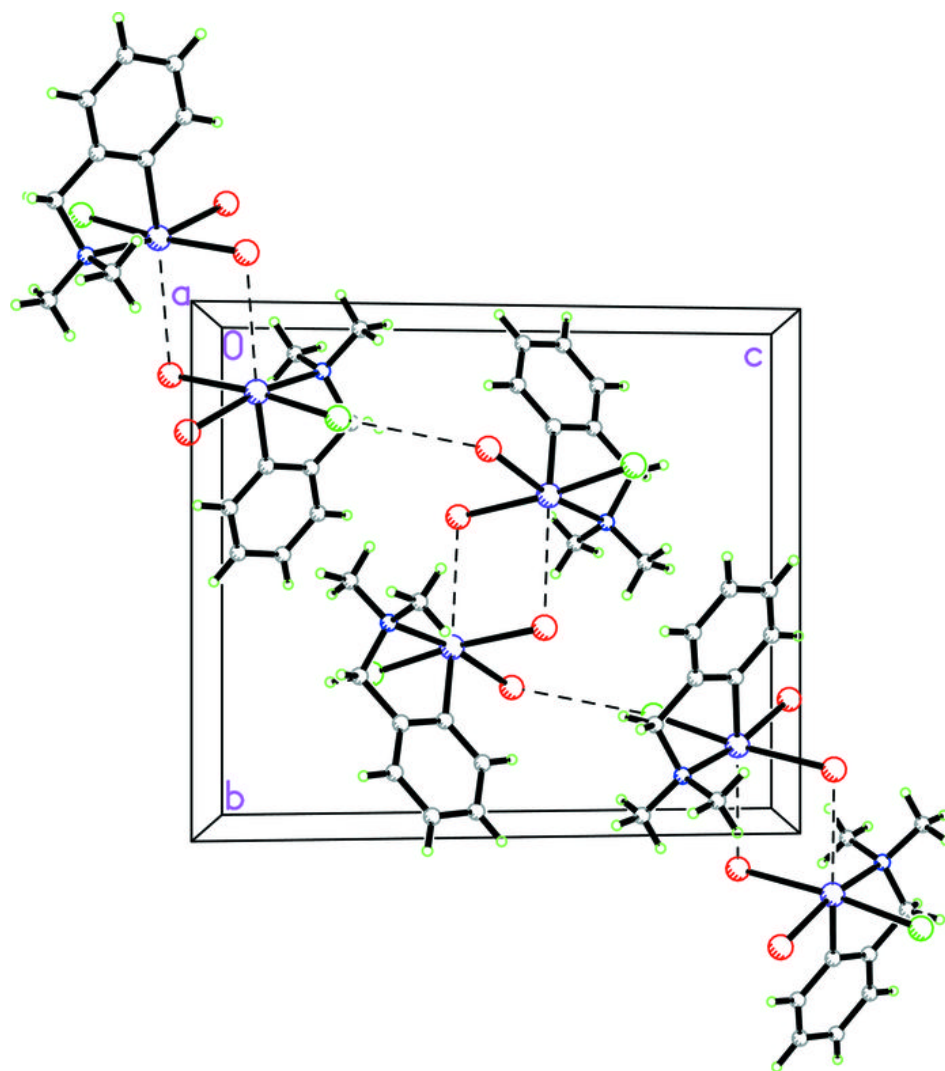


Fig. 4

