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1-[(*Z*)-2-Butyltellanyl-1-chloroethenyl]-cyclohex-1-ene

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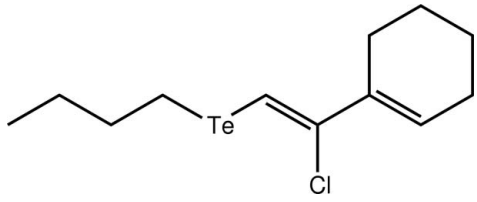
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.023; wR factor = 0.069; data-to-parameter ratio = 18.9.

The Te^{II} atom in the title molecule, $C_{12}H_{19}ClTe$, is coordinated in a V-shaped geometry by C atoms derived from the disparate organic substituents. A short intramolecular C—H···Cl contact occurs owing to the proximity of the ethene bond in the six-membered ring to the Cl atom. In the crystal, molecules assemble into layers parallel to the *ac* plane, with the closest interactions between them being of the Te···Te type [3.9993 (16) Å].

Related literature

For background to the synthesis, see: Guadagnin *et al.* (2008). For related crystal structures, see: Zeni *et al.* (1999); Barrientos-Astigarraga *et al.* (2002). For ring conformational analysis, see: Cremer & Pople (1975). The van der Waals radius for Te was taken from Bondi (1964).



Experimental

Crystal data

$C_{12}H_{19}ClTe$
M_r = 326.32
Triclinic, $P\overline{1}$
a = 7.666 (3) Å
b = 7.687 (3) Å
c = 12.266 (4) Å
α = 95.499 (15)°
β = 105.060 (14)°
γ = 111.832 (13)°
V = 632.8 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.53 mm^{-1}
T = 100 K
0.3 × 0.3 × 0.2 mm

Data collection

Rigaku Saturn724 (2 × 2 bin mode) diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.575, T_{max} = 1.000
3588 measured reflections
2421 independent reflections
2406 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.069
S = 1.17
2421 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.95 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Te—C1	2.077 (3)	Te—C9	2.148 (3)
C1—Te—C9	94.09 (12)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···Cl	0.95	2.56	3.024 (3)	110

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *MarvinSketch* (ChemAxon, 2010) and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2453).

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supplementary materials

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1-[(*Z*)-2-Butyltellanyl-1-chloroethenyl]cyclohex-1-ene

Julio Zukerman-Schpector, Ignez Caracelli, Rafael Carlos Guadagnin, Hélio A. Stefani and Edward R. T. Tiekink

Comment

The title compound, (I), was synthesized by reduction with sodium borohydride of the corresponding 2-halovinyl tellurium dichloride (Guadagnin *et al.*, 2008).

The Te^{II} atom in (I), Fig. 1, is coordinated by C atoms derived from the organic substituents which define a V-shape, Table 1. The conformation about the C1═C2 bond [1.334 (4) Å] is *Z*. The ethene bond in the six-membered ring is orientated toward the Cl atom enabling the formation of an intramolecular C—H···Cl interaction, Table 2. The conformation of the six-membered ring is a half-chair with the C5 atom lying 0.641 (5) Å above the plane of the remaining five atoms (r.m.s. deviation = 0.0738 Å), with puckering parameters: q_2 = 0.381 (4) Å and q_3 = 0.311 (4) Å, and amplitudes: Q = 0.492 (4) Å, θ = 50.8 (5) ° and φ_2 = 144.3 (6) ° (Cremer & Pople, 1975).

In the crystal packing, molecules assemble into layers parallel to the *ac* plane, Fig. 2. Within layers, Te···Te^{i} contacts of 3.9993 (16) Å, *i.e.* less than the sum of the van der Waals radius for Te of 4.4 Å (Bondi, 1964), are noted; *i*: -*x*, -*y*, 2 - *z*.

Experimental

The title compound was prepared as described in a previous study (Guadagnin *et al.*, 2008). Crystals of (I) were obtained by slow evaporation from its $CHCl_3$ solution held at room temperature.

Refinement

C-bound H-atoms were placed in calculated positions (C—H = 0.95–0.99 Å) and were included in the refinement in the riding model approximation with U_{iso}(H) = 1.2–1.5U_{eq}(C). Owing to poor agreement, three reflections, *i.e.* (2 $\bar{8}$ 3), ($\bar{1}$ 4 4) and ($\bar{1}$ 5 6), were omitted from the final refinement.

Computing details

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2005); cell refinement: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2005); data reduction: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2005); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: MarvinSketch (ChemAxon, 2010) and *publCIF* (Westrip, 2010).

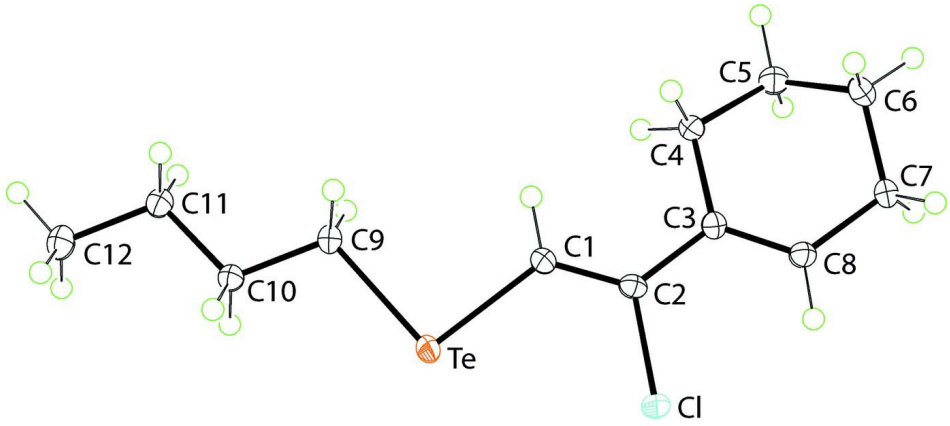

Figure 1

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

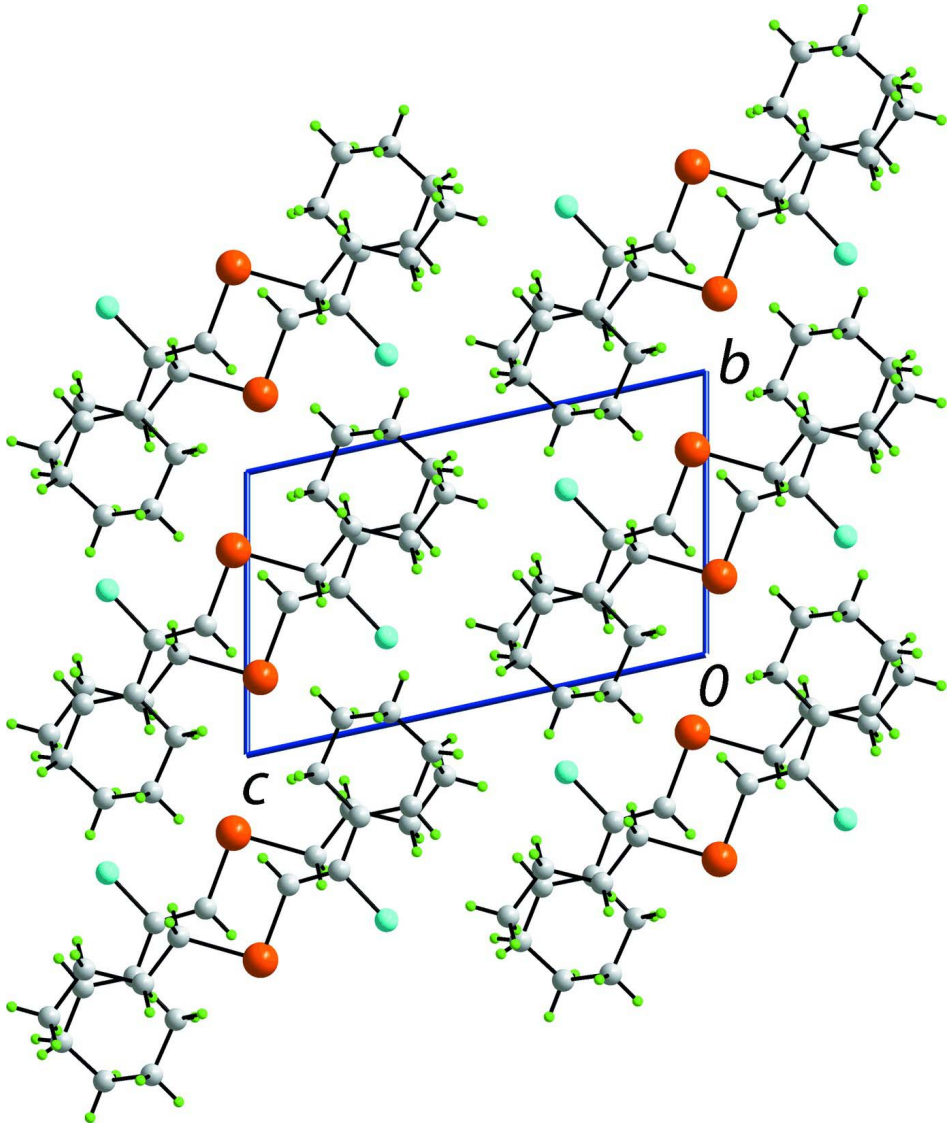

Figure 2

A view in projection down the *a* axis of the unit-cell contents for (I).

1-[(*Z*)-2-Butyltellanyl-1-chloroethenyl]cyclohex-1-ene

Crystal data

$C_{12}H_{19}ClTe$
$M_r = 326.32$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.666\ (3)$ Å
$b = 7.687\ (3)$ Å
$c = 12.266\ (4)$ Å
$\alpha = 95.499\ (15)°$
$\beta = 105.060\ (14)°$
$\gamma = 111.832\ (13)°$
$V = 632.8\ (4)$ Å^3
$Z = 2$
$F(000) = 320$
$D_x = 1.713$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8499 reflections
$\theta = 1.7–29.8°$
$\mu = 2.53$ mm^{-1}
$T = 100$ K
Irregular, yellow
0.3 × 0.3 × 0.2 mm

Data collection

Rigaku Saturn724 (2x2 bin mode) diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 28.5714 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.575, T_{max} = 1.000
3588 measured reflections
2421 independent reflections
2406 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 26.0°, θ_{min} = 2.9°
h = −8→9
k = −9→7
l = −15→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.069
S = 1.17
2421 reflections
128 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
$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 1.4833P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.95 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.

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 $F^2 > 2\sigma(F^2)$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Te	0.10592 (3)	0.26493 (3)	0.970657 (16)	0.01857 (9)
Cl	0.04726 (12)	0.30822 (11)	0.69597 (6)	0.02053 (17)
C10	0.1785 (5)	0.2722 (4)	1.2266 (3)	0.0163 (6)
H10A	0.2188	0.1662	1.2121	0.020*
H10B	0.0323	0.2162	1.2066	0.020*
C2	0.2010 (4)	0.5213 (4)	0.7990 (3)	0.0143 (6)
C4	0.3968 (5)	0.8795 (4)	0.8452 (3)	0.0171 (6)
H4A	0.5292	0.8862	0.8866	0.020*
H4B	0.3262	0.8801	0.9022	0.020*
C3	0.2828 (4)	0.6957 (4)	0.7553 (3)	0.0140 (6)
C6	0.4941 (5)	1.0420 (5)	0.6892 (3)	0.0213 (7)
H6A	0.5152	1.1599	0.6582	0.026*
H6B	0.6223	1.0306	0.7137	0.026*
C11	0.2714 (5)	0.3691 (5)	1.3547 (3)	0.0190 (6)
H11A	0.4177	0.4269	1.3747	0.023*
H11B	0.2292	0.4736	1.3698	0.023*

C9	0.2398 (5)	0.4113 (5)	1.1492 (3)	0.0184 (6)
H9A	0.3860	0.4681	1.1688	0.022*
H9B	0.1980	0.5167	1.1623	0.022*
C5	0.4221 (5)	1.0565 (5)	0.7922 (3)	0.0218 (7)
H5A	0.2936	1.0674	0.7675	0.026*
H5B	0.5188	1.1733	0.8511	0.026*
C12	0.2110 (5)	0.2269 (5)	1.4310 (3)	0.0216 (7)
H12A	0.0667	0.1735	1.4136	0.032*
H12B	0.2755	0.2930	1.5125	0.032*
H12C	0.2521	0.1230	1.4159	0.032*
C8	0.2582 (4)	0.6929 (4)	0.6429 (3)	0.0155 (6)
H8	0.1827	0.5730	0.5896	0.019*
C1	0.2312 (5)	0.5094 (4)	0.9097 (3)	0.0174 (6)
H1	0.3183	0.6237	0.9659	0.021*
C7	0.3432 (5)	0.8689 (5)	0.5959 (3)	0.0183 (6)
H7A	0.2337	0.9002	0.5536	0.022*
H7B	0.4068	0.8400	0.5402	0.022*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Te	0.02669 (14)	0.01289 (13)	0.01485 (13)	0.00616 (9)	0.00697 (9)	0.00480 (8)
Cl	0.0278 (4)	0.0125 (3)	0.0153 (3)	0.0037 (3)	0.0050 (3)	0.0000 (3)
C10	0.0192 (14)	0.0146 (14)	0.0144 (14)	0.0061 (12)	0.0055 (12)	0.0032 (11)
C2	0.0138 (13)	0.0120 (13)	0.0167 (14)	0.0048 (11)	0.0054 (11)	0.0016 (11)
C4	0.0169 (14)	0.0158 (15)	0.0147 (14)	0.0026 (12)	0.0055 (11)	0.0026 (11)
C3	0.0147 (13)	0.0152 (14)	0.0144 (14)	0.0076 (11)	0.0061 (11)	0.0039 (11)
C6	0.0216 (15)	0.0183 (16)	0.0213 (16)	0.0039 (13)	0.0074 (13)	0.0084 (13)
C11	0.0221 (15)	0.0183 (15)	0.0153 (15)	0.0078 (13)	0.0049 (12)	0.0037 (12)
C9	0.0218 (15)	0.0181 (15)	0.0138 (14)	0.0061 (12)	0.0054 (12)	0.0055 (12)
C5	0.0265 (16)	0.0158 (15)	0.0193 (16)	0.0057 (13)	0.0064 (13)	0.0018 (12)
C12	0.0237 (16)	0.0266 (17)	0.0172 (15)	0.0112 (14)	0.0085 (13)	0.0073 (13)
C8	0.0165 (14)	0.0138 (14)	0.0151 (14)	0.0058 (11)	0.0043 (11)	0.0022 (11)
C1	0.0220 (15)	0.0123 (14)	0.0152 (14)	0.0047 (12)	0.0052 (12)	0.0036 (11)
C7	0.0214 (15)	0.0171 (15)	0.0148 (14)	0.0051 (12)	0.0069 (12)	0.0056 (12)

Geometric parameters (Å, º)

Te—C1	2.077 (3)	C6—H6B	0.9900
Te—C9	2.148 (3)	C11—C12	1.526 (4)
Cl—C2	1.750 (3)	C11—H11A	0.9900
C10—C9	1.523 (4)	C11—H11B	0.9900
C10—C11	1.526 (4)	C9—H9A	0.9900
C10—H10A	0.9900	C9—H9B	0.9900
C10—H10B	0.9900	C5—H5A	0.9900
C2—C1	1.334 (4)	C5—H5B	0.9900
C2—C3	1.471 (4)	C12—H12A	0.9800
C4—C3	1.503 (4)	C12—H12B	0.9800
C4—C5	1.532 (5)	C12—H12C	0.9800
C4—H4A	0.9900	C8—C7	1.509 (4)

C4—H4B	0.9900	C8—H8	0.9500
C3—C8	1.338 (4)	C1—H1	0.9500
C6—C7	1.514 (4)	C7—H7A	0.9900
C6—C5	1.515 (5)	C7—H7B	0.9900
C6—H6A	0.9900		

C1—Te—C9	94.09 (12)	C10—C9—Te	110.3 (2)
C9—C10—C11	112.3 (3)	C10—C9—H9A	109.6
C9—C10—H10A	109.1	Te—C9—H9A	109.6
C11—C10—H10A	109.1	C10—C9—H9B	109.6
C9—C10—H10B	109.1	Te—C9—H9B	109.6
C11—C10—H10B	109.1	H9A—C9—H9B	108.1
H10A—C10—H10B	107.9	C6—C5—C4	110.7 (3)
C1—C2—C3	126.5 (3)	C6—C5—H5A	109.5
C1—C2—Cl	116.5 (2)	C4—C5—H5A	109.5
C3—C2—Cl	117.0 (2)	C6—C5—H5B	109.5
C3—C4—C5	112.1 (3)	C4—C5—H5B	109.5
C3—C4—H4A	109.2	H5A—C5—H5B	108.1
C5—C4—H4A	109.2	C11—C12—H12A	109.5
C3—C4—H4B	109.2	C11—C12—H12B	109.5
C5—C4—H4B	109.2	H12A—C12—H12B	109.5
H4A—C4—H4B	107.9	C11—C12—H12C	109.5
C8—C3—C2	122.8 (3)	H12A—C12—H12C	109.5
C8—C3—C4	121.6 (3)	H12B—C12—H12C	109.5
C2—C3—C4	115.7 (3)	C3—C8—C7	123.9 (3)
C7—C6—C5	110.2 (3)	C3—C8—H8	118.1
C7—C6—H6A	109.6	C7—C8—H8	118.1
C5—C6—H6A	109.6	C2—C1—Te	126.3 (2)
C7—C6—H6B	109.6	C2—C1—H1	116.9
C5—C6—H6B	109.6	Te—C1—H1	116.9
H6A—C6—H6B	108.1	C8—C7—C6	113.1 (3)
C12—C11—C10	111.6 (3)	C8—C7—H7A	109.0
C12—C11—H11A	109.3	C6—C7—H7A	109.0
C10—C11—H11A	109.3	C8—C7—H7B	109.0
C12—C11—H11B	109.3	C6—C7—H7B	109.0
C10—C11—H11B	109.3	H7A—C7—H7B	107.8
H11A—C11—H11B	108.0		

C1—C2—C3—C8	174.6 (3)	C7—C6—C5—C4	61.8 (4)
Cl—C2—C3—C8	−5.9 (4)	C3—C4—C5—C6	−48.2 (4)
C1—C2—C3—C4	−5.6 (4)	C2—C3—C8—C7	−179.0 (3)
Cl—C2—C3—C4	173.9 (2)	C4—C3—C8—C7	1.2 (5)
C5—C4—C3—C8	17.1 (4)	C3—C2—C1—Te	177.3 (2)
C5—C4—C3—C2	−162.7 (3)	Cl—C2—C1—Te	−2.2 (4)
C9—C10—C11—C12	−179.1 (3)	C9—Te—C1—C2	−177.3 (3)
C11—C10—C9—Te	179.5 (2)	C3—C8—C7—C6	12.0 (4)
C1—Te—C9—C10	179.5 (2)	C5—C6—C7—C8	−42.7 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···Cl	0.95	2.56	3.024 (3)	110