# Crystal structure of (2*E*)-3-bromo-2-[bromo(chloro)phenyl-λ$^4$-tellanyl]-2-propen-1-ol, BrCH=C(TeBrClPh)($CH_2OH$)

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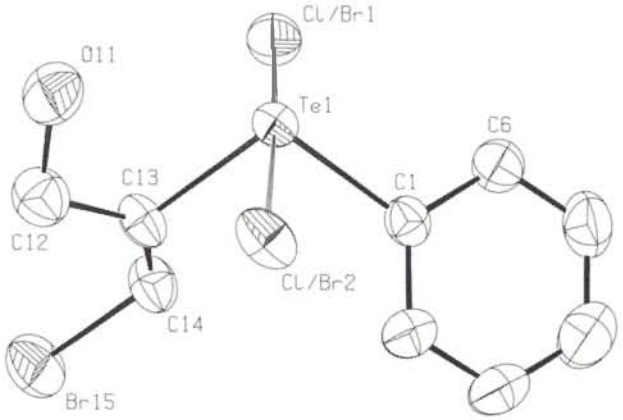


**Abstract**

$C_9H_9Br_2ClOTe$, orthorhombic, *Pbca* (No. 61), $a$ = 11.460(2) Å, $b$ = 8.4396(5) Å, $c$ = 26.296(2) Å, $V$ = 2543.2 Å$^3$, $Z$ = 8, $R_{gt}(F)$ = 0.047, $wR_{ref}(F^2)$ = 0.133, $T$ = 293 K.

## Source of material

The title compound is formed when bromine (1 mmol) in benzene (1 mL) was mixed for 1.5 h at room temperature with BrCH=(TePh)$CH_2OH$ (0.5 mmol), made by the in situ reaction of HC C-$CH_2OH$ (1 mmol), PhTeBr (0.5 mmol) and $ZnCl_2$ (10 mol) in THF (3 mL) at 333 K in 15 h. The product of the last reaction is not stable and is analogous to previously synthesized sulfur and selenium compounds [1-3]. Slow evaporation of a dichlorometane/petroleum ether solution at room temperature yielded crystals suitable for X-ray diffraction.

## Discussion

The single crystal X-ray experiment was carried out to determine the stereochemistry of the compound. The two halogen atoms, the C1 and C13 atoms and electron lone pair on the tellurium atom create an approximately trigonal geometry about the chalcogen center. It was not possible to distinguish between the chlorine and bromine atoms bonded to tellurium atom due to apparent disorder. They were modelled at 50% occupancy each. Bond distances and angles fit well in the ranges of corresponding compounds.

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | yellow block, size 0.18 × 0.25 × 0.32 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| μ: | 88.01 cm$^{-1}$ |
| Diffractometer, scan mode: | Enraf-Nonius CAD4, ω |
| $2\theta_{max}$: | 53.94° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 3134, 2767 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2000 |
| $N(param)_{refined}$: | 131 |
| Programs: | PLATON [4], SHELXS-97 [5], SHELXSL-97 [6] |

**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(2) | 8*c* | 0.4706 | 0.3807 | 0.3242 | 0.064 |
| H(3) | 8*c* | 0.4755 | 0.4230 | 0.2382 | 0.077 |
| H(4) | 8*c* | 0.6116 | 0.2937 | 0.1884 | 0.085 |
| H(5) | 8*c* | 0.7561 | 0.1482 | 0.2258 | 0.072 |
| H(6) | 8*c* | 0.7528 | 0.1009 | 0.3123 | 0.053 |
| H(11) | 8*c* | 0.5570 | 0.2668 | 0.5027 | 0.093 |
| H(12A) | 8*c* | 0.383(2) | 0.312(6) | 0.4816(4) | 0.064 |
| H(12B) | 8*c* | 0.354(4) | 0.131(4) | 0.4911(9) | 0.064 |
| H(14) | 8*c* | 0.396(3) | 0.103(2) | 0.353(3) | 0.053 |

**Table 3.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | Occ. | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Te(1) | 8*c* | | 0.61772(3) | 0.19356(5) | 0.40624(2) | 0.0293(2) | 0.0311(3) | 0.0337(3) | 0.0002(2) | -0.0009(2) | -0.0033(2) |
| Cl(1) | 8*c* | 0.5 | 0.60935(9) | -0.1132(1) | 0.38351(5) | 0.0482(6) | 0.0352(6) | 0.0491(7) | 0.0047(4) | 0.0028(5) | 0.0001(5) |
| Br(1) | 8*c* | 0.5 | 0.60935 | -0.1132 | 0.38351 | 0.0482 | 0.0352 | 0.0491 | 0.0047 | 0.0028 | 0.0001 |
| Cl(2) | 8*c* | 0.5 | 0.58891(9) | 0.4923(1) | 0.42203(5) | 0.0425(5) | 0.0313(6) | 0.0769(8) | -0.0015(5) | 0.0077(5) | -0.0149(6) |
| Br(2) | 8*c* | 0.5 | 0.58891 | 0.4923 | 0.42203 | 0.0425 | 0.0313 | 0.0769 | -0.0015 | 0.0077 | -0.0149 |
| C(1) | 8*c* | | 0.6098(5) | 0.2351(9) | 0.3269(3) | 0.034(3) | 0.032(4) | 0.043(4) | -0.003(3) | 0.005(3) | 0.000(3) |
| C(2) | 8*c* | | 0.5275(7) | 0.332(1) | 0.3044(3) | 0.055(5) | 0.057(6) | 0.047(5) | 0.013(4) | 0.002(4) | 0.013(4) |

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**Table 3.** Continued.

| Atom | Site | Occ. | *x* | *y* | *z* | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C(3) | 8*c* | | 0.5300(8) | 0.356(1) | 0.2533(4) | 0.072(6) | 0.071(6) | 0.051(5) | 0.019(5) | –0.002(5) | 0.020(5) |
| C(4) | 8*c* | | 0.6132(8) | 0.282(1) | 0.2235(4) | 0.084(7) | 0.075(8) | 0.054(6) | 0.003(6) | 0.005(5) | 0.014(6) |
| C(5) | 8*c* | | 0.6973(7) | 0.192(1) | 0.2457(3) | 0.065(5) | 0.057(6) | 0.057(5) | 0.007(4) | 0.024(4) | 0.001(5) |
| C(6) | 8*c* | | 0.6964(6) | 0.1650(9) | 0.2974(3) | 0.049(4) | 0.040(4) | 0.044(4) | 0.004(3) | 0.003(3) | –0.001(4) |
| O(11) | 8*c* | | 0.5178(5) | 0.1860(8) | 0.5055(2) | 0.063(4) | 0.083(5) | 0.039(3) | –0.002(3) | –0.007(3) | –0.005(3) |
| C(12) | 8*c* | | 0.4128(7) | 0.204(1) | 0.4779(3) | 0.050(4) | 0.058(5) | 0.052(5) | 0.000(4) | 0.001(4) | –0.007(4) |
| C(13) | 8*c* | | 0.4364(6) | 0.1687(9) | 0.4230(3) | 0.029(3) | 0.041(4) | 0.042(4) | –0.002(3) | 0.004(3) | –0.014(3) |
| C(14) | 8*c* | | 0.3649(6) | 0.122(1) | 0.3891(3) | 0.034(4) | 0.054(5) | 0.044(4) | –0.006(3) | 0.004(3) | –0.007(4) |
| Br(15) | 8*c* | | 0.20443(7) | 0.0868(1) | 0.40239(4) | 0.0343(4) | 0.0816(7) | 0.0735(6) | –0.0121(4) | 0.0015(4) | 0.0036(5) |

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