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Short Communication

Jens Beckmann*, Enno Lork and Ole Mallow

Molecular structure of *n*-tributylphosphine telluride

Abstract: The molecular of the title compound *n*-Bu_3PTe was established by X-ray crystallography and compared with the previously known trialkylphosphine tellurides.

Keywords: chalcogenides; trialkylphosphine telluride; X-ray crystallography.

***Corresponding author: Jens Beckmann,** Institute of Inorganic & Physical Chemistry, Bremen University, Leobener Straße, 28359 Bremen, Germany, e-mail: j.beckmann@uni-bremen.de
Enno Lork and Ole Mallow: Institute of Inorganic & Physical Chemistry, Bremen University, Leobener Straße, 28359 Bremen, Germany

The title compound *n*-Bu_3PTe was the first trialkylphosphine telluride ever prepared (Zingaro, 1963). Its characterization was achieved by ^{125}Te nuclear magnetic resonance and ^{125m}Te Mößbauer spectroscopy (Jones and Sharma, 1987). In organometallic synthesis, *n*-Bu_3PTe has been utilized as a mild transfer reagent for atomic tellurium (Sasamori et al., 2005; Tajima et al., 2006). A literature search brought forward that only three trialkylphosphine tellurides have been investigated by X-ray crystallography, namely, *t*-Bu_3PTe (Kuhn et al., 1987), *i*-Pr_3PTe (Kuhn et al., 1990), and $Me_2P(Te)CH_2CH_2P(Te)Me_2$ (Steigerwald et al., 1994). Here, we report the molecular structure of *n*-Bu_3PTe, which is shown in Figure 1. Selected bond parameters are collected in the caption. Crystal and refinement data are listed in Table 1. The spatial arrangement of the P atom is distorted tetrahedral. The P−Te bond length of *n*-Bu_3PTe [2.368 (1) Å] compares well with those of *t*-Bu_3PTe [2.368 (4) Å] (Kuhn et al., 1987), *i*-Pr_3PTe [2.366 (1) Å] (Kuhn et al., 1990), and $Me_2P(Te)CH_2CH_2P(Te)Me_2$ [2.357 (2) Å] (Steigerwald et al., 1994) and points to

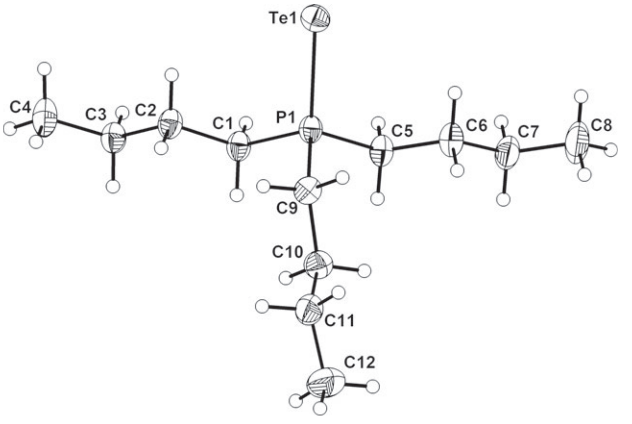

Figure 1 Molecular structure of *n*-Bu_3PTe showing 50% probability ellipsoids and the crystallographic numbering scheme. Selected bond parameters (Å) are as follows: P1−Te1 2.368 (1), P1−C1 1.817 (3), P1−C5 1.826 (3), P1−C9 1.828 (3), C1−P1−Te1 114.78 (9), C5−P1−Te1 113.9 (1), C9−P1−Te1 109.90 (9), C1−P1−C5 102.4 (1), C1−P1−C9 107.1 (1), C5−P1−C9 108.3 (1).

Formula	$C_{12}H_{27}PTe$
Formula weight, g/mol	329.91
Crystal system	Triclinic
Crystal size, mm	0.40×0.40×0.40
Space group	*P*-1
a, Å	7.468 (2)
b, Å	9.503 (3)
c, Å	12.415 (4)
α	105.56 (2°)
β	91.74 (2°)
γ	110.79 (3°)
V, $Å^3$	785.8 (4)
Z	2
ρ_{calcd}, Mg m^{-3}	1.394
T, K	173
μ (Mo-Kα), mm^{-1}	1.966
F(000)	332
θ range, degrees	2.50–27.49
Index ranges	$-9 \le h \le 8$ $-11 \le k \le 11$ $-16 \le l \le 16$
Number of reflections collected	4454
Completeness to θ_{max}	98.4%
Number of independent reflections	3561
Number of observed reflections with ($I > 2\sigma(I)$)	3449
Number of refined parameters	130
GooF (F^2)	1.113
R_1 (F) ($I > 2\sigma(I)$)	0.0307
wR_2 (F^2) (all data)	0.0808
$(\Delta/\sigma)_{max}$	<0.001
Largest difference peak/hole, e $Å^{-3}$	0.898/-1.479

Table 1 Crystal data and structure refinement of *n*-Bu_3PTe.

a formal bond order of about 1.5 (Kuhn et al., 1987). The distortion is reflected by the mean Te−P−C and C−P−C angles [112.9(1)° and 105.9(1)°] that are in good agreement with those of $Me_2P(Te)CH_2CH_2P(Te)Me_2$ [113.5(3)° and 105.2(4)°] (Steigerwald et al., 1994). In contrast, the mean Te−P−C and C−P−C angles of *t*-Bu_3PTe [108.7(4)° and 110.2(5)°] (Kuhn et al., 1987) and *i*-Pr_3PTe [110.9(1)° and 110.7(1)°] (Kuhn et al., 1990) are much closer to the ideal tetrahedral angle of 109.3°.

Experimental

The title compound *n*-Bu_3PTe was prepared by the reaction of *n*-Bu_3P with tellurium powder (Zingaro, 1963). Single crystals were obtained by slow evaporation of a toluene solution under the inert conditions of a glove box.

X-ray crystallography

Intensity data of *n*-Bu_3PTe were collected on a Siemens P4 diffractometer with graphite-monochromated Mo-Kα (0.7107 Å) radiation. Data were reduced and corrected for absorption (Walker and Stuart, 1983). The structure was solved by direct methods and difference Fourier synthesis with subsequent full-matrix least-squares refinements on F^2, using all data (Sheldrick, 2008). All nonhydrogen atoms were refined using anisotropic displacement parameters. Hydrogen atoms attached to carbon atoms were included in geometrically calculated positions using a riding model. Crystal and refinement data are collected in Table 1. Figures were created using DIAMOND (Brandenburg and Putz, 2006). Crystallographic data (excluding structure factors) for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC number 898395. Copies of this information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or http://www.ccdc.cam.ac.uk).

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