C6	0.4539 (8)	−0.6439 (7)	0.2602 (8)	3.9 (2)
C7	0.3458 (8)	−0.5824 (6)	0.2040 (8)	3.2 (2)
C8	0.2134 (8)	−0.6048 (6)	0.2097 (8)	3.4 (2)
C9	0.1774 (8)	−0.7057 (6)	0.1551 (9)	3.2 (2)
C10	0.1782 (8)	−0.7053 (6)	0.0275 (9)	3.6 (2)
C11	0.1496 (8)	−0.5505 (6)	0.0867 (8)	3.4 (2)
C12	0.5412 (9)	−0.6100 (8)	0.1687 (8)	4.4 (2)
C13	0.5308 (1)	−0.8047 (8)	0.170 (1)	5.3 (3)
C14	0.1157 (8)	−0.3897 (6)	0.1561 (9)	3.6 (2)
C15	0.1438 (8)	−0.2866 (6)	0.1355 (9)	3.3 (2)
C16	0.0926 (8)	−0.2183 (6)	0.2081 (9)	4.0 (2)
C17	0.1097 (8)	−0.1205 (7)	0.1918 (9)	4.0 (2)
C18	0.1809 (9)	−0.0923 (6)	0.1048 (9)	4.1 (2)
C19	0.235 (1)	−0.1568 (7)	0.0310 (9)	4.8 (3)
C20	0.2153 (9)	−0.2553 (6)	0.0486 (8)	4.0 (2)

Table 2. *Selected geometric parameters (Å, °)*

Br—C18	1.899 (6)	C5—C6	1.518 (9)
O1—C14	1.172 (8)	C6—C7	1.524 (9)
O2—C11	1.460 (7)	C6—C12	1.569 (9)
O2—C14	1.367 (8)	C7—C8	1.546 (9)
C1—C2	1.556 (9)	C8—C9	1.537 (8)
C1—C10	1.517 (8)	C8—C11	1.559 (8)
C1—C11	1.540 (8)	C9—C10	1.343 (9)
C2—C3	1.553 (8)	C14—C15	1.486 (8)
C2—C7	1.585 (8)	C15—C16	1.403 (8)
C3—C4	1.516 (9)	C15—C20	1.393 (9)
C3—C12	1.551 (9)	C16—C17	1.382 (9)
C4—C5	1.512 (9)	C17—C18	1.379 (9)
C4—C13	1.549 (9)	C18—C19	1.394 (9)
C5—C13	1.521 (9)	C19—C20	1.399 (9)
C11—O2—C14	115.7 (5)	C7—C8—C11	100.6 (5)
C2—C1—C10	112.1 (5)	C9—C8—C11	94.3 (5)
C2—C1—C11	99.8 (5)	C8—C9—C10	108.7 (5)
C10—C1—C11	95.9 (5)	C1—C10—C9	107.4 (6)
C1—C2—C3	126.1 (5)	O2—C11—C1	109.9 (5)
C1—C2—C7	103.6 (5)	O2—C11—C8	114.4 (5)
C3—C2—C7	102.1 (5)	C1—C11—C8	95.3 (4)
C2—C3—C4	110.0 (5)	C3—C12—C6	93.9 (5)
C2—C3—C12	98.6 (5)	C4—C13—C5	59.0 (4)
C4—C3—C12	102.6 (5)	O1—C14—O2	124.3 (6)
C3—C4—C5	104.5 (5)	O1—C14—C15	125.9 (6)
C3—C4—C13	118.3 (6)	O2—C14—C15	109.8 (6)
C5—C4—C13	59.6 (4)	C14—C15—C16	116.6 (6)
C4—C5—C6	104.8 (5)	C14—C15—C20	124.0 (6)
C4—C5—C13	61.4 (4)	C16—C15—C20	119.5 (5)
C6—C5—C13	119.7 (6)	C15—C16—C17	120.8 (6)
C5—C6—C7	110.4 (5)	C16—C17—C18	118.1 (6)
C5—C6—C12	101.5 (5)	Br—C18—C17	119.2 (5)
C7—C6—C12	98.5 (5)	Br—C18—C19	117.1 (5)
C2—C7—C6	104.0 (5)	C17—C18—C19	123.7 (6)
C2—C7—C8	102.7 (5)	C18—C19—C20	117.0 (6)
C6—C7—C8	126.5 (5)	C15—C20—C19	121.0 (6)
C7—C8—C9	111.3 (5)		

Lorentz and polarization corrections were applied. The structure was solved by direct methods. Non-H atoms were refined anisotropically. Programs used were from the *Enraf–Nonius CAD*-4 *SDP* package (Frenz, 1978).

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1-Iodo-2-*p*-tolyl-1-tellura-2-azaindene

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Abstract

The structure of $C_{14}H_{12}INTe$ consists of discrete molecules in which the Te atom is three-coordinate with Te—C and Te—I distances of 2.102 (5) and 2.936 (1) Å, respectively, and a Te···N interaction of 2.230 (4) Å. The I atom is *trans* to the N atom [I—Te···N 170.3 (1)°].

Comment

Organotellurium compounds may be stabilized by reduction of the Lewis acid of the Te atom by intramolecular coordination with a heteroatom, e.g. nitrogen (McWhinnie, 1992). In this context, the factors affecting the strength of putative Te· · ·N interactions are important. We report here the crystal structure of the title compound, (I), synthesized according to the method of Maksimenko, Sadekov, Maslakov, Mehrotra, Kompan, Struchkov, Lindeman & Minkin (1988), as part of an ongoing study of organotellurium compounds containing an N atom sterically capable of coordinating to the central Te atom. Previous work (McWhinnie, 1992; Maslakov, McWhinnie, Perry, Shaikh, McWhinnie & Hamor, 1993) has indicated the particular importance of the ligand bonded *trans* to the Te· · ·N vector in determining the strength of this interaction.
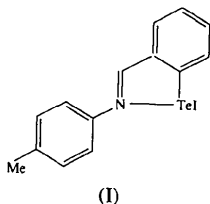
(I)

Fig. 1 shows the atom-numbering scheme. The Te atom is bonded to one C atom and one I atom with distances Te—C(1) 2.102 (5) and Te—I 2.936 (1) Å, and is involved in a Te· · ·N interaction of 2.230 (4) Å. The interactions involving Te may be compared with those found in the related compounds 2-(ClTe)C_6H_4CH=N(C_6H_4Me-4), (II) (Maksimenko *et al.*, 1988), and 2-(BrTe)C_6H_4CH$_2$NH(C_6H_4Me-4), (III) (Maslakov *et al.*, 1993). In compound (II), which differs from the title compound only with respect to the nature of the attached halogen atom, the Te—C and Te· · ·N distances are 2.098 and 2.229 Å, respectively, averaged over two independent molecules in the unit cell; these distances are virtually identical to the corresponding distances in the title compound. In compound (III), the Te—C bond length is similar at 2.125 Å, but the Te· · ·N distance is significantly longer at 2.375 Å. If, as seems likely, the *trans* influence of Br is similar to that of Cl and I (McWhinnie, 1992), the difference in the Te· · ·N separation between the title compound and compound (II) on the one hand, and compound (III) on the other, can be attributed (Maslakov *et al.*, 1993) to the difference in hybridization state of the N atom: sp^2 in both the title compound and compound (II), and sp^3 in compound (III).

The overall geometry of the molecule can be described in terms of two planar residues: the telluraazaindene and the C(7)–C(13) *p*-toluene moieties. The interplanar angle is 38.8°, the I atom being displaced by 0.222 (2) Å from the telluraazaindene plane.

The I atom does not appear to be involved in any intermolecular secondary bonding interactions, although I· · ·H distances down to 3.13 Å occur between centrosymmetrically related molecules. The Te—I bond distance of 2.936 (4) Å is longer than the sum of the corresponding covalent radii (2.70 Å) but falls in the range 2.75–3.15 Å found to be characteristic of essentially covalent bonding (Jones & Hamor, 1982; Alcock & Harrison, 1984; Foss & Maartmann-Moe, 1986, Hu, Jin & Li, 1991).
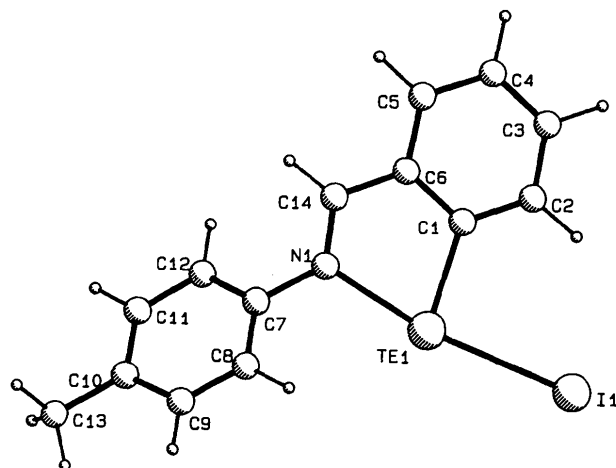

Fig. 1. View of the molecule perpendicular to the planar telluraazaindene moiety.

Experimental

The title compound was synthesized according to the method of Maksimenko *et al.* (1988), and recrystallized from chloroform.

Crystal data

$C_{14}H_{12}INTe$	Mo $K\alpha$ radiation
$M_r = 448.8$	$\lambda = 0.71069$ Å
Triclinic	Cell parameters from 92
$P\bar{1}$	reflections
$a = 8.127$ (5) Å	$\theta = 6–18°$
$b = 9.952$ (2) Å	$\mu = 4.35$ mm^{-1}
$c = 9.992$ (3) Å	$T = 293$ K
$\alpha = 72.17$ (2)°	Chunky block
$\beta = 76.76$ (3)°	0.6 × 0.5 × 0.5 mm
$\gamma = 68.31$ (3)°	Light brown
$V = 708.7$ (5) Å^3	
$Z = 2$	
$D_x = 2.103$ Mg m^{-3}	

Data collection

Enraf–Nonius CAD-4	2092 observed reflections
diffractometer	$[F > 5\sigma(F)]$
ω–2θ scans	$R_{int} = 0.009$

Absorption correction:
refined from ΔF
(*DIFABS*; Walker &
Stuart, 1983)
$T_{min} = 0.52$, $T_{max} = 1.00$
2675 measured reflections
2484 independent reflections

$\theta_{max} = 25°$
$h = 0 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -11 \rightarrow 11$
3 standard reflections
frequency: 120 min
intensity decay: $< 3\%$

Refinement

Refinement on F
$R = 0.0278$
$wR = 0.0382$
$S = 0.67$
2092 reflections
169 parameters
Only H-atom U's refined

$w = 1/[\sigma^2(F) + 0.0015F^2]$
$(\Delta/\sigma)_{max} = 0.06$
$\Delta\rho_{max} = 0.66$ e Å^{-3}
$\Delta\rho_{min} = -1.07$ e Å^{-3}
Atomic scattering factors
from *International Tables
for X-ray Crystallography*
(1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent
isotropic displacement parameters* (Å^2)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Te	0.04417 (4)	0.72426 (3)	0.48724 (4)	0.046
I	−0.21613 (5)	0.82044 (4)	0.72481 (4)	0.065
N(1)	0.2476 (5)	0.6122 (4)	0.3297 (4)	0.046
C(1)	0.1798 (7)	0.5157 (5)	0.6112 (6)	0.047
C(2)	0.1465 (8)	0.4648 (6)	0.7562 (6)	0.056
C(3)	0.2469 (9)	0.3222 (6)	0.8218 (7)	0.065
C(4)	0.3799 (8)	0.2307 (6)	0.7459 (7)	0.061
C(5)	0.4152 (7)	0.2807 (6)	0.6017 (6)	0.056
C(6)	0.3163 (7)	0.4236 (5)	0.5326 (6)	0.048
C(7)	0.2531 (7)	0.6814 (5)	0.1793 (5)	0.047
C(8)	0.2228 (7)	0.8329 (6)	0.1351 (6)	0.054
C(9)	0.2251 (8)	0.9026 (6)	−0.0069 (6)	0.056
C(10)	0.2511 (7)	0.8236 (6)	−0.1078 (6)	0.055
C(11)	0.2791 (8)	0.6714 (6)	−0.0598 (6)	0.058
C(12)	0.2795 (7)	0.6003 (6)	0.0823 (6)	0.053
C(13)	0.2507 (9)	0.9000 (8)	−0.2632 (7)	0.069
C(14)	0.3454 (7)	0.4793 (6)	0.3829 (6)	0.050

Table 2. *Selected geometric parameters* (Å, °)

Te—I	2.936 (1)	C(5)—C(6)	1.397 (7)
Te—N(1)	2.230 (4)	C(6)—C(14)	1.424 (8)
Te—C(1)	2.102 (5)	C(7)—C(8)	1.377 (7)
N(1)—C(7)	1.447 (7)	C(7)—C(12)	1.376 (7)
N(1)—C(14)	1.285 (7)	C(8)—C(9)	1.375 (8)
C(1)—C(2)	1.379 (8)	C(9)—C(10)	1.395 (8)
C(1)—C(6)	1.406 (7)	C(10)—C(11)	1.387 (8)
C(2)—C(3)	1.389 (8)	C(10)—C(13)	1.505 (8)
C(3)—C(4)	1.376 (8)	C(11)—C(12)	1.379 (8)
C(4)—C(5)	1.372 (8)		
I—Te—N(1)	170.3 (1)	C(1)—C(6)—C(14)	118.0 (4)
I—Te—C(1)	94.8 (1)	C(5)—C(6)—C(14)	122.2 (5)
N(1)—Te—C(1)	76.3 (2)	N(1)—C(7)—C(8)	118.4 (4)
Te—N(1)—C(7)	121.2 (3)	N(1)—C(7)—C(12)	121.3 (4)
Te—N(1)—C(14)	114.5 (3)	C(8)—C(7)—C(12)	120.2 (5)
C(7)—N(1)—C(14)	124.0 (4)	C(7)—C(8)—C(9)	119.9 (5)
Te—C(1)—C(2)	126.5 (4)	C(8)—C(9)—C(10)	121.2 (5)
Te—C(1)—C(6)	113.9 (4)	C(9)—C(10)—C(11)	117.5 (5)
C(2)—C(1)—C(6)	119.6 (5)	C(9)—C(10)—C(13)	121.3 (5)
C(1)—C(2)—C(3)	119.2 (5)	C(11)—C(10)—C(13)	121.2 (5)
C(2)—C(3)—C(4)	121.7 (6)	C(10)—C(11)—C(12)	121.7 (5)
C(3)—C(4)—C(5)	119.6 (5)	C(7)—C(12)—C(11)	119.4 (5)
C(4)—C(5)—C(6)	120.1 (5)	N(1)—C(14)—C(6)	117.3 (4)
C(1)—C(6)—C(5)	119.8 (5)		

H atoms were placed in calculated positions (C—H 1.08 Å),
riding on their respective bonded atoms. The methyl sub-
stituent was refined as a rigid rotating group.

Computer programs used include *SHELX76* (Sheldrick,
1976), *SHELX86* (Sheldrick, 1985) and *PLUTO* (Motherwell
& Clegg, 1978).

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3-Methyl-4*H*-pyrido[2,3-*e*]-1,2,4-thiadiazine 1,1-Dioxide

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Abstract

The title compound, $C_7H_7N_3O_2S$, was prepared for
comparison with diazoxide, an antihypertensive agent,
from a structural and pharmacological point of view.