ligand in the present compound are as follows: B(c)—B(d) 1·8249 (19), B(h)—B(i) 1·9837 (19), B(a)···B(b) 3·352 (2) Å; height of Pd above the B(a)B(h)B(i)B(b) plane 0·5693 (22) Å.

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Structure of Di-μ-bromo-(tetrabromo-1κ⁴Br)bis(N,N-dimethylselenourea-2κ²Se)-ditellurium(II,IV)–Acetonitrile–Methanol (2/3/1)

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Abstract. $2[Te_2Br_6(C_3H_8N_2Se)_2] \cdot 3C_2H_3N \cdot CH_3OH$, $M_r = 2228·7$, monoclinic, $P2_1$, $a = 9·973$ (3), $b = 16·659$ (6), $c = 16·930$ (6) Å, $\beta = 101·03°$, $V = 2760·8$ (16) Å³, $Z = 2$, $D_x = 2·681$ Mg m⁻³, Mo $K\alpha$, $\lambda = 0·71073$ Å, $\mu = 13·11$ mm⁻¹, $F(000) = 2016$, $T = 193$ K, $R = 0·053$ for 3379 reflections and 305 parameters. The structure consists of two crystallographically distinct units. In each of them, a Te^{IV} species has a sixfold, nearly octahedral configuration of Br atoms around it. Two of these Br atoms are shared (*cis*) with a Te^{II} atom to which are also attached two molecules of N,N-dimethylselenourea, producing a distorted square-planar configuration of ligands around Te^{II}. The two crystallographically distinct units are similar, but one of them is coordinated by two CH_3CN moieties and the other by one CH_3CN and one CH_3OH moiety.

Introduction. During the preparation of thin films of Te–Se alloys, a number of products of the reactions between Te^{IV} halides and substituted selenoureas have been isolated. One of these, the title compound, is unusual in that both Te^{IV} and Te^{II} are present in the same molecule and share two Br atoms. There

appear to be no previously reported cases of such structures involving tellurium, although the compound $[(C_2H_5)_2N]_2Se_2Br_8$ contains an anion with Se^{II} and Se^{IV} sharing two Br atoms, which is remarkably similar to the uncharged species found here (Hauge, Maroy & Odegard, 1988). The purpose of the present study is to compare the structure of this mixed valence compound with those that contain Te^{II} and Te^{IV} in more conventional materials and also to compare the structure with that of the analagous selenium compound mentioned above.

Experimental. When $TeBr_4$ was reacted with N,N-dimethylselenourea (DMSeU) in C_2H_5OH, an insoluble product was formed. After separating the solid, refluxing in CH_3OH and filtering, a few orange crystals of the title compound grew from solution upon standing. A single crystal was selected, attached with Dow stopcock grease to a glass fiber, mounted on a Nicolet $R3m/V$ diffractometer and cooled to $T = 193$ K with a stream of N_2 gas. Unit-cell dimensions were obtained from measurements of 2θ for 25 reflections, $8 \le 2\theta \le 30°$, using graphite-monochromatized Mo $K\alpha$ radiation. Intensities were measured for reflections in the range $4·0 \le 2\theta \le 50°$, $-11 \le h \le 9$, $-19 \le k \le 0$, $-20 \le l \le 0$, using a

Wyckoff-type scan with a variable scan speed, 2·00 to 14·65° min^{-1} in ω, a fixed scan range, $\Delta\omega = 0·60°$, and backgrounds obtained with a stationary crystal, stationary counter at the beginning and end of the scan, each for 25% of the total scan time. The intensities of three standard reflections which were measured every 97 reflections remained nearly unchanged throughout data collection. Intensities of 4088 reflections were measured, of which 4079 were independent, and 3379 had $I > 1·5\sigma(I)$; $R_{int} = 0·043$. Close to the end of data collection an icing problem occurred, the crystal fell from its mount and its physical dimensions could not be measured. Prior to this, ψ-scan data had been collected and an empirical absorption correction was applied to the data (ellipsoid approximation, min. $T = 0·709$, max. $T = 0·855$) as well as Lorentz and polarization corrections. The composition of the crystal was originally unknown. The structure was solved by examination of the Patterson function and by the trial-and-error testing of models suggested by it, coupled with electron-density and least-squares calculations. At first, the space group $P2_1/m$ was selected, but as the outline of the structure developed, it became clear that either the structure was disordered or the space group $P2_1$ was correct, with two independent molecules of $(DMSeU)_2TeBr_2TeBr_4$ in the unit cell. The structure refined satisfactorily in $P2_1$, but difference electron density maps revealed the presence of three molecules of CH_3CN and one molecule of CH_3OH in the asymmetric unit. Since the crystals had been recrystallized from CH_3OH, it was not surprising to observe it in the crystals.

The unexpected appearance of CH_3CN was traced back to the use of DMSeU that had been recrystallized from CH_3CN and C_6H_6. (An analagous compound that contains CH_3CN and C_2H_5OH has been prepared simply by diffusion between solutions of $TeBr_4$ in C_2H_5OH and DMSeU in CH_3CN at room temperature.) Least-squares refinements were carried out on the coordinates and temperature factors of all non-H atoms, with Te, Br and Se anisotropic, O, N and C isotropic, on the scale factor and Rogers's η (Rogers, 1981), with the H atoms of the NH_2 groups placed in idealized positions. Difference electron density maps were calculated and 16 of 36 H atoms in CH_3 groups were identified and used to obtain positions for all methyl H atoms which were then held fixed in all further refinements. The H atom attached to O was not found. Final refinements (carried out until the change in any parameter was less than 0·01 of its σ) of the scale factor, Rogers's $\eta = 0·93$ (10), coordinates and temperature factors of all non-H atoms with Te, Br and Se anisotropic and O, N and C isotropic gave $R = 0·053$, $wR = 0·050$, 3379 reflections with $I > 1·5\sigma(I)$, 305 parameters, goodness-of-fit = 1·24, quantity minimized $\sum w(|F_o| - |F_c|)^2$, w^{-1}

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic displacement parameters* ($\text{Å}^2 \times 10^3$) *for* $2[Te_2Br_6(C_3H_8N_2Se)_2].3C_2H_3N.CH_3OH$

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Te(1)	4418 (2)	2500	4991 (1)	25 (1)
Br(1)	5503 (3)	3546 (3)	6089 (2)	39 (1)
Br(2)	5493 (3)	1333 (3)	5960 (2)	44 (1)
Br(3)	6615 (3)	2548 (3)	4325 (2)	41 (1)
Br(4)	2104 (2)	2431 (3)	5645 (1)	39 (1)
Br(5)	3275 (3)	1363 (2)	3826 (2)	37 (1)
Br(6)	3256 (3)	3758 (2)	4010 (2)	37 (1)
Te(2)	720 (2)	2580 (2)	3225 (1)	38 (1)
Se(1)	−937 (3)	3714 (2)	2915 (2)	38 (1)
Se(2)	−975 (3)	1466 (2)	2816 (2)	36 (1)
Te(3)	−3034 (2)	3714 (2)	−136 (1)	23 (1)
Br(7)	−5399 (3)	2999 (3)	−111 (2)	39 (1)
Br(8)	−3428 (3)	4704 (3)	1010 (2)	41 (1)
Br(9)	−580 (3)	4447 (2)	−125 (2)	37 (1)
Br(10)	−4187 (3)	4707 (2)	−1265 (2)	35 (1)
Br(11)	−2579 (3)	2663 (3)	−1343 (2)	37 (1)
Br(12)	−1792 (3)	2658 (2)	1068 (1)	36 (1)
Te(4)	−2 (2)	1891 (2)	−117 (1)	51 (1)
Se(3)	1241 (3)	1502 (3)	−1197 (2)	50 (1)
Se(4)	1845 (3)	1518 (3)	1030 (2)	49 (1)
C(1)	−1138 (26)	4045 (16)	3974 (16)	34 (7)
C(2)	−1315 (25)	1057 (15)	3823 (15)	26 (6)
C(3)	1793 (22)	2552 (17)	−1540 (13)	29 (6)
C(4)	2599 (24)	2536 (18)	1336 (14)	37 (6)
N(1)	−2178 (19)	4534 (12)	3996 (11)	24 (5)
N(2)	−304 (22)	3808 (14)	4595 (13)	41 (6)
N(3)	−2268 (22)	590 (14)	3834 (13)	34 (6)
N(4)	−380 (21)	1233 (13)	4510 (12)	31 (6)
N(5)	2670 (18)	2565 (14)	−1995 (11)	31 (5)
N(6)	1151 (22)	3223 (14)	−1345 (12)	36 (6)
N(7)	3809 (21)	2602 (16)	1780 (12)	45 (6)
N(8)	1856 (27)	3203 (17)	1180 (16)	63 (8)
C(5)	−2435 (28)	4818 (17)	4744 (17)	41 (8)
C(6)	−3129 (37)	4802 (24)	3302 (22)	77 (11)
C(7)	−2555 (32)	220 (20)	4579 (19)	55 (9)
C(8)	−3289 (29)	396 (18)	3141 (17)	43 (8)
C(9)	3007 (30)	3296 (18)	−2330 (17)	47 (8)
C(10)	3498 (31)	1823 (20)	−2111 (19)	57 (9)
C(11)	4719 (31)	1912 (20)	1937 (19)	56 (9)
C(12)	4370 (42)	3401 (26)	2036 (25)	92 (14)
N(9)	9816 (24)	4265 (14)	6379 (15)	44 (6)
C(13)	9294 (25)	4448 (16)	6856 (16)	32 (7)
C(14)	8599 (28)	4626 (19)	7531 (17)	48 (8)
N(10)	9819 (35)	882 (21)	6336 (21)	94 (11)
C(15)	9332 (30)	1438 (21)	6493 (18)	51 (8)
C(16)	8906 (34)	2267 (21)	6661 (20)	70 (10)
N(11)	1918 (25)	4937 (15)	8722 (15)	52 (7)
C(17)	2548 (33)	5313 (21)	9198 (20)	57 (9)
C(18)	3350 (37)	5710 (24)	9884 (23)	80 (12)
O(1)	7950 (33)	−135 (21)	8541 (20)	133 (12)
C(19)	7558 (37)	325 (25)	7843 (25)	86 (12)

$= \sigma^2(F) + 0·0005F^2$ with $\sigma^2(F)$ estimated from $\sigma(I)$. For all 4079 data, $R = 0·069$, $wR = 0·052$, and the residuals on the final difference map varied from 1·1 to $-1·7$ e Å^{-3}. Calculations were performed with *SHELXTL-Plus* (Sheldrick, 1987). Scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). The refined coordinates and equivalent isotropic temperature factors for the structure are listed in Table 1.*
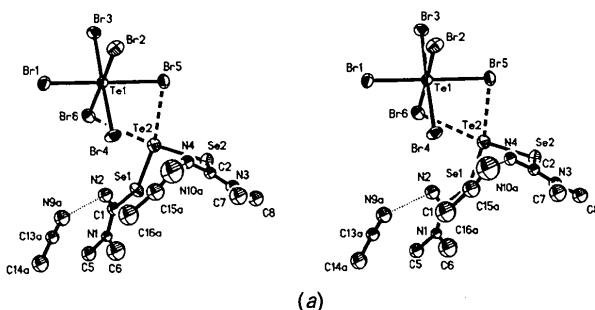
* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, bond lengths and angles involving H atoms and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53520 (25 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond lengths* (Å) *and bond angles* (°) *for* 2[Te$_2$Br$_6$(C$_3$H$_8$N$_2$Se)$_2$].3C$_2$H$_3$N.CH$_3$OH

Te(1)—Br(1)	2·626 (4)		Te(1)—Br(2)	2·636 (4)
Te(1)—Br(3)	2·650 (3)		Te(1)—Br(4)	2·747 (3)
Te(1)—Br(5)	2·814 (4)		Te(1)—Br(6)	2·785 (4)
Te(2)—Se(1)	2·498 (4)		Te(2)—Se(2)	2·517 (4)
Se(1)—C(1)	1·922 (28)		Se(2)—C(2)	1·925 (26)
Te(3)—Br(7)	2·651 (4)		Te(3)—Br(8)	2·633 (4)
Te(3)—Br(9)	2·732 (4)		Te(3)—Br(10)	2·621 (4)
Te(3)—Br(11)	2·794 (4)		Te(3)—Br(12)	2·796 (4)
Te(4)—Se(3)	2·483 (5)		Te(4)—Se(4)	2·486 (4)
Se(3)—C(3)	1·956 (28)		Se(4)—C(4)	1·886 (29)
C(1)—N(1)	1·324 (33)		C(1)—N(2)	1·273 (32)
C(2)—N(3)	1·232 (34)		C(2)—N(4)	1·376 (30)
C(3)—N(5)	1·271 (32)		C(3)—N(6)	1·360 (35)
C(4)—N(7)	1·299 (29)		C(4)—N(8)	1·333 (40)
N(1)—C(5)	1·421 (36)		N(1)—C(6)	1·434 (39)
N(3)—C(7)	1·479 (41)		N(3)—C(8)	1·436 (33)
N(5)—C(9)	1·411 (38)		N(5)—C(10)	1·520 (39)
N(7)—C(11)	1·457 (40)		N(7)—C(12)	1·476 (49)
N(9)—C(13)	1·085 (28)		C(13)—C(14)	1·475 (42)
N(10)—C(15)	1·102 (49)		C(15)—C(16)	1·489 (49)
N(11)—C(17)	1·115 (39)		C(17)—C(18)	1·439 (47)
O(1)—C(19)	1·400 (52)			

Br(1)—Te(1)—Br(2)	89·2 (1)		Br(1)—Te(1)—Br(3)	91·1 (1)
Br(2)—Te(1)—Br(3)	90·9 (1)		Br(1)—Te(1)—Br(4)	90·4 (1)
Br(2)—Te(1)—Br(4)	89·5 (1)		Br(3)—Te(1)—Br(4)	178·5 (1)
Br(1)—Te(1)—Br(5)	179·3 (1)		Br(2)—Te(1)—Br(5)	90·1 (1)
Br(3)—Te(1)—Br(5)	88·8 (1)		Br(4)—Te(1)—Br(5)	89·8 (1)
Br(1)—Te(1)—Br(6)	89·5 (1)		Br(2)—Te(1)—Br(6)	178·1 (1)
Br(3)—Te(1)—Br(6)	90·4 (1)		Br(4)—Te(1)—Br(6)	89·2 (1)
Br(5)—Te(1)—Br(6)	91·3 (1)		Se(1)—Te(2)—Se(2)	96·7 (1)
Te(2)—Se(1)—C(1)	101·8 (8)		Te(2)—Se(2)—C(2)	103·9 (7)
Br(7)—Te(3)—Br(8)	90·6 (1)		Br(7)—Te(3)—Br(9)	178·7 (1)
Br(8)—Te(3)—Br(9)	88·6 (1)		Br(7)—Te(3)—Br(10)	91·6 (1)
Br(8)—Te(3)—Br(10)	92·1 (1)		Br(9)—Te(3)—Br(10)	89·5 (1)
Br(7)—Te(3)—Br(11)	90·0 (1)		Br(8)—Te(3)—Br(11)	179·2 (1)
Br(9)—Te(3)—Br(11)	90·8 (1)		Br(10)—Te(3)—Br(11)	88·4 (1)
Br(7)—Te(3)—Br(12)	88·7 (1)		Br(8)—Te(3)—Br(12)	88·0 (1)
Br(9)—Te(3)—Br(12)	90·3 (1)		Br(10)—Te(3)—Br(12)	179·7 (1)
Br(11)—Te(3)—Br(12)	91·6 (1)		Se(3)—Te(4)—Se(4)	96·3 (1)
Te(4)—Se(3)—C(3)	101·2 (8)		Te(4)—Se(4)—C(4)	100·8 (7)
Se(1)—C(1)—N(1)	115·2 (17)		Se(1)—C(1)—N(2)	120·9 (21)
N(1)—C(1)—N(2)	123·9 (25)		Se(2)—C(2)—N(3)	120·3 (18)
Se(2)—C(2)—N(4)	117·9 (18)		N(3)—C(2)—N(4)	121·4 (24)
Se(3)—C(3)—N(5)	117·4 (21)		Se(3)—C(3)—N(6)	119·4 (18)
N(5)—C(3)—N(6)	122·9 (25)		Se(4)—C(4)—N(7)	120·9 (22)
Se(4)—C(4)—N(8)	121·1 (18)		N(7)—C(4)—N(8)	117·6 (27)
C(1)—N(1)—C(5)	120·5 (20)		C(1)—N(1)—C(6)	124·5 (24)
C(5)—N(1)—C(6)	115·0 (23)		C(2)—N(3)—C(7)	123·5 (22)
C(2)—N(3)—C(8)	123·9 (24)		C(7)—N(3)—C(8)	112·3 (22)
C(3)—N(5)—C(9)	120·2 (25)		C(3)—N(5)—C(10)	121·2 (24)
C(9)—N(5)—C(10)	118·2 (22)		C(4)—N(7)—C(11)	121·0 (26)
C(4)—N(7)—C(13)	120·3 (27)		C(11)—N(7)—C(12)	118·0 (24)
N(9)—C(13)—C(14)	175·1 (30)		N(10)—C(15)—C(16)	169·0 (37)
N(11)—C(17)—C(18)	172·3 (37)			

Discussion. Bond distances and bond angles are presented in Table 2. Fig. 1(*a,b*) presents stereoviews of portions of the structure.

(*a*) *N,N-Dimethylselenourea* (DMSeU). Each of the four independent molecules of DMSeU is approximately planar and coordinated through Se to Te^{II}. The largest average deviation from planarity, 0·072 Å, was found for [Se(3), C(3), N(5), N(6), C(9), C(10)], and the smallest, 0·007 Å, for [Se(1), C(1), N(1), N(2), C(5), C(6)]. Within the DMSeU units, the average bond distances are Se—C = 1·923 (14) Å, C—NH$_2$ = 1·336 (24) Å, C—N(CH$_3$)$_2$ = 1·283 (19) Å, N—CH$_3$ = 1·451 (13) Å. The long Se—C distance, with Se coordinated to Te^{II}, fits well with other reported values. In structures without such coordination such as *N*-phenyl-*N'*-benzoyl-selenourea (Hope, 1965), C—Se = 1·82 Å, and tris-

(acetylacetonato)cobalt(III)selenourea (Wright & Meyers, 1980), C—Se = 1·852 Å. In contrast, with tetramethylselenourea coordinated to Te^{II}, longer Se—C distances have been found: 1·872 Å by Foss, Maartman-Moe & Maroy (1986) and 1·924 Å by Eide, Foss, Maartman-Moe, Maberg & Scheie (1987). The C—N distances seem to be normal.

(*b*) Te^{IV} *and* Te^{II}. Sixfold, approximately octahedral coordination is frequently observed for Te^{IV} (Mangion, Zingaro & Meyers, 1975), with Te^{IV}—Br ≃2·70 Å, as in [TeBr$_6$]$^{2-}$. In the present structure, Te(1) and Te(3) are six coordinated, with average Te—Br = 2·707 Å. These bonds divide naturally into three classes: (1) long bonds with Br shared between Te^{IV} and Te^{II}, Te^{IV}—Br = 2·796 Å; (2) short bonds that are *trans* to these, Te^{IV}—Br = 2·636 (5) Å; and (3) the remaining pair of bonds that vary from Te(3)—Br(10) = 2·621 (4) Å to Te(1)—Br(4) = 2·747 (3) Å. Fourfold, approximately planar coordination is frequently observed for Te^{II} (Husebye, 1983, 1988) and in this structure Te(2) and Te(4) are each coordinated by two Se atoms and two Br atoms, arranged in planar *cis* configurations. The average distance Te^{II}—Se is equal to 2·496 (8) Å, which is slightly shorter than the sum of covalent radii, 2·51 Å, and Te^{II}···Br is equal to 3·24 (3) Å, which is much longer than the sum of covalent radii,

(*a*)

(*b*)

Fig. 1(*a*). Stereoview of (DMSeU)$_2$Te$_2$Br$_6$ complex coordinated by two molecules of CH$_3$CN. (Thermal ellipsoids at 0·50 probability.) (*b*) Stereoview of (DMSeU)$_2$Te$_2$Br$_6$ complex coordinated by one molecule of CH$_3$CN and one molecule of CH$_3$OH. (Thermal ellipsoids at 0·50 probability.)

2·51 Å, and much shorter than the sum of van der Waals radii, 4·15 Å (Pauling, 1960).

The structure of this entire group of atoms, namely $Se_2Te^{II}Br_2Te^{IV}Br_4$, is very similar to that found for the unit $Br_2Se^{II}Br_2Se^{IV}Br_4$ in $[(C_2H_5)_2N]_2Se_2Br_8$ (Hauge, Maroy & Odegard, 1988). In that structure, the terminal Se^{II}—Br bond lengths are 2·461 (2) and 2·427 (2) Å, while the bridging Se^{II}—Br bond lengths are 2·993 (2) and 3·010 Å; the bridging Se^{IV}—Br bond distances are 2·748 (2) and 2·720 (2) Å, the bonds *trans* to them are 2·459 (2) and 2·442 (2) Å and the third pair of Se^{IV}—Br bond distances is 2·522 (2) and 2·600 (2) Å. For Se and Br, the sum of the covalent radii is 2·31 Å and the sum of the van der Waals radii is 3·95 Å (Pauling, 1960). The dihedral angle between the $Se^{II}Br_4$ plane and the equatorial $Se^{IV}Br_4$ plane is 57°. The corresponding angles in the present structure are 58° for the planes that share Br(5) and Br(6), and 37° for the planes that share Br(11) and Br(12). The various DMSeU planes make dihedral angles with their Se_2-$Te^{II}Br_2$ planes that range from 68·0 to 71·4°.

(*c*) CH_3CN *and* CH_3OH. Four molecules of solvation were found in the structure, three CH_3CN and one CH_3OH. For CH_3CN, the average distances and angles are C—C = 1·10 (3) Å, C—N = 1·47 (2) Å and C—C—N = 173 (2)° and for CH_3OH, C—O = 1·40 (5) Å. All of these values appear to be normal. Each of the four solvent molecules has one close contact with one of the four available H atoms of the NH_2 groups of DMSeU. The N···H contacts from CH_3CN vary from 2·12 to 2·26 Å, while the angles

C—N···H vary from 99 to 139°. The contact O1···H8*Ea* = 1·99 Å and C19—O1···H8*Ea* = 128°. All of these distances are considerably shorter than van der Waals contacts, and may be hydrogen bonds. The angles N···H—N vary from 151 to 167° and N8—H8*Ea*···O1 = 150°, all values that deviate considerably from 180°.

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Structure of Bis(2,2'-bipyridine)dichlororhodium(III) Chloride Dihydrate

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Abstract. $[RhCl_2(C_{10}H_8N_2)_2]Cl.2H_2O$, $M_r = 557.7$, triclinic, $P\bar{1}$, $a = 12.9712 (5)$, $b = 12.402 (1)$, $c = 6.9998 (4)$ Å, $\alpha = 100.123 (5)$, $\beta = 93.607 (3)$, $\gamma = 90.668 (4)°$, $V = 1106.0 (1)$ Å^3, $Z = 2$, $D_x = 1.67$ Mg m^{-3}, Mo *Kα* radiation (graphite crystal monochromator), $\lambda = 0.71069$ Å, $\mu = 11.49$ cm^{-1}, $F(000) = 560$, $T = 293$ K. Final $R = 0.052$ for 3633 independent observed reflections and 325 variables.

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