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New aryltellurenyl iodides with uncommon valences: synthetic and structural characteristics of $[RTeTeI_2R]$, $[R_2TeTeR_2][Te_4I_{14}]$ and $[RTe(I)I_2]$ (R = 2,6-dimethoxyphenyl)

G. Manzoni de Oliveira[*], *Eliandro Faoro, E. Schulz Lang*[*]

Departamento de Química, Laboratório de Materiais Inorgânicos, Universidade Federal de Santa Maria, 97115-900 Santa Maria, RS, Brazil.

[*] Corresponding authors.
E-mail adresses: manzonideo@smail.ufsm.br; eslang@base.ufsm.br

Contents

Experimental Section

***Equipments*:** Elemental analyses were made by a Shimadzu EA 112 at the Universidade Federal de Santa Maria - Brazil. Infrared analyses were made by a Tensor 27 - Bruker.

***Preparation of* 1–3**: $(RTe)_2$ (R = 2,6-dimethoxyphenyl) 0.212 g, 0.4 mmol were dissolved in 5 mL of CH_2Cl_2 for **1**, 5 mL of toluene for **2** and 5 mL of CH_2Cl_2 for **3**. Resublimed iodine (0.102 g, 0.4 mmol for **1**; 0.223 g, 0.9 mmol for **2**; 0.102 g, 0.4 mmol for **3**) was added. **1**: after 2 h stirring at −10 ºC the mixture was kept at −18 ºC under Ar for recrystallization of black crystals {**1** is also obtained with good yield through the iodine transfer reaction between 2 mesTeI and $(RTe)_2$}. **2**: after 14 h stirring at RT a red precipitate was isolated by filtration, dissolved in a mixture 1:1 of CH_2Cl_2/acetone and black crystals were obtained at −18 ºC under Ar. **3**: the mixture was refluxed under stirring by 3 h and the red color turned brown (formation of RTeI). Resublimed I_2 (0.204 g, 0.8 mmol) was added. After 1 h stirring the solid was filtrated and dissolved in a mixture 2:1 of CH_2Cl_2/acetone which yielded red crystals at −18 ºC under Ar. Yields: 304 mg, 0.39 mmol of **1** (97 %, m.p. 155 ºC); 239 mg, 0.08 mmol of **2** (55 %, m.p. 86 ºC); 492 mg, 0.76 mmol of **3** (95 %, m.p. 137 ºC).

Analytical data:

Compound 1: IR (KBr): 3059 [ν(C–H)$_{Ar.}$], 2932 [ν_{as}(C–H)$_{Me}$], 2831 [ν_{s}(C–H)$_{Me}$], 1587 [ν(C=C)], 1473 [δ_{s}(C=C–H)], 1255 [ν_{as}(C–O)], 1105 [δ_{as}(C–O–C)], 767, 731 [$\delta_{o.p.}$(C=C–H)]. Elemental analysis (%) calcd for $C_{16}H_{18}I_2O_4Te_2$ (783.30 g mol^{-1}): C 24.53, H 2.32; found: C 24.44, H 2.35.

Compound 2: IR (KBr): 3005 [ν(C–H)$_{Ar.}$], 2931 [ν_{as}(C–H)$_{Me}$], 2828 [ν_{s}(C–H)$_{Me}$], 1587 [ν(C=C)], 1472 [δ_{s}(C=C–H)], 1256 [ν_{as}(C–O)], 1102 [δ_{as}(C–O–C)], 766, 740 [$\delta_{o.p.}$(C=C–H)]. Elemental analysis (%) calcd for $C_{32}H_{36}I_{14}O_8Te_6$ (3090.81 g mol^{-1}): C 12.43, H 1.17; found: C 12.38, H 1.21. This reaction gives as subproduct red crystals of the already described compound RTe(I_2)R.[12b]

Compound 3: IR (KBr): 3003 [ν(C–H)$_{Ar.}$], 2931 [ν_{as}(C–H)$_{Me.}$], 2825 [ν_{s}(C–H)$_{Me.}$], 1587 [ν(C=C)], 1472 [δ_{s}(C=C–H)], 1255 [ν_{as}(C–O)], 1105 [δ_{as}(C–O–C)], 766, 741 [$\delta_{o.p.}$(C=C–H)]. Elemental analysis (%) calcd for $C_8H_9I_3O_2Te1$ (645.45 g mol^{-1}): C 14.89, H 1.41; found: C 14.71, H 1.49.

X-ray crystallographic data

Crystallographic measurements were made on a Bruker Kappa Apex II CCD area-detector diffractometer with graphite monochromatized Mo Kα radiation (λ = 0.71073 Å). The structures were solved by direct methods (SHELXS-97)[*] and additional atoms were located in the difference Fourier map and refined on F^2 (SHELXL-97)[*]. Metal atoms were refined anisotropically; carbon atoms were refined isotropically and hydrogen atoms as riding atoms at geometrically defined positions with isotropic thermal parameters 20% larger than their parent atoms.

[*] Sheldrick, G. M. *Acta Cryst*. **2008**, *A64*, 112–122.

Crystal data for **1**:

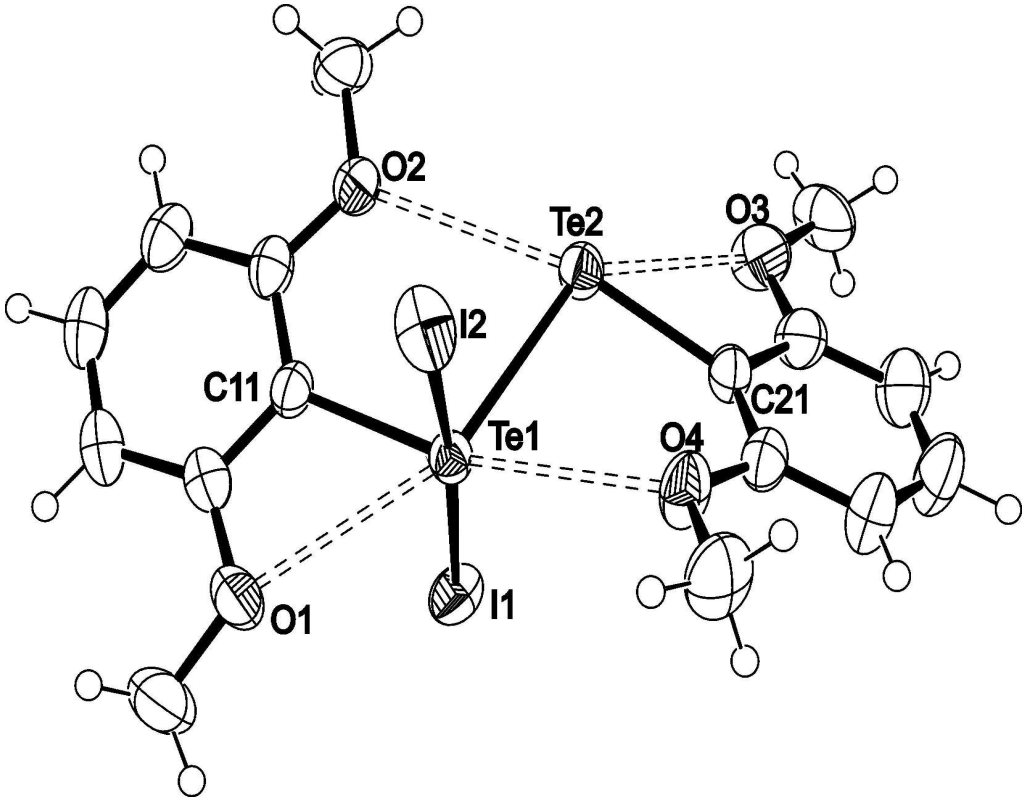

Figure 1. ORTEP projection for the molecular structure of **1**.

Table 1. Crystal data and structure refinement for **1**.

Empirical formula	C16 H18 I2 O4 Te2	
Formula weight	783.30	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.4629(5) Å	α= 66.165(3)°.
	b = 10.7699(7) Å	β= 78.888(3)°.
	c = 11.9210(7) Å	γ = 81.055(3)°.
Volume	1086.39(11) $Å^3$	
Z	2	
Density (calculated)	2.395 Mg/m^3	
Absorption coefficient	5.542 mm^{-1}	
F(000)	712	
Crystal size	0.193 x 0.171 x 0.132 mm^3	
Theta range for data collection	1.89 to 29.99°.	
Index ranges	-13<=h<=12, -14<=k<=15, -16<=l<=16	
Reflections collected	22343	
Independent reflections	6234 [R(int) = 0.0343]	
Completeness to theta = 29.99°	98.1 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.746 and 0.638	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6234 / 0 / 218	
Goodness-of-fit on F^2	1.099	
Final R indices [I>2sigma(I)]	R1 = 0.0336, wR2 = 0.0808	
R indices (all data)	R1 = 0.0535, wR2 = 0.1085	
Extinction coefficient	0.0041(3)	
Largest diff. peak and hole	1.584 and -1.039 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Te(1)	2066(1)	6969(1)	2067(1)	32(1)
Te(2)	837(1)	9588(1)	1627(1)	38(1)
I(2)	509(1)	6548(1)	375(1)	54(1)
I(1)	3836(1)	7070(1)	3843(1)	48(1)
O(2)	3004(4)	9564(4)	-438(3)	46(1)
O(1)	4599(4)	5091(4)	1873(4)	50(1)
C(11)	3907(5)	7337(5)	698(4)	35(1)
C(16)	4103(5)	8565(5)	-315(5)	38(1)
C(12)	4953(5)	6241(5)	881(5)	40(1)
C(21)	-602(5)	9072(5)	3323(5)	37(1)
C(26)	-1278(5)	7864(6)	3926(5)	42(1)
C(22)	-1003(6)	10146(6)	3731(5)	47(1)
O(4)	-829(4)	6891(4)	3446(4)	51(1)
O(3)	-314(5)	11294(4)	3034(4)	59(1)
C(15)	5400(6)	8705(6)	-1134(5)	48(1)
C(13)	6235(6)	6377(6)	61(6)	50(1)
C(14)	6433(6)	7603(7)	-914(6)	55(2)
C(25)	-2315(7)	7687(7)	4956(6)	60(2)
C(23)	-2051(8)	9993(7)	4752(6)	65(2)
C(24)	-2684(7)	8758(8)	5355(6)	73(2)
C(18)	3197(6)	10904(6)	-1397(5)	50(1)
C(17)	5728(7)	4043(6)	2265(7)	67(2)
C(27)	-672(8)	12469(6)	3356(7)	65(2)
C(28)	-1567(8)	5680(7)	3948(7)	71(2)

Table 3. Bond lengths [Å] and angles [°] for **1**.

Te(1)-C(11)	2.110(4)
Te(1)-Te(2)	2.7572(4)
Te(1)-I(2)	2.9220(5)
Te(1)-I(1)	2.9845(5)
Te(2)-C(21)	2.126(5)
O(2)-C(16)	1.358(6)
O(2)-C(18)	1.446(6)
O(1)-C(12)	1.355(7)
O(1)-C(17)	1.423(7)
C(11)-C(12)	1.391(7)
C(11)-C(16)	1.393(7)
C(16)-C(15)	1.400(7)
C(12)-C(13)	1.390(7)
C(21)-C(26)	1.395(7)
C(21)-C(22)	1.402(7)
C(26)-O(4)	1.363(6)
C(26)-C(25)	1.383(7)
C(22)-O(3)	1.362(7)
C(22)-C(23)	1.384(8)
O(4)-C(28)	1.428(7)
O(3)-C(27)	1.440(6)
C(15)-C(14)	1.385(8)
C(13)-C(14)	1.372(9)
C(25)-C(24)	1.391(9)
C(23)-C(24)	1.397(10)
C(11)-Te(1)-Te(2)	101.02(13)
C(11)-Te(1)-I(2)	89.13(13)
Te(2)-Te(1)-I(2)	94.786(14)
C(11)-Te(1)-I(1)	89.18(13)
Te(2)-Te(1)-I(1)	92.050(14)
I(2)-Te(1)-I(1)	173.153(15)
C(21)-Te(2)-Te(1)	95.54(13)
C(16)-O(2)-C(18)	119.6(4)
C(12)-O(1)-C(17)	117.3(5)
C(12)-C(11)-C(16)	121.1(4)
C(12)-C(11)-Te(1)	114.5(4)
C(16)-C(11)-Te(1)	124.4(4)
O(2)-C(16)-C(11)	117.0(4)
O(2)-C(16)-C(15)	124.0(5)
C(11)-C(16)-C(15)	119.1(5)
O(1)-C(12)-C(13)	125.2(5)
O(1)-C(12)-C(11)	115.0(4)
C(13)-C(12)-C(11)	119.7(5)
C(26)-C(21)-C(22)	120.2(5)
C(26)-C(21)-Te(2)	125.3(4)
C(22)-C(21)-Te(2)	113.9(4)
O(4)-C(26)-C(25)	123.5(5)
O(4)-C(26)-C(21)	115.7(4)
C(25)-C(26)-C(21)	120.8(5)
O(3)-C(22)-C(23)	125.5(5)
O(3)-C(22)-C(21)	114.7(5)
C(23)-C(22)-C(21)	119.8(6)
C(26)-O(4)-C(28)	118.5(4)
C(22)-O(3)-C(27)	119.2(5)
C(14)-C(15)-C(16)	118.5(6)
C(14)-C(13)-C(12)	118.6(5)
C(13)-C(14)-C(15)	123.0(5)

C(26)-C(25)-C(24)	118.0(6)
C(22)-C(23)-C(24)	118.7(6)
C(25)-C(24)-C(23)	122.5(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Te(1)	29(1)	30(1)	35(1)	-12(1)	0(1)	-4(1)
Te(2)	38(1)	30(1)	42(1)	-14(1)	3(1)	-4(1)
I(2)	45(1)	66(1)	69(1)	-44(1)	-14(1)	-1(1)
I(1)	47(1)	59(1)	37(1)	-16(1)	-5(1)	-13(1)
O(2)	37(2)	42(2)	43(2)	-5(2)	9(2)	-5(2)
O(1)	43(2)	42(2)	60(3)	-19(2)	-6(2)	7(2)
C(11)	29(2)	42(3)	31(2)	-14(2)	2(2)	-5(2)
C(16)	29(2)	51(3)	38(3)	-22(2)	0(2)	-8(2)
C(12)	33(2)	45(3)	47(3)	-25(2)	-8(2)	1(2)
C(21)	34(2)	42(3)	35(3)	-18(2)	0(2)	0(2)
C(26)	34(3)	49(3)	40(3)	-18(2)	1(2)	-6(2)
C(22)	56(3)	47(3)	40(3)	-22(2)	-4(3)	2(3)
O(4)	45(2)	46(2)	63(3)	-24(2)	16(2)	-20(2)
O(3)	83(3)	42(2)	55(3)	-28(2)	-4(2)	-2(2)
C(15)	38(3)	64(4)	42(3)	-21(3)	4(2)	-15(3)
C(13)	34(3)	62(4)	62(4)	-38(3)	0(3)	2(2)
C(14)	35(3)	78(4)	58(4)	-40(4)	10(3)	-8(3)
C(25)	51(3)	72(4)	54(4)	-29(3)	15(3)	-17(3)
C(23)	73(4)	73(4)	58(4)	-43(4)	4(3)	4(4)
C(24)	66(4)	97(6)	48(4)	-33(4)	19(3)	-8(4)
C(18)	46(3)	47(3)	46(3)	-6(3)	-3(3)	-10(2)
C(17)	60(4)	51(4)	78(5)	-15(3)	-18(4)	12(3)
C(27)	87(5)	51(3)	68(4)	-38(3)	-19(4)	18(3)
C(28)	65(4)	57(4)	82(5)	-22(4)	14(4)	-27(3)

Crystal data for **2**:

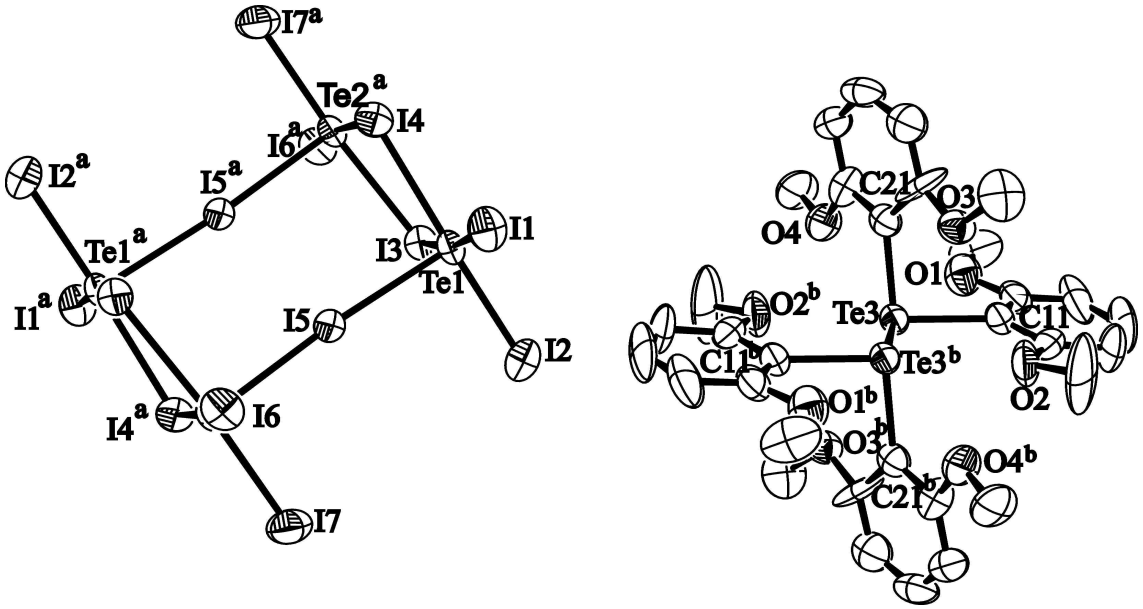

Figure 2. ORTEP projection for the molecular structure of **2**. The hydrogen atoms were omitted. Symmetry operations to generate the equivalent atoms: (*a*) 1–*x*, 1–*y*, 1–*z*; (*b*) 3–*x*, –*y*, –*z*.

Table 1. Crystal data and structure refinement for **2**.

Empirical formula	C32 H36 I14 O8 Te6	
Formula weight	3090.81	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.3543(7) Å	α= 64.698(3)°.
	b = 12.7746(7) Å	β= 70.118(3)°.
	c = 14.2133(9) Å	γ = 81.693(4)°.
Volume	1598.36(17) $Å^3$	
Z	1	
Density (calculated)	3.211 Mg/m^3	
Absorption coefficient	9.499 mm^{-1}	
F(000)	1346	
Crystal size	0.141 x 0.114 x 0.094 mm^3	
Theta range for data collection	1.67 to 28.16°.	
Index ranges	-13<=h<=10, -16<=k<=16, -18<=l<=18	
Reflections collected	22983	
Independent reflections	7408 [R(int) = 0.0509]	
Completeness to theta = 28.16°	94.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7041 and 0.5133	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7408 / 0 / 272	
Goodness-of-fit on F^2	0.983	
Final R indices [I>2sigma(I)]	R1 = 0.0554, wR2 = 0.1313	
R indices (all data)	R1 = 0.1215, wR2 = 0.1833	
Extinction coefficient	0.00084(14)	
Largest diff. peak and hole	2.668 and -1.523 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(21)	15968(13)	0(12)	1490(10)	45(3)
C(11)	17805(14)	264(12)	-871(11)	49(3)
O(3)	16279(10)	-1745(8)	1321(7)	51(2)
O(4)	15791(11)	1868(9)	1461(8)	66(3)
O(1)	18372(10)	1682(9)	-470(8)	69(3)
O(2)	16970(11)	-1142(11)	-1141(10)	79(4)
C(25)	15827(14)	199(13)	3137(11)	53(4)
C(22)	16189(15)	-1304(18)	2005(10)	80(7)
C(26)	15852(15)	682(12)	2064(11)	52(4)
C(24)	15972(15)	-987(15)	3588(12)	65(5)
C(23)	16176(16)	-1686(15)	3009(13)	67(5)
C(16)	18096(16)	-508(15)	-1355(11)	60(4)
C(12)	18846(16)	947(14)	-1000(12)	60(4)
C(13)	20158(18)	836(15)	-1575(16)	87(6)
C(15)	19402(18)	-630(19)	-1956(14)	93(6)
C(14)	20366(18)	46(18)	-2038(16)	94(7)
C(27)	16679(18)	-2936(13)	1692(14)	80(5)
C(28)	15954(19)	2603(14)	1914(13)	77(5)
C(17)	19382(19)	2372(16)	-506(13)	89(6)
C(18)	17363(19)	-2160(20)	-1390(20)	164(13)
I(5)	5340(1)	4036(1)	3986(1)	42(1)
Te(1)	8213(1)	3375(1)	4101(1)	43(1)
Te(3)	15838(1)	861(1)	-101(1)	42(1)
I(3)	8785(1)	5841(1)	3836(1)	51(1)
Te(2)	2502(1)	4662(1)	3717(1)	43(1)
I(4)	7310(1)	2796(1)	6583(1)	54(1)
I(6)	1896(1)	2347(1)	4257(1)	62(1)
I(1)	7961(1)	1030(1)	4596(1)	65(1)
I(2)	9229(1)	4143(1)	1789(1)	70(1)
I(7)	3560(1)	5349(1)	1425(1)	76(1)

Table 3. Bond lengths [Å] and angles [°] for **2**.

C(21)-C(26)	1.397(17)
C(21)-C(22)	1.52(2)
C(21)-Te(3)	2.093(13)
C(11)-C(16)	1.375(19)
C(11)-C(12)	1.40(2)
C(11)-Te(3)	2.162(13)
O(3)-C(22)	1.288(15)
O(3)-C(27)	1.430(17)
O(4)-C(26)	1.391(17)
O(4)-C(28)	1.400(16)
O(1)-C(12)	1.382(17)
O(1)-C(17)	1.437(17)
O(2)-C(16)	1.388(18)
O(2)-C(18)	1.459(19)
C(25)-C(26)	1.372(18)
C(25)-C(24)	1.38(2)
C(22)-C(23)	1.29(2)
C(24)-C(23)	1.41(2)
C(16)-C(15)	1.36(2)
C(12)-C(13)	1.35(2)
C(13)-C(14)	1.38(3)
C(15)-C(14)	1.36(3)
I(5)-Te(1)	3.0121(13)
I(5)-Te(2)	3.0412(13)
Te(1)-I(1)	2.7984(12)
Te(1)-I(2)	2.8382(14)
Te(1)-I(4)	3.0971(13)
Te(1)-I(3)	3.1295(12)
Te(3)-Te(3)#1	2.8559(16)
I(3)-Te(2)#2	3.0779(12)
Te(2)-I(7)	2.8266(14)
Te(2)-I(6)	2.8282(12)
Te(2)-I(3)#2	3.0779(12)
Te(2)-I(4)#2	3.1153(12)
I(4)-Te(2)#2	3.1153(12)
C(26)-C(21)-C(22)	121.1(12)
C(26)-C(21)-Te(3)	116.6(10)
C(22)-C(21)-Te(3)	122.3(9)
C(16)-C(11)-C(12)	120.4(13)
C(16)-C(11)-Te(3)	129.5(11)
C(12)-C(11)-Te(3)	109.2(10)
C(22)-O(3)-C(27)	112.8(14)
C(26)-O(4)-C(28)	117.5(12)
C(12)-O(1)-C(17)	116.8(13)
C(16)-O(2)-C(18)	112.6(12)
C(26)-C(25)-C(24)	115.6(13)
O(3)-C(22)-C(23)	137(2)
O(3)-C(22)-C(21)	109.9(13)
C(23)-C(22)-C(21)	113.3(15)
C(25)-C(26)-O(4)	123.5(12)
C(25)-C(26)-C(21)	121.5(13)
O(4)-C(26)-C(21)	115.0(12)
C(25)-C(24)-C(23)	124.0(14)
C(22)-C(23)-C(24)	124.3(18)
C(15)-C(16)-C(11)	120.6(16)
C(15)-C(16)-O(2)	125.2(16)
C(11)-C(16)-O(2)	114.2(12)

C(13)-C(12)-O(1)	126.5(16)
C(13)-C(12)-C(11)	120.7(16)
O(1)-C(12)-C(11)	112.8(13)
C(12)-C(13)-C(14)	115.4(18)
C(14)-C(15)-C(16)	116.0(18)
C(15)-C(14)-C(13)	126.9(16)
Te(1)-I(5)-Te(2)	175.65(4)
I(1)-Te(1)-I(2)	97.04(4)
I(1)-Te(1)-I(5)	95.79(4)
I(2)-Te(1)-I(5)	90.32(4)
I(1)-Te(1)-I(4)	89.35(4)
I(2)-Te(1)-I(4)	172.72(4)
I(5)-Te(1)-I(4)	92.51(3)
I(1)-Te(1)-I(3)	170.02(5)
I(2)-Te(1)-I(3)	89.12(4)
I(5)-Te(1)-I(3)	92.01(3)
I(4)-Te(1)-I(3)	84.08(3)
C(21)-Te(3)-C(11)	95.1(5)
C(21)-Te(3)-Te(3)#1	94.9(4)
C(11)-Te(3)-Te(3)#1	97.9(4)
Te(2)#2-I(3)-Te(1)	95.19(3)
I(7)-Te(2)-I(6)	96.79(4)
I(7)-Te(2)-I(5)	92.23(4)
I(6)-Te(2)-I(5)	92.84(4)
I(7)-Te(2)-I(3)#2	174.21(4)
I(6)-Te(2)-I(3)#2	87.76(4)
I(5)-Te(2)-I(3)#2	91.11(3)
I(7)-Te(2)-I(4)#2	90.45(4)
I(6)-Te(2)-I(4)#2	170.29(4)
I(5)-Te(2)-I(4)#2	93.35(3)
I(3)#2-Te(2)-I(4)#2	84.64(3)
Te(1)-I(4)-Te(2)#2	95.09(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1 #2 -x+3,-y,-z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(21)	35(8)	46(8)	45(8)	-10(7)	-10(6)	-5(6)
C(11)	37(8)	58(9)	47(8)	-19(7)	-15(7)	11(7)
O(3)	62(7)	39(5)	53(6)	-16(5)	-24(5)	4(5)
O(4)	81(8)	65(7)	70(7)	-46(6)	-29(6)	17(6)
O(1)	53(7)	70(7)	74(7)	-25(6)	-9(6)	-7(6)
O(2)	51(7)	114(10)	108(9)	-85(8)	-30(7)	36(7)
C(25)	52(9)	64(10)	44(9)	-19(8)	-13(7)	-12(8)
C(22)	51(10)	171(19)	24(7)	-45(10)	14(7)	-72(11)
C(26)	52(9)	48(9)	54(9)	-26(8)	1(7)	-16(7)
C(24)	48(10)	89(13)	45(9)	-5(9)	-22(7)	-17(9)
C(23)	53(10)	72(11)	62(11)	-14(9)	-13(8)	-9(9)
C(16)	47(9)	93(12)	41(8)	-32(8)	-11(7)	6(9)
C(12)	47(10)	63(10)	52(9)	-10(8)	-18(8)	16(8)
C(13)	53(12)	63(11)	106(15)	-11(11)	-18(11)	23(9)
C(15)	52(11)	130(18)	71(12)	-47(12)	12(10)	24(12)
C(14)	30(10)	96(15)	104(15)	-27(12)	24(10)	3(10)
C(27)	88(14)	41(9)	101(13)	-23(9)	-20(11)	-11(9)
C(28)	102(14)	79(12)	81(12)	-56(10)	-38(11)	8(11)
C(17)	100(15)	94(14)	69(11)	-21(10)	-16(10)	-54(12)
C(18)	71(14)	250(30)	310(30)	-260(30)	-39(19)	36(17)
I(5)	44(1)	37(1)	45(1)	-18(1)	-11(1)	-1(1)
Te(1)	34(1)	43(1)	58(1)	-25(1)	-16(1)	6(1)
Te(3)	37(1)	46(1)	47(1)	-23(1)	-16(1)	7(1)
I(3)	49(1)	45(1)	57(1)	-20(1)	-14(1)	-2(1)
Te(2)	36(1)	44(1)	55(1)	-23(1)	-19(1)	7(1)
I(4)	62(1)	43(1)	58(1)	-18(1)	-22(1)	-1(1)
I(6)	66(1)	51(1)	81(1)	-32(1)	-30(1)	-4(1)
I(1)	67(1)	47(1)	86(1)	-35(1)	-22(1)	4(1)
I(2)	64(1)	77(1)	63(1)	-36(1)	-2(1)	-4(1)
I(7)	98(1)	75(1)	56(1)	-24(1)	-33(1)	9(1)

Crystal data for **3:**

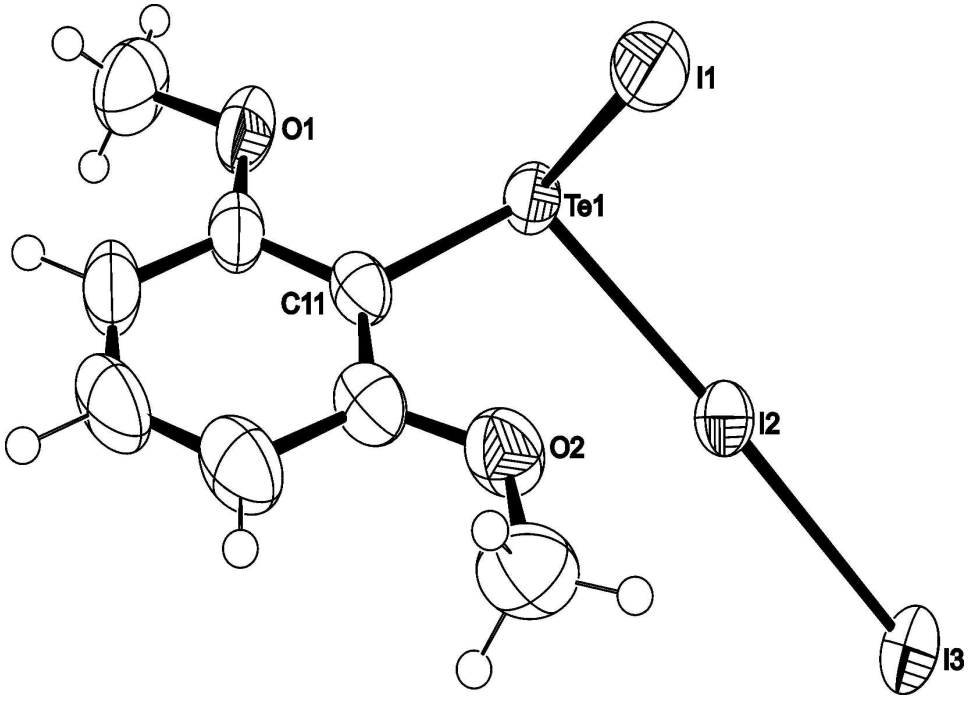

Figure 3. ORTEP projection for the molecular structure of **3**.

Table 1. Crystal data and structure refinement for **3**.

Empirical formula	C8 H9 I3 O2 Te	
Formula weight	645.45	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.110(5) Å	α= 73.550(5)°.
	b = 9.529(5) Å	β= 80.002(5)°.
	c = 9.681(5) Å	γ = 62.359(5)°.
Volume	713.1(7) $Å^3$	
Z	2	
Density (calculated)	3.006 Mg/m^3	
Absorption coefficient	8.557 mm^{-1}	
F(000)	568	
Crystal size	0.183 x 0.092 x 0.06 mm^3	
Theta range for data collection	2.20 to 28.77°.	
Index ranges	-12<=h<=12, -12<=k<=12, -12<=l<=13	
Reflections collected	13277	
Independent reflections	3676 [R(int) = 0.0342]	
Completeness to theta = 28.77°	99.1 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3676 / 0 / 127	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0336, wR2 = 0.0710	
R indices (all data)	R1 = 0.0517, wR2 = 0.0800	
Largest diff. peak and hole	1.045 and -1.236 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(2)	4565(1)	7043(1)	5333(1)	42(1)
Te(1)	5803(1)	6046(1)	8104(1)	42(1)
I(3)	3172(1)	7630(1)	2414(1)	51(1)
I(1)	5189(1)	9100(1)	8311(1)	64(1)
O(2)	8107(5)	7237(5)	5740(5)	58(1)
O(1)	8414(5)	3366(5)	10049(5)	57(1)
C(13)	11004(8)	3400(8)	8877(8)	65(2)
C(12)	9287(7)	3965(7)	8968(7)	48(1)
C(11)	8378(6)	5251(7)	7877(6)	41(1)
C(15)	10841(8)	5424(9)	6644(8)	66(2)
C(16)	9120(7)	5990(7)	6712(7)	48(1)
C(18)	8780(9)	8126(9)	4615(7)	73(2)
C(14)	11731(8)	4135(10)	7718(9)	74(2)
C(17)	9284(9)	1934(8)	11094(8)	79(2)

Table 3. Bond lengths [Å] and angles [°] for **3**.

I(2)-Te(1)	2.8255(14)
I(2)-I(3)	3.0980(15)
Te(1)-C(11)	2.096(5)
Te(1)-I(1)	2.7574(16)
O(2)-C(16)	1.342(7)
O(2)-C(18)	1.417(7)
O(1)-C(12)	1.360(7)
O(1)-C(17)	1.417(7)
C(13)-C(14)	1.384(10)
C(13)-C(12)	1.393(8)
C(12)-C(11)	1.390(8)
C(11)-C(16)	1.397(8)
C(15)-C(14)	1.376(10)
C(15)-C(16)	1.397(8)
Te(1)-I(2)-I(3)	171.153(18)
C(11)-Te(1)-I(1)	93.14(14)
C(11)-Te(1)-I(2)	108.50(15)
I(1)-Te(1)-I(2)	96.25(2)
C(16)-O(2)-C(18)	119.0(5)
C(12)-O(1)-C(17)	119.1(5)
C(14)-C(13)-C(12)	119.2(6)
O(1)-C(12)-C(11)	116.7(5)
O(1)-C(12)-C(13)	125.3(6)
C(11)-C(12)-C(13)	118.0(6)
C(12)-C(11)-C(16)	122.5(5)
C(12)-C(11)-Te(1)	115.7(4)
C(16)-C(11)-Te(1)	121.8(4)
C(14)-C(15)-C(16)	118.2(7)
O(2)-C(16)-C(15)	124.3(6)
O(2)-C(16)-C(11)	116.9(5)
C(15)-C(16)-C(11)	118.8(6)
C(15)-C(14)-C(13)	123.3(6)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(2)	42(1)	34(1)	49(1)	-6(1)	-7(1)	-15(1)
Te(1)	36(1)	43(1)	40(1)	-2(1)	-6(1)	-15(1)
I(3)	56(1)	39(1)	59(1)	2(1)	-23(1)	-22(1)
I(1)	79(1)	44(1)	63(1)	-20(1)	-18(1)	-11(1)
O(2)	48(2)	59(3)	62(3)	-10(2)	5(2)	-24(2)
O(1)	56(2)	46(3)	57(3)	0(2)	-23(2)	-13(2)
C(13)	43(3)	62(4)	78(5)	-25(4)	-25(3)	0(3)
C(12)	39(3)	43(3)	59(4)	-18(3)	-17(3)	-6(3)
C(11)	32(3)	45(3)	53(3)	-21(3)	-4(2)	-15(2)
C(15)	44(4)	77(5)	85(5)	-32(4)	3(3)	-29(3)
C(16)	40(3)	52(4)	62(4)	-24(3)	-2(3)	-23(3)
C(18)	77(5)	74(5)	67(5)	-7(4)	14(4)	-41(4)
C(14)	31(3)	104(6)	98(6)	-55(5)	-2(4)	-23(4)
C(17)	89(5)	52(4)	72(5)	3(4)	-26(4)	-15(4)