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Crystallographic Details

Data Collection

A colorless prismatic crystal of $C_{31}H_{22}O_2Te$ having approximate dimensions of 0.60 x 0.50 x 0.30 mm was mounted on a glass fiber. All measurements were made on an Enraf-Nonius CAD4-FR diffractometer with graphite monochromated Mo-KALPHA radiation. Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 25 carefully centered reflections in the range 12.00 < 2THETA < 21.00° corresponded to a primitive triclinic cell with dimensions:

a = 10.590(2) Å	ALPHA = 85.54(1)°
b = 10.910(2) Å	BETA = 78.76(1)°
c = 11.843(1) Å	GAMMA = 64.35(1)
V = 1209.8(3) Å^3	

For Z = 2 and F.W. = 554.11, the calculated density is 1.52 g/cm^3. Based on a statistical analysis of intensity distribution,and the successful solution and refinement of thestructure, the space group was determined to be:

$P\bar{1}$ (#2)

The data were collected at a temperature of 296 ± 1 K using the OMEGA-2THETA scan technique to a maximum 2THETA value of 49.9°.Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.27° with a take-off angle of 2.8°. Scans of (0.80 + 0.52 tan THETA)° were made at a speed of 2.0-20.0°/min (in omega). Moving-crystal moving counter background measurements were made by scanning an additional 25 above and below the scan range. The counter aperture consisted of a variable horizontal slit with a width ranging from 2.5 to 2.7 mm and a vertical slit set to 4.0 mm. The diameter of the incident beam collimator was 0.8 mm and the crystal to detector distance was 21 cm. For intense reflections an attenuator was automatically inserted in front of the detector.

Data Reduction

A total of 4492 reflections was collected. The intensities of three representative reflection were measured after every 120 minutes of X-ray exposure time. Over the course of data collection, the standards decreased by 1.0%. A linear correction factor was applied to the data to account for this phenomenon.

The linear absorption coefficient, MU, for Mo-KALPHA radiation is 12.6 cm^{-1}. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.84 to 1.00. The data were corrected for Lorentz and polarization effects. A correction for secondary extinction was applied (coefficient = 3.15050e-07).

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[3] was based on 4155 observed reflections (I > 3.00sigma(I)) and 308 variable parameters and converged (largest parameter shift was 0.02 times its esd) with unweighted and weighted agreement factors of:

$$R = \text{SIGMA } ||Fo| - |Fc|| \ / \ \text{SIGMA } |Fo| = 0.025$$

$$R_w = [(\text{SIGMA } w \ (|Fo| - |Fc|)^2 \ / \ \text{SIGMA } w \ Fo^2)]^{1/2} = 0.029$$

The standard deviation of an observation of unit weight[4] was 4.25. The weighting scheme was based on counting statistics. Plots of SIGMA w $(|Fo| - |Fc|)^2$ versus |Fo|,reflection order in data collection, sin THETA/LAMBDA and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.78 and -0.47 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for DELTAf' and DELTAf" were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the teXsan[9] crystallographic software package of

References

(1) SIR92: Altomare, A., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., Polidori, G. (1994). J. Appl. Cryst., in preparation.

(2) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least-Squares:

Function minimized: $Sw(|F_o|-|F_c|)^2$ where

$w = 1/[sigma^2(Fo)] = [sigma^2_c(Fo) + p^2Fo^2/4]^{-1}$

$sigma_c(Fo)$ = e.s.d. based on counting statistics

p = p-factor

(4) Standard deviation of an observation of unit weight:

$[Sw(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations

N_v = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{31}H_{22}O_2Te$
Formula Weight	554.11
Crystal Color, Habit	colorless, prismatic
Crystal Dimensions	0.60 X 0.50 X 0.30 mm
Crystal System	triclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2THETA range)	25 (12.0 - 21.0°)
Omega Scan Peak Width at Half-height	0.27°
Lattice Parameters	a = 10.590(2)Å
	b = 10.910(2) Å
	c = 11.843(1) Å
	ALPHA = 85.54(1)°
	BETA = 78.76(1)°
	GAMMA = 64.35(1)°
	V = 1209.8(3) $Å^3$
Space Group	$P\bar{1}$ (#2)
Z value	2
D_{calc}	1.521 g/cm^3
F_{000}	552.00
MU(MoKALPHA)	12.56 cm^{-1}

B. Intensity Measurements

Diffractometer	Enraf-Nonius CAD4-FR
Radiation	MoKALPHA (LAMBDA = 0.71069 Å)
	graphite monochromated
Attenuator	Zr foil (factor = 13.40)
Take-off Angle	2.8°

Detector Aperture	2.5 - 2.7 mm horizontal
	4.0 mm vertical
Crystal to Detector Distance	21 mm
Temperature	296.0 K
Scan Type	OMEGA-2THETA
Scan Rate	2.0-20.0°/min (in OMEGA)
Scan Width	(0.80 + 0.52 tan THETA)°
$2THETA_{max}$	49.9°
No. of Reflections Measured	Total: 4492
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.84 - 1.00)
	Decay (1.0% decrease)
	Secondary Extinction
	(coefficient: 3.15050e-07)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	SIGMA w $(\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$1/^2$sigma(Fo) = $4Fo^2/sigma^2(Fo^2)$
p-factor	0.0000
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00sigma(I))	4155
No. Variables	308
Reflection/Parameter Ratio	13.49
Residuals: R; Rw	0.025 ; 0.029
Goodness of Fit Indicator	4.25
Max Shift/Error in Final Cycle	0.02
Maximum peak in Final Diff. Map	0.78 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.47 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Te(1)	0.22548(2)	0.44537(2)	0.83573(2)	2.884(5)
O(1)	0.3906(3)	0.2240(3)	0.7437(2)	4.57(6)
O(2)	0.5594(3)	0.2601(3)	0.7980(2)	4.71(7)
C(1)	0.0382(4)	0.6297(3)	0.8769(3)	3.19(7)
C(2)	0.0290(4)	0.7520(4)	0.9124(3)	4.08(8)
C(3)	-0.1027(5)	0.8635(4)	0.9346(4)	5.2(1)
C(4)	-0.2250(5)	0.8518(4)	0.9241(4)	5.4(1)
C(5)	-0.2173(4)	0.7296(4)	0.8921(3)	4.60(9)
C(6)	-0.0861(4)	0.6175(4)	0.8684(3)	3.36(7)
C(7)	-0.0665(4)	0.4824(4)	0.8359(3)	3.30(7)
C(8)	-0.1775(4)	0.4453(4)	0.8332(3)	4.15(9)
C(9)	-0.1491(4)	0.3150(5)	0.8050(3)	4.55(10)
C(10)	-0.0115(4)	0.2184(4)	0.7759(4)	4.61(10)
C(11)	0.1021(4)	0.2507(4)	0.7773(3)	3.87(8)
C(12)	0.0731(3)	0.3802(3)	0.8085(3)	3.11(7)
C(13)	0.2737(3)	0.5157(3)	0.6669(3)	3.18(7)
C(14)	0.2460(4)	0.4613(4)	0.5779(3)	4.20(9)
C(15)	0.2667(5)	0.5099(5)	0.4660(3)	5.2(1)
C(16)	0.3161(5)	0.6081(5)	0.4455(3)	5.3(1)
C(17)	0.3443(4)	0.6607(4)	0.5343(3)	4.49(9)
C(18)	0.3238(4)	0.6158(3)	0.6486(3)	3.33(7)
C(19)	0.3525(4)	0.6793(3)	0.7413(3)	3.25(7)
C(20)	0.4234(3)	0.6009(3)	0.8279(3)	3.17(7)
C(21)	0.4377(4)	0.6639(4)	0.9193(3)	3.74(8)
C(22)	0.3874(5)	0.8033(4)	0.9226(4)	4.60(9)
C(23)	0.3243(5)	0.8806(4)	0.8353(4)	5.2(1)
C(24)	0.3055(5)	0.8199(4)	0.7458(3)	4.54(9)
C(25)	0.5172(4)	0.1938(3)	0.7484(3)	3.19(7)
C(26)	0.6285(4)	0.0676(4)	0.6803(3)	3.78(8)
C(27)	0.5884(5)	-0.0135(5)	0.6268(5)	7.6(2)
C(28)	0.6899(8)	-0.1278(7)	0.5662(7)	11.1(2)
C(29)	0.8311(7)	-0.1631(6)	0.5569(6)	9.0(2)
C(30)	0.8731(5)	-0.0844(6)	0.6082(5)	7.5(1)
C(31)	0.7725(5)	0.0306(4)	0.6707(4)	5.5(1)
H(1)	0.1236	0.7608	0.9228	4.8721
H(2)	-0.1099	0.9594	0.9602	6.2362
H(3)	-0.3266	0.9390	0.9410	6.5206
H(4)	-0.3135	0.7211	0.8853	5.4947
H(5)	-0.2863	0.5200	0.8533	4.9458
H(6)	-0.2361	0.2885	0.8058	5.4517
H(7)	0.0085	0.1176	0.7521	5.5192
H(8)	0.2106	0.1754	0.7543	4.6328
H(9)	0.2090	0.3823	0.5949	5.0009
H(10)	0.2437	0.4702	0.3959	6.2711
H(11)	0.3323	0.6449	0.3591	6.3509
H(12)	0.3836	0.7378	0.5163	5.3501
H(13)	0.4670	0.4915	0.8235	3.7813
H(14)	0.4885	0.6030	0.9881	4.4585
H(15)	0.3976	0.8521	0.9938	5.4733
H(16)	0.2885	0.9895	0.8361	6.2404
H(17)	0.2538	0.8822	0.6784	5.3832
H(18)	0.4772	0.0118	0.6321	9.1586
H(19)	0.6564	-0.1911	0.5261	13.5338
H(20)	0.9086	-0.2519	0.5081	10.9076
H(21)	0.9847	-0.1111	0.6017	9.1164
H(22)	0.8079	0.0917	0.7121	6.6254

$B_{eq} = 8/3\ PI^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos GAMMA + 2U_{13}(aa^*cc^*)\cos BETA + 2U_{23}(bb^*cc^*)\cos ALPHA)$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Te(1)	0.0344(1)	0.0450(1)	0.0320(1)	-0.01951(10)	-0.00438(8)	0.00200(8)
O(1)	0.040(1)	0.059(2)	0.075(2)	-0.020(1)	-0.008(1)	-0.012(1)
O(2)	0.051(2)	0.060(2)	0.072(2)	-0.024(1)	-0.011(1)	-0.016(1)
C(1)	0.042(2)	0.047(2)	0.028(2)	-0.018(2)	0.000(1)	0.000(1)
C(2)	0.053(2)	0.057(2)	0.042(2)	-0.025(2)	0.005(2)	-0.008(2)
C(3)	0.070(3)	0.055(2)	0.063(3)	-0.021(2)	0.007(2)	-0.015(2)
C(4)	0.055(3)	0.055(2)	0.074(3)	-0.005(2)	0.001(2)	-0.010(2)
C(5)	0.043(2)	0.062(2)	0.060(2)	-0.014(2)	-0.005(2)	-0.002(2)
C(6)	0.039(2)	0.051(2)	0.032(2)	-0.015(2)	-0.004(1)	0.001(1)
C(7)	0.038(2)	0.058(2)	0.030(2)	-0.021(2)	-0.007(1)	0.005(1)
C(8)	0.037(2)	0.076(3)	0.046(2)	-0.024(2)	-0.009(2)	-0.003(2)
C(9)	0.053(2)	0.080(3)	0.057(2)	-0.041(2)	-0.016(2)	0.001(2)
C(10)	0.059(3)	0.065(3)	0.065(3)	-0.038(2)	-0.015(2)	-0.002(2)
C(11)	0.046(2)	0.049(2)	0.055(2)	-0.023(2)	-0.010(2)	0.001(2)
C(12)	0.036(2)	0.050(2)	0.036(2)	-0.022(2)	-0.007(1)	0.006(1)
C(13)	0.039(2)	0.046(2)	0.032(2)	-0.016(2)	-0.003(1)	0.001(1)
C(14)	0.062(2)	0.066(2)	0.036(2)	-0.033(2)	-0.004(2)	-0.004(2)
C(15)	0.081(3)	0.088(3)	0.035(2)	-0.040(3)	-0.010(2)	-0.003(2)
C(16)	0.078(3)	0.090(3)	0.034(2)	-0.041(3)	-0.005(2)	0.011(2)
C(17)	0.062(2)	0.067(2)	0.043(2)	-0.032(2)	-0.005(2)	0.012(2)
C(18)	0.039(2)	0.046(2)	0.036(2)	-0.016(2)	-0.003(1)	0.006(1)
C(19)	0.039(2)	0.042(2)	0.040(2)	-0.018(2)	0.001(1)	0.003(1)
C(20)	0.034(2)	0.039(2)	0.046(2)	-0.016(1)	-0.002(1)	-0.001(1)
C(21)	0.044(2)	0.047(2)	0.053(2)	-0.020(2)	-0.009(2)	-0.003(2)
C(22)	0.063(3)	0.047(2)	0.066(3)	-0.024(2)	-0.009(2)	-0.012(2)
C(23)	0.083(3)	0.039(2)	0.074(3)	-0.023(2)	-0.011(2)	-0.001(2)
C(24)	0.067(3)	0.043(2)	0.057(2)	-0.020(2)	-0.012(2)	0.011(2)
C(25)	0.044(2)	0.036(2)	0.047(2)	-0.020(2)	-0.014(2)	0.004(1)
C(26)	0.046(2)	0.045(2)	0.052(2)	-0.019(2)	-0.007(2)	-0.002(2)
C(27)	0.067(3)	0.091(4)	0.134(5)	-0.029(3)	-0.012(3)	-0.057(3)
C(28)	0.102(5)	0.114(5)	0.197(8)	-0.026(4)	-0.016(5)	-0.102(5)
C(29)	0.093(5)	0.095(4)	0.124(5)	-0.008(4)	0.000(4)	-0.059(4)
C(30)	0.051(3)	0.087(4)	0.120(5)	-0.007(3)	0.005(3)	-0.026(3)
C(31)	0.047(2)	0.065(3)	0.094(3)	-0.018(2)	-0.009(2)	-0.016(2)

The general temperature factor expression:

$\exp(-2PI^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Te(1)	O(1)	2.469(3)	Te(1)	C(1)	2.131(3)
Te(1)	C(12)	2.110(3)	Te(1)	C(13)	2.133(3)
O(1)	C(25)	1.246(4)	O(2)	C(25)	1.232(4)
C(1)	C(2)	1.387(5)	C(1)	C(6)	1.403(5)
C(2)	C(3)	1.391(6)	C(3)	C(4)	1.384(6)
C(4)	C(5)	1.379(6)	C(5)	C(6)	1.391(5)
C(6)	C(7)	1.468(5)	C(7)	C(8)	1.406(5)
C(7)	C(12)	1.406(4)	C(8)	C(9)	1.374(6)
C(9)	C(10)	1.372(6)	C(10)	C(11)	1.396(5)
C(11)	C(12)	1.374(5)	C(13)	C(14)	1.385(5)
C(13)	C(18)	1.393(5)	C(14)	C(15)	1.402(5)
C(15)	C(16)	1.369(6)	C(16)	C(17)	1.375(6)
C(17)	C(18)	1.411(4)	C(18)	C(19)	1.486(5)
C(19)	C(20)	1.398(4)	C(19)	C(24)	1.395(5)
C(20)	C(21)	1.393(5)	C(21)	C(22)	1.378(5)
C(22)	C(23)	1.368(6)	C(23)	C(24)	1.381(6)
C(25)	C(26)	1.527(5)	C(26)	C(27)	1.372(6)
C(26)	C(31)	1.382(5)	C(27)	C(28)	1.379(7)
C(28)	C(29)	1.357(9)	C(29)	C(30)	1.349(8)
C(30)	C(31)	1.391(6)	Te(1)	O(2)	3.182(3)

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Te(1)	C(1)	159.9(1)	O(1)	Te(1)	C(12)	81.7(1)
O(1)	Te(1)	C(13)	81.4(1)	C(1)	Te(1)	C(12)	80.9(1)
C(1)	Te(1)	C(13)	91.5(1)	C(12)	Te(1)	C(13)	99.3(1)
C(2)	C(1)	C(6)	119.8(3)	C(1)	C(2)	C(3)	119.9(4)
C(2)	C(3)	C(4)	120.1(4)	C(3)	C(4)	C(5)	120.4(4)
C(4)	C(5)	C(6)	120.1(4)	C(1)	C(6)	C(5)	119.6(3)
C(1)	C(6)	C(7)	115.9(3)	C(5)	C(6)	C(7)	124.5(3)
C(6)	C(7)	C(8)	124.9(3)	C(6)	C(7)	C(12)	118.3(3)
C(8)	C(7)	C(12)	116.7(3)	C(7)	C(8)	C(9)	120.9(3)
C(8)	C(9)	C(10)	120.9(3)	C(9)	C(10)	C(11)	120.2(4)
C(10)	C(11)	C(12)	118.7(3)	C(7)	C(12)	C(11)	122.5(3)
C(14)	C(13)	C(18)	122.1(3)	C(13)	C(14)	C(15)	119.0(4)
C(14)	C(15)	C(16)	120.0(4)	C(15)	C(16)	C(17)	120.5(3)
C(16)	C(17)	C(18)	121.5(4)	C(13)	C(18)	C(17)	116.8(3)
C(13)	C(18)	C(19)	124.2(3)	C(17)	C(18)	C(19)	119.0(3)
C(18)	C(19)	C(20)	121.3(3)	C(18)	C(19)	C(24)	120.5(3)
C(20)	C(19)	C(24)	118.2(3)	C(19)	C(20)	C(21)	120.1(3)
C(20)	C(21)	C(22)	120.2(3)	C(21)	C(22)	C(23)	120.2(4)
C(22)	C(23)	C(24)	120.2(4)	C(19)	C(24)	C(23)	121.0(4)
O(1)	C(25)	O(2)	125.7(3)	O(1)	C(25)	C(26)	116.1(3)
O(2)	C(25)	C(26)	118.0(3)	C(25)	C(26)	C(27)	120.9(4)
C(25)	C(26)	C(31)	121.5(3)	C(27)	C(26)	C(31)	117.6(4)
C(26)	C(27)	C(28)	120.4(5)	C(27)	C(28)	C(29)	121.6(6)
C(28)	C(29)	C(30)	119.1(5)	C(29)	C(30)	C(31)	120.2(5)
C(26)	C(31)	C(30)	121.1(4)	Te(1)	O(2)	C(25)	77.9(2)
O(1)	C(25)	O(2)	125.7(3)				

Table 5. Torsion or Conformation Angles

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
O(1)	C(25)	C(26)	C(27)	-6.0(6)	C(13)	C(18)	C(19)	C(20)	43.9(5)
O(1)	C(25)	C(26)	C(31)	174.3(4)	C(13)	C(18)	C(19)	C(24)	-134.3(4)
O(2)	C(25)	C(26)	C(27)	177.5(4)	C(14)	C(13)	C(18)	C(17)	0.5(5)
O(2)	C(25)	C(26)	C(31)	-2.2(6)	C(14)	C(13)	C(18)	C(19)	178.8(3)
C(1)	C(2)	C(3)	C(4)	1.6(6)	C(14)	C(15)	C(16)	C(17)	-0.7(7)
C(1)	C(6)	C(5)	C(4)	-0.2(6)	C(15)	C(14)	C(13)	C(18)	-1.1(6)
C(1)	C(6)	C(7)	C(8)	173.7(3)	C(15)	C(16)	C(17)	C(18)	0.1(7)
C(1)	C(6)	C(7)	C(12)	-4.3(4)	C(16)	C(17)	C(18)	C(19)	-178.4(4)
C(2)	C(1)	C(6)	C(5)	2.1(5)	C(17)	C(18)	C(19)	C(20)	-137.8(4)
C(2)	C(1)	C(6)	C(7)	-177.0(3)	C(17)	C(18)	C(19)	C(24)	43.9(5)
C(2)	C(3)	C(4)	C(5)	0.3(7)	C(18)	C(19)	C(20)	C(21)	-174.3(3)
C(3)	C(2)	C(1)	C(6)	-2.8(5)	C(18)	C(19)	C(24)	C(23)	176.2(4)
C(3)	C(4)	C(5)	C(6)	-0.9(7)	C(19)	C(20)	C(21)	C(22)	-2.7(5)
C(4)	C(5)	C(6)	C(7)	178.8(4)	C(19)	C(24)	C(23)	C(22)	-1.2(7)
C(5)	C(6)	C(7)	C(8)	-5.3(5)	C(20)	C(19)	C(24)	C(23)	-2.0(6)
C(5)	C(6)	C(7)	C(12)	176.7(3)	C(20)	C(21)	C(22)	C(23)	-0.7(6)
C(6)	C(7)	C(8)	C(9)	-178.0(3)	C(21)	C(20)	C(19)	C(24)	4.0(5)
C(6)	C(7)	C(12)	C(11)	179.9(3)	C(21)	C(22)	C(23)	C(24)	2.6(7)
C(7)	C(8)	C(9)	C(10)	-1.6(6)	C(25)	C(26)	C(27)	C(28)	-179.6(6)
C(7)	C(12)	C(11)	C(10)	-1.9(5)	C(25)	C(26)	C(31)	C(30)	-179.8(4)
C(8)	C(7)	C(12)	C(11)	1.8(5)	C(26)	C(27)	C(28)	C(29)	0(1)
C(8)	C(9)	C(10)	C(11)	1.5(6)	C(26)	C(31)	C(30)	C(29)	-0.9(9)
C(9)	C(8)	C(7)	C(12)	0.0(5)	C(27)	C(26)	C(31)	C(30)	0.5(8)
C(9)	C(10)	C(11)	C(12)	0.2(6)	C(27)	C(28)	C(29)	(30)	0(1)
C(13)	C(14)	C(15)	C(16)	1.2(7)	C(28)	C(27)	C(26)	C(31)	0.1(9)
C(13)	C(18)	C(17)	C(16)	0.0(6)	C(28)	C(29)	C(30)	C(31)	1(1)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Crystallographic Details

Data Collection

A colorless rod crystal of $C_{26}H_{20}O_2Te$ having approximate dimensions of 1.00 x 0.80 x 0.80 mm was mounted on a glass fiber. All measurements were made on an Enraf-Nonius CAD4-FR with graphite monochromated Mo-KALPHA radiation.Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 25 carefully centered reflections in the range 12.00 < 2THETA < 21.00° corresponded to an I-centered tetragonal cell (laue class: 4/m) with dimensions:

a = 30.731(1) Å

c = 10.189(1) Å

V = 9622.4(8) $Å^3$

For Z = 16 and F.W. = 492.04, the calculated density is 1.36 g/cm^3. Based on the systematic absences of:

hkl: h+k+l ± 2n

hk0: h ± 2n

00l: l ± 4n

and the successful solution and refinement of thestructure, the space group was determined to be:

$I4_1/a$ (#88)

The data were collected at a temperature of 296 ± 1 K using the OMEGA scan technique to a maximum 2THETA value of 49.9°.Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.26° with a take-off angle of 2.8°. Scans of (0.50 + 0.40 tan THETA)° were made at a speed of 2-20°/min (in omega). Moving-crystal moving counter background measurements were made by scanning an additional 25 above and below the scan range. The counter aperture consisted of a variable horizontal slit with a width ranging from 1.3 to 1.9 mm and a vertical slit set to 4.0 mm. The diameter of the incident beam collimator was 1.2 mm and the crystal to detector distance was 21 cm. For intense reflections an attenuator was automatically inserted in front of the detector (attenuator factor =

13.4).

Data Reduction

A total of 4010 reflections was collected. The intensities of three representative reflection were measured after every 120 minutes of X-ray exposure time. Over the course of data collection, the standards decreased by 2.4%. A linear correction factor was applied to the data to account for this phenomenon. The linear absorption coefficient, MU, for Mo-KALPHA radiation is 12.5 cm^{-1}. An empirical absorption correction using the program DIFABS[1] was applied which resulted in transmission factors ranging from 0.92 to 1.00. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques[3]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[4](on *F*) was based on 3013 observed reflections (I > 3.00sigma(I)) and 262 variable parameters and converged with unweighted and weighted agreement factors of:

$$R = \text{SIGMA } ||Fo| - |Fc|| \ / \ \text{SIGMA } |Fo| = 0.027$$

$$R_w = [(\text{SIGMA } w \ (|Fo| - |Fc|)^2 \ / \ \text{SIGMA } w \ Fo^2)]^{1/2} = 0.034$$

The standard deviation of an observation of unit weight[5] was 2.82. The weighting scheme was based on counting statistics. Plots of SIGMA w $(|Fo| - |Fc|)^2$ versus |Fo|,reflection order in data collection, sin THETA/LAMBDA and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.48 and -0.27 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for DELTAf' and DELTAf" were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[9]. All calculations were performed using the teXsan[10] crystallographic software package of Molecular Structure Corporation.

References

(1) DIFABS: Walker, N. & Stuart, Acta Cryst. A39, 158-166 (1983). An empirical absorption correction program.

(2) SIR92: Altomare, A., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., Polidori, G. (1994). J. Appl. Cryst., in preparation.

(3) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(4) Least-Squares:

Function minimized: $Sw(|F_o|-|F_c|)^2$ where

$w = 1/[sigma^2(Fo)] = [sigma^2{}_c(Fo) + p^2Fo^2/4]^{-1}$

$sigma_c(Fo)$ = e.s.d. based on counting statistics

p = p-factor

(5) Standard deviation of an observation of unit weight:

$[Sw(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations

N_v = number of variables

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(8) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(9) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(10) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{26}H_{20}O_2Te$
Formula Weight	492.04
Crystal Color, Habit	colorless, rod
Crystal Dimensions	0.80 X 0.80 X 1.00 mm
Crystal System	tetragonal
Lattice Type	I-centered
No. of Reflections Used for Unit Cell Determination (2THETA range)	25 (12.0 - 21.0°)
Omega Scan Peak Width at Half-height	0.30°
Lattice Parameters	a = 30.731(1)Å c = 10.189(1) Å V = 9622.4(8) $Å^3$
Space Group	$I4_1/a$ (#88)
Z value	16
D_{calc}	1.358 g/cm^3
F_{000}	3904.00
MU(MoKALPHA)	12.53 cm^{-1}

B. Intensity Measurements

Diffractometer	CAD4-FR
Radiation	MoKALPHA (LAMBDA = 0.71069 Å) graphite monochromated
Attenuator	Zr foil (factor = 13.40)
Take-off Angle	2.8°
Detector Aperture	1.3 - 1.9 mm horizontal 4.0 mm vertical
Crystal to Detector Distance	21 mm
Temperature	296.0 K

Scan Type	OMEGA
Scan Rate	2.0-20.0°/min (in OMEGA)
Scan Width	(0.50 + 0.40 tan THETA)°
$2THETA_{max}$	49.9°
No. of Reflections Measured	Total: 4010
Corrections	Lorentz-polarization Absorption (trans. factors: 0.92 - 1.00) Decay (2.4 % decrease)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	SIGMA w $(\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$1/^2$sigma(Fo) = $4Fo^2/sigma^2(Fo^2)$
p-factor	0.0000
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00sigma(I))	3013
No. Variables	262
Reflection/Parameter Ratio	11.50
Residuals: R; Rw	0.027 ; 0.034
Goodness of Fit Indicator	2.82
Maximum peak in Final Diff. Map	0.48 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.27 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Te(1)	0.02146(1)	0.06042(1)	0.01681(3)	3.122(7)
O(1)	0.0464(1)	0.0136(1)	0.2017(3)	4.68(9)
O(2)	0.0705(1)	-0.0302(1)	0.0470(4)	5.2(1)
C(1)	0.0002(2)	0.1172(2)	-0.0890(5)	3.5(1)
C(2)	0.0034(2)	0.1240(2)	-0.2230(6)	4.6(1)
C(3)	-0.0134(2)	0.1619(2)	-0.2757(7)	6.2(2)
C(4)	-0.0330(3)	0.1923(2)	-0.1962(8)	7.0(2)
C(5)	-0.0375(2)	0.1851(2)	-0.0623(7)	5.8(2)
C(6)	-0.0205(2)	0.1470(2)	-0.0066(6)	3.8(1)
C(7)	-0.0236(2)	0.1359(2)	0.1329(5)	3.6(1)
C(8)	-0.0432(2)	0.1625(2)	0.2276(7)	4.7(1)
C(9)	-0.0450(2)	0.1491(2)	0.3558(7)	5.4(2)
C(10)	-0.0282(2)	0.1095(2)	0.3935(6)	5.1(2)
C(11)	-0.0086(2)	0.0826(2)	0.3019(5)	4.2(1)
C(12)	-0.0066(2)	0.0961(2)	0.1728(5)	3.3(1)
C(13)	0.0864(2)	0.0853(2)	0.0364(5)	3.2(1)
C(14)	0.0990(2)	0.0993(2)	0.1607(5)	4.0(1)
C(15)	0.1400(2)	0.1168(2)	0.1783(6)	4.9(1)
C(16)	0.1680(2)	0.1197(2)	0.0741(7)	5.5(2)
C(17)	0.1555(2)	0.1052(2)	-0.0490(6)	5.1(2)
C(18)	0.1144(2)	0.0878(2)	-0.0705(5)	3.7(1)
C(19)	0.1026(2)	0.0734(2)	-0.2054(5)	3.8(1)
C(20)	0.0843(2)	0.0333(2)	-0.2295(6)	4.4(1)
C(21)	0.0736(2)	0.0211(2)	-0.3570(6)	5.5(2)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(22)	0.0810(2)	0.0487(2)	-0.4609(6)	5.8(2)
C(23)	0.0993(2)	0.0891(2)	-0.4378(6)	5.6(2)
C(24)	0.1101(2)	0.1013(2)	-0.3113(6)	5.0(2)
C(25)	0.0675(2)	-0.0185(2)	0.1611(6)	3.9(1)
C(26)	0.0901(3)	-0.0451(2)	0.2672(8)	7.9(2)
H(1)	0.0187	0.1001	-0.2854	5.4619
H(2)	-0.0110	0.1677	-0.3800	7.4588
H(3)	-0.0451	0.2222	-0.2385	8.3934
H(4)	-0.0540	0.2087	-0.0015	7.0193
H(5)	-0.0569	0.1935	0.1997	5.6357
H(6)	-0.0599	0.1699	0.4283	6.5285
H(7)	-0.0303	0.0994	0.4948	6.1061
H(8)	0.0050	0.0517	0.3309	5.0138
H(9)	0.0770	0.0964	0.2427	4.8386
H(10)	0.1500	0.1281	0.2740	5.8523
H(11)	0.2000	0.1335	0.0878	6.6416
H(12)	0.1781	0.1074	-0.1297	6.0774
H(13)	0.0782	0.0112	-0.1492	5.2315
H(14)	0.0592	-0.0104	-0.3746	6.5977
H(15)	0.0727	0.0389	-0.5596	7.0145
H(16)	0.1052	0.1111	-0.5184	6.7343
H(17)	0.1245	0.1328	-0.2941	6.0108
H(18)	0.0686	-0.0565	0.3278	9.4302
H(19)	0.1057	-0.0691	0.2269	9.4302
H(20)	0.1105	-0.0268	0.3144	9.4302

B_{eq} = 8/3 $PI^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos GAMMA + 2U_{13}(aa^*cc^*)\cos BETA + 2U_{23}(bb^*cc^*)\cos ALPHA)$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Te(1)	0.0428(2)	0.0362(2)	0.0397(2)	-0.0015(1)	-0.0010(1)	-0.0015(1)
O(1)	0.078(3)	0.053(2)	0.047(2)	0.013(2)	-0.002(2)	0.002(2)
O(2)	0.071(3)	0.067(3)	0.058(3)	0.016(2)	0.002(2)	-0.006(2)
C(1)	0.040(3)	0.045(3)	0.049(3)	-0.005(2)	-0.007(2)	0.005(3)
C(2)	0.058(3)	0.066(4)	0.049(3)	-0.003(3)	-0.005(3)	0.009(3)
C(3)	0.087(5)	0.084(5)	0.065(4)	-0.004(4)	-0.010(4)	0.028(4)
C(4)	0.107(6)	0.067(4)	0.092(6)	0.009(4)	-0.022(5)	0.031(4)
C(5)	0.078(4)	0.059(4)	0.085(5)	0.017(3)	-0.007(4)	0.007(4)
C(6)	0.043(3)	0.045(3)	0.058(3)	0.002(2)	-0.006(3)	0.004(3)
C(7)	0.035(3)	0.046(3)	0.057(3)	0.001(2)	-0.002(2)	-0.005(3)
C(8)	0.047(3)	0.055(3)	0.076(4)	0.005(3)	-0.001(3)	-0.016(3)
C(9)	0.056(4)	0.082(5)	0.069(4)	0.002(3)	0.006(3)	-0.026(4)
C(10)	0.061(4)	0.084(5)	0.048(3)	0.000(3)	0.007(3)	-0.007(3)
C(11)	0.051(3)	0.060(3)	0.048(3)	0.002(3)	0.005(3)	0.000(3)
C(12)	0.037(3)	0.045(3)	0.044(3)	-0.002(2)	0.001(2)	-0.004(2)
C(13)	0.040(3)	0.039(3)	0.044(3)	-0.003(2)	-0.003(2)	0.001(2)
C(14)	0.051(3)	0.055(3)	0.048(3)	-0.002(3)	-0.006(3)	-0.002(3)
C(15)	0.058(4)	0.069(4)	0.058(4)	-0.011(3)	-0.014(3)	-0.006(3)
C(16)	0.043(3)	0.087(5)	0.080(5)	-0.016(3)	-0.011(3)	-0.002(4)
C(17)	0.045(3)	0.079(4)	0.068(4)	-0.010(3)	0.008(3)	-0.005(3)
C(18)	0.046(3)	0.049(3)	0.047(3)	0.000(3)	0.002(2)	-0.002(2)
C(19)	0.049(3)	0.052(3)	0.045(3)	0.001(3)	0.008(2)	-0.004(3)
C(20)	0.069(4)	0.042(3)	0.054(3)	0.002(3)	0.009(3)	-0.005(3)
C(21)	0.090(5)	0.057(4)	0.062(4)	-0.008(3)	0.008(4)	-0.017(3)
C(22)	0.091(5)	0.083(5)	0.048(4)	-0.004(4)	0.003(3)	-0.012(3)
C(23)	0.090(5)	0.074(4)	0.049(4)	-0.010(4)	0.016(3)	0.003(3)
C(24)	0.078(4)	0.063(4)	0.050(3)	-0.014(3)	0.014(3)	-0.003(3)
C(25)	0.052(3)	0.040(3)	0.056(3)	0.000(3)	-0.005(3)	-0.002(3)
C(26)	0.137(7)	0.082(5)	0.080(5)	0.038(5)	-0.037(5)	-0.003(4)

The general temperature factor expression:
$\exp(-2PI^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Te(1)	O(1)	2.491(4)	Te(1)	C(1)	2.152(5)
Te(1)	C(12)	2.116(5)	Te(1)	C(13)	2.146(5)
O(1)	C(25)	1.250(6)	O(2)	C(25)	1.220(6)
C(1)	C(2)	1.385(7)	C(1)	C(6)	1.396(7)
C(2)	C(3)	1.381(8)	C(3)	C(4)	1.376(10)
C(4)	C(5)	1.389(10)	C(5)	C(6)	1.403(8)
C(6)	C(7)	1.465(7)	C(7)	C(8)	1.400(7)
C(7)	C(12)	1.390(7)	C(8)	C(9)	1.370(9)
C(9)	C(10)	1.375(9)	C(10)	C(11)	1.386(8)
C(11)	C(12)	1.380(7)	C(13)	C(14)	1.392(7)
C(13)	C(18)	1.390(7)	C(14)	C(15)	1.381(7)
C(15)	C(16)	1.369(8)	C(16)	C(17)	1.385(8)
C(17)	C(18)	1.388(7)	C(18)	C(19)	1.490(7)
C(19)	C(20)	1.379(7)	C(19)	C(24)	1.396(7)
C(20)	C(21)	1.390(8)	C(21)	C(22)	1.375(9)
C(22)	C(23)	1.384(9)	C(23)	C(24)	1.382(8)
C(25)	C(26)	1.524(8)	Te(1)	O(2)	3.181(4)
Te(1)	O(2)'	3.046(4)			

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Te(1)	C(1)	160.1(2)	O(1)	Te(1)	C(12)	81.8(2)
O(1)	Te(1)	C(13)	81.2(2)	C(1)	Te(1)	C(12)	80.3(2)
C(1)	Te(1)	C(13)	92.3(2)	C(12)	Te(1)	C(13)	97.2(2)
C(2)	C(1)	C(6)	121.6(5)	C(1)	C(2)	C(3)	119.0(6)
C(2)	C(3)	C(4)	120.5(6)	C(3)	C(4)	C(5)	121.0(6)
C(4)	C(5)	C(6)	119.5(6)	C(1)	C(6)	C(5)	118.4(5)
C(1)	C(6)	C(7)	117.4(5)	C(5)	C(6)	C(7)	124.2(5)
C(6)	C(7)	C(8)	124.2(5)	C(6)	C(7)	C(12)	117.6(5)
C(8)	C(7)	C(12)	118.2(5)	C(7)	C(8)	C(9)	119.9(6)
C(8)	C(9)	C(10)	121.1(6)	C(9)	C(10)	C(11)	120.2(6)
C(10)	C(11)	C(12)	118.8(5)	C(7)	C(12)	C(11)	121.8(5)
C(14)	C(13)	C(18)	121.5(5)	C(13)	C(14)	C(15)	119.6(5)
C(14)	C(15)	C(16)	119.8(5)	C(15)	C(16)	C(17)	120.5(5)
C(16)	C(17)	C(18)	121.2(5)	C(13)	C(18)	C(17)	117.4(5)
C(13)	C(18)	C(19)	123.8(5)	C(17)	C(18)	C(19)	118.8(5)
C(18)	C(19)	C(20)	121.9(5)	C(18)	C(19)	C(24)	119.5(5)
C(20)	C(19)	C(24)	118.6(5)	C(19)	C(20)	C(21)	120.2(5)
C(20)	C(21)	C(22)	121.0(6)	C(21)	C(22)	C(23)	119.3(6)
C(22)	C(23)	C(24)	119.9(6)	C(19)	C(24)	C(23)	121.0(5)
O(1)	C(25)	O(2)	126.0(5)	O(1)	C(25)	C(26)	115.2(5)
O(2)	C(25)	C(26)	118.8(5)	Te(1)	O(1)	C(1)	111.4(3)
O(1)	C(25)	O(2)	126.0(5)	O(2)	Te(1)	O(2)'	101.15(9)
Te(1)	O(2)	Te(1)'	78.85(9)	O(1)	Te(1)	O(2)'	105.7(1)
O(1)	Te(1)	O(2)	43.6(1)				

Table 5. Torsion or Conformation Angles

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
Te(1)	C(1)	C(7)	C(2)	2(1)	C(4)	Te(1)	C(1)	C(7)	-1.1(6)
Te(1)	C(1)	C(7)	C(20)	-176.9(7)	C(4)	Te(1)	C(1)	C(11)	-176.8(8)
Te(1)	C(1)	C(11)	C(23)	176.7(8)	C(4)	Te(1)	C(6)	C(8)	-151.5(7)
Te(1)	C(4)	C(2)	C(7)	0(1)	C(4)	Te(1)	C(6)	C(27)	27.4(7)
Te(1)	C(4)	C(2)	C(12)	179.3(6)	C(4)	C(2)	C(7)	C(20)	177.1(9)
Te(1)	C(4)	C(13	C(21)	-179.0(7)	C(4)	C(2)	C(12)	C(24)	0(1)
Te(1)	C(6)	C(8)	C(3)	0(1)	C(4)	C(13)	C(21)	C(24)	0(2)
Te(1)	C(6)	C(8)	C(28)	178.5(7)	C(6)	Te(1)	C(1)	C(7)	-97.7(6)
Te(1)	C(6)	C(27)	C(30)	-177.8(7)	C(6)	Te(1)	C(1)	C(11)	86.6(8)
C(1)	Te(1)	C(4)	C(2)	0.5(6)	C(6)	Te(1)	C(4)	C(13)	-89.5(8)
C(1)	Te(1)	C(4)	C(13)	179.6(8)	C(6)	C(8)	C(3)	C(10)	-50(1)
C(1)	Te(1)	C(6)	C(8)	-71.5(7)	C(6)	C(8)	C(3)	C(17)	130(1)
C(1)	Te(1)	C(6)	C(27)	107.4(7)	C(6)	C(8)	C(28)	C(29)	0(1)
C(1)	C(7)	C(2)	C(4)	-1(1)	C(6)	C(27)	C(30)	C(29)	-1(2)
C(1)	C(7)	C(2)	C(12)	179.8(8)	C(7)	C(1)	C(11)	C(23)	1(1)
C(1)	C(7)	C(20)	C(26)	-1(2)	C(7)	C(2)	C(4)	C(13)	-179.0(8)
C(1)	C(11)	C(23)	C(26)	0(2)	C(7)	C(2)	C(12)	C(24)	178.8(9)
C(2)	C(4)	Te(1)	C(6)	91.4(6)	C(7)	C(20)	C(26)	C(23)	2(2)
C(2)	C(4)	C(13)	C(21)	0(1)	C(8)	C(3)	C(10)	C(14)	-179.9(9)
C(2)	C(7)	C(1)	C(11)	177.5(8)	C(8)	C(3)	C(17)	C(18)	-180(1)
C(2)	C(7)	C(20)	C(26)	-179(1)	C(8)	C(6)	C(27)	C(30)	1(1)
C(2)	C(12)	C(24)	C(21)	0(2)	C(8)	C(28)	C(29)	C(30)	0(2)
C(3)	C(8)	C(6)	C(27)	-179.3(8)	C(10)	C(3)	C(8)	C(28)	131(1)
C(3)	C(8)	C(28)	C(29)	179(1)	C(10)	C(3)	C(17)	C(18)	0(2)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Table 5. Torsion or Conformation Angles (continue)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
C(3)	C(10)	C(14)	C(15)	-1(2)	C(10)	C(14)	C(15)	C(18)	1(2)
C(3)	C(17)	C(18)	C(15)	0(2)	C(11)	C(1)	C(7)	C(20)	-1(1)
C(11)	C(23)	C(26)	C(20)	-1(2)					
C(12)	C(2)	C(4)	C(13)	0(1)					
C(12)	C(2)	C(7)	C(20)	-2(1)					
C(12)	C(24)	C(21)	C(13)	0(2)					
C(14)	C(10)	C(3)	C(17)	0(1)					
C(14)	C(15)	C(18)	C(17)	0(2)					
C(17)	C(3)	C(8)	C(28)	-49(1)					
C(27)	C(6)	C(8)	C(28)	0(1)					
C(27)	C(30)	C(29)	C(28)	1(2)					

Table 6. Non-bonded Intermolecular Contacts out to 3.27 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
Te(1)	O(2)'	3.046(4)	5				