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Experimental

Data Collection

A colorless needle crystal of $C_{21}H_{46}Cl_{12}Te_6O_{2.50}N$ having approximate dimensions of 0.20 x 0.50 x 1.20 mm was mounted on a glass fiber. All measurements were made on an Enraf-Nonius CAD4 diffractometer with graphite monochromated Mo-Kα 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 $12.00 < 2\theta < 21.00°$ corresponded to atriclinic cell with dimensions:

a = 8.782(1) Å	α = 60.83(3)°
b = 12.426(5) Å	β = 87.65(3)°
c = 12.723(4) Å	γ = 85.37(3)
V = 1208.4(7) Å^3	

For Z = 1 and F.W. = 1543.64, the calculated density is 2.12 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P1 (#1)

The data were collected at a temperature of 296 $\pm$ 1°C using the ω-2θ scan technique to a maximum 2θ value of 49.9°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.24° with a take-off angle of 2.8°. Scans of $(1.20 + 0.65 \tan \theta)°$ were made at a speed of 4.0°/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 2.0 to 2.5 mm and a vertical slit set to 4.0 mm. The diameter of the incident beam collimator was 1.4 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 4543 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 20.1%. A polynomial correction factor was applied to the data to account for this phenomenon.

The linear absorption coefficient, μ, for Mo-Kα radiation is 42.6 cm^{-1}. An empirical absorption correction using the program DIFABS[1] was applied which resulted in transmission factors ranging from 0.52 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]. Some non-

hydrogen atoms were refined anisotropically, while the rest were refined isotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[4] was based on 4037 observed reflections ($I > 5.00\sigma(I)$) and 256 variable parameters and converged (largest parameter shift was 1.32 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma||Fo| - |Fc||/\Sigma|Fo| = 0.079$$

$$R_w = \sqrt{(\Sigma w(|Fo| - |Fc|)^2/\Sigma wFo^2)} = 0.092$$

The standard deviation of an observation of unit weight[5] was 12.01. 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 2.52 and -1.96 $e^-/\AA^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6] . Anomalous dispersion effects were included in Fcalc[7]; the values for Δf' and Δf" 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: $\Sigma w(|Fo| - |Fc|)^2$

where w = $\frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$

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

p = p-factor

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

$$\sqrt{\Sigma w(|Fo| - |Fc|)^2/(No - Nv)}$$

where: No = number of observations

Nv = 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	$C_{21}H_{46}Cl_{12}Te_6O_{2.50}N$
Formula Weight	1543.64
Crystal Color, Habit	colorless, needle
Crystal Dimensions	0.20 X 0.50 X 1.20 mm
Crystal System	triclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	25 (12.0 - 21.0°)
Omega Scan Peak Width at Half-height	0.24°
Lattice Parameters	a = 8.782(1)Å b = 12.426(5) Å c = 12.723(4) Å α = 60.83(3)° β = 87.65(3)° γ = 85.37(3)°
	V = 1208.4(7) $Å^3$
Space Group	P1 (#1)
Z value	1
D_{calc}	2.121 g/cm^3
F_{000}	715.00
μ(MoKα)	42.58 cm^{-1}

B. Intensity Measurements

Diffractometer	CAD4
Radiation	MoKα (λ = 0.71069 Å)

	graphite monochromated
Attenuator	Zr foil (factor = 13.40)
Take-off Angle	2.8°
Detector Aperture	2.0 - 2.5 mm horizontal 4.0 mm vertical
Crystal to Detector Distance	21 mm
Temperature	296.0°C
Scan Type	ω-2θ
Scan Rate	4.0°/min (in ω)
Scan Width	$(1.20 + 0.65 \tan \theta)°$
$2\theta_{max}$	49.9°
No. of Reflections Measured	Total: 4543
Corrections	Lorentz-polarization Absorption (trans. factors: 0.5242 - 1.0000) Decay (20.11% decline)

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	$w = \frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$
p-factor	0.0000
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>5.00σ(I))	4037
No. Variables	256
Reflection/Parameter Ratio	15.77
Residuals: R; Rw	0.079 ; 0.092
Goodness of Fit Indicator	12.01

Max Shift/Error in Final Cycle	1.32
Maximum peak in Final Diff. Map	2.52 $e^-/\mathring{A}^3$
Minimum peak in Final Diff. Map	-1.96 $e^-/\mathring{A}^3$

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

atom	x	y	z	B_{eq}	occ
Te(1)	0.3920	0.8461	0.5197	2.59(2)	1.0000
Te(2)	0.9794(1)	0.69095(8)	0.31751(8)	2.57(1)	1.0000
Te(3)	0.4521(1)	0.34147(8)	0.51178(8)	2.70(2)	1.0000
Te(4)	-0.0476(1)	0.14396(7)	-0.09390(7)	2.77(2)	1.0000
Te(5)	-0.1081(1)	0.65767(9)	-0.10238(8)	2.78(2)	1.0000
Te(6)	0.4792(1)	0.29981(8)	0.10013(8)	2.49(1)	1.0000
Cl(1)	0.1877(4)	0.8864(3)	0.3707(3)	4.62(7)	1.0000
Cl(2)	0.5981(4)	0.8007(4)	0.6667(3)	5.05(8)	1.0000
Cl(3)	0.9695(4)	0.5780(3)	0.5379(3)	3.81(6)	1.0000
Cl(4)	0.9696(4)	0.8113(3)	0.0855(3)	3.97(6)	1.0000
Cl(5)	0.2589(4)	0.4742(4)	0.3538(3)	5.03(8)	1.0000
Cl(6)	0.6573(4)	0.2310(4)	0.6659(3)	6.08(8)	1.0000
Cl(7)	-0.2411(4)	0.1195(3)	0.0641(3)	4.80(7)	1.0000
Cl(8)	0.1574(4)	0.1869(4)	-0.2478(3)	5.58(9)	1.0000
Cl(9)	-0.3113(4)	0.5473(3)	0.0478(3)	4.55(7)	1.0000
Cl(10)	0.0981(4)	0.7594(3)	-0.2515(3)	4.85(7)	1.0000
Cl(11)	0.4703(4)	0.1862(3)	0.3324(3)	3.40(6)	1.0000
Cl(12)	0.4704(3)	0.4065(3)	-0.1194(3)	3.47(5)	1.0000
O(1)	0.5027	0.7597	-0.8063	7.4571	1.0000
O(2)	0.997(2)	0.245(1)	0.225(1)	3.2(3)	0.5000
O(3)	0.943(2)	0.138(1)	0.415(1)	2.9(2)	0.5000
O(4)	1.034(3)	0.156(2)	0.470(2)	7.6(6)	0.5000
N(1)	0.4417	0.8460	-1.0016	4.8856	1.0000
C(1)	0.550(1)	0.8779(10)	0.3794(9)	2.7(2)	1.0000

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

atom	x	y	z	B_{eq}	occ
C(2)	0.707(1)	0.7974(9)	0.4192(9)	3.1(2)	1.0000
C(3)	0.799(2)	0.816(1)	0.311(1)	4.7(2)	1.0000
C(4)	0.832(2)	0.556(1)	0.306(1)	4.2(2)	1.0000
C(5)	0.732(2)	0.501(1)	0.403(1)	4.7(3)	1.0000
C(6)	0.626(1)	0.426(1)	0.379(1)	3.4(2)	1.0000
C(7)	0.407(1)	0.454(1)	0.598(1)	3.7(2)	1.0000
C(8)	0.407(1)	0.5935(9)	0.5238(8)	1.8(1)	1.0000
C(9)	0.371(1)	0.653(1)	0.597(1)	3.8(2)	1.0000
C(10)	-0.102(2)	0.337(1)	-0.169(1)	4.6(3)	1.0000
C(11)	-0.115(1)	0.4120(8)	-0.1064(8)	1.8(1)	1.0000
C(12)	-0.123(2)	0.546(1)	-0.177(1)	4.4(2)	1.0000
C(13)	0.058(1)	0.550(1)	0.042(1)	3.5(2)	1.0000
C(14)	0.203(1)	0.5032(9)	0.0004(9)	2.7(2)	1.0000
C(15)	0.295(1)	0.4168(9)	0.1078(9)	2.9(2)	1.0000
C(16)	0.350(2)	0.148(1)	0.113(1)	5.4(3)	1.0000
C(17)	0.225(2)	0.194(1)	0.018(1)	4.9(3)	1.0000
C(18)	0.122(1)	0.096(1)	0.045(1)	3.7(2)	1.0000
C(19)	0.420(1)	0.786(1)	-0.886(1)	4.1(3)	1.0000
C(20)	0.348(3)	0.844(2)	-1.090(2)	8.7(5)	1.0000
C(21)	0.560(2)	0.923(2)	-1.065(2)	7.3(4)	1.0000
H(1)	0.5016	0.8591	0.3227	3.4484	1.0000
H(2)	0.5707	0.9636	0.3394	3.4484	1.0000
H(3)	0.7633	0.8217	0.4674	3.7084	1.0000
H(4)	0.6881	0.7104	0.4667	3.7084	1.0000

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

atom	x	y	z	B_{eq}	occ
H(5)	0.8444	0.8954	0.2816	5.5457	1.0000
H(6)	0.7281	0.8230	0.2517	5.5457	1.0000
H(7)	0.7734	0.5991	0.2326	5.0681	1.0000
H(8)	0.8995	0.4908	0.3034	5.0681	1.0000
H(9)	0.7902	0.4470	0.4754	5.4939	1.0000
H(10)	0.6734	0.5644	0.4129	5.4939	1.0000
H(11)	0.6875	0.3611	0.3736	4.3778	1.0000
H(12)	0.5757	0.4806	0.3036	4.3778	1.0000
H(13)	0.3081	0.4356	0.6364	4.6942	1.0000
H(14)	0.4853	0.4280	0.6603	4.6942	1.0000
H(15)	0.5078	0.6151	0.4884	2.3410	1.0000
H(16)	0.3318	0.6224	0.4611	2.3410	1.0000
H(17)	0.4387	0.6117	0.6668	4.4482	1.0000
H(18)	0.2664	0.6369	0.6239	4.4482	1.0000
H(19)	-0.0272	0.3758	-0.2321	5.3913	1.0000
H(20)	-0.2026	0.3514	-0.2066	5.3913	1.0000
H(21)	-0.2066	0.3902	-0.0569	2.0397	1.0000
H(22)	-0.0261	0.3866	-0.0539	2.0397	1.0000
H(23)	-0.2182	0.5708	-0.2201	5.4635	1.0000
H(24)	-0.0383	0.5658	-0.2350	5.4635	1.0000
H(25)	0.0867	0.6012	0.0753	3.9934	1.0000
H(26)	0.0088	0.4788	0.1053	3.9934	1.0000
H(27)	0.1743	0.4614	-0.0426	3.2633	1.0000
H(28)	0.2613	0.5729	-0.0526	3.2633	1.0000

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

atom	x	y	z	B_{eq}	occ
H(29)	0.2233	0.3624	0.1667	3.5846	1.0000
H(30)	0.3366	0.4664	0.1376	3.5846	1.0000
H(31)	0.4208	0.0894	0.1017	6.5432	1.0000
H(32)	0.3040	0.1056	0.1921	6.5432	1.0000
H(33)	0.1661	0.2644	0.0174	6.0813	1.0000
H(34)	0.2708	0.2205	-0.0610	6.0813	1.0000
H(35)	0.0691	0.0749	0.1209	4.0857	1.0000
H(36)	0.1840	0.0216	0.0555	4.0857	1.0000
H(37)	0.3186	0.7613	-0.8654	4.2136	1.0000
H(38)	0.2974	0.9260	-1.1360	12.2852	1.0000
H(39)	0.3968	0.8116	-1.1314	12.2852	1.0000
H(40)	0.2601	0.7899	-1.0395	12.2852	1.0000
H(41)	0.6296	0.9266	-1.0097	8.9360	1.0000
H(42)	0.6158	0.8936	-1.1144	8.9360	1.0000
H(43)	0.5162	1.0076	-1.1183	8.9360	1.0000

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Te(1)	0.0359(4)	0.0288(3)	0.0408(4)	0.0029(3)	-0.0011(3)	-0.0229(3)
Te(2)	0.0300(4)	0.0350(3)	0.0308(3)	-0.0041(3)	0.0036(3)	-0.0147(3)
Te(3)	0.0434(4)	0.0245(3)	0.0338(4)	-0.0061(3)	0.0028(3)	-0.0132(3)
Te(4)	0.0360(4)	0.0377(4)	0.0338(4)	-0.0052(3)	-0.0022(3)	-0.0185(3)
Te(5)	0.0307(4)	0.0344(4)	0.0402(4)	0.0027(3)	-0.0006(3)	-0.0184(3)
Te(6)	0.0308(4)	0.0326(3)	0.0323(3)	-0.0001(3)	-0.0056(3)	-0.0165(3)
Cl(1)	0.053(2)	0.055(2)	0.061(2)	-0.014(1)	-0.014(1)	-0.020(1)
Cl(2)	0.045(2)	0.100(3)	0.058(2)	-0.004(2)	-0.014(1)	-0.047(2)
Cl(3)	0.041(2)	0.055(2)	0.0323(9)	-0.002(1)	-0.010(1)	-0.008(1)
Cl(4)	0.054(2)	0.054(2)	0.030(1)	0.004(1)	0.004(1)	-0.012(1)
Cl(5)	0.067(2)	0.077(2)	0.059(2)	0.023(2)	-0.017(1)	-0.046(2)
Cl(6)	0.065(2)	0.081(2)	0.052(2)	-0.003(2)	-0.020(1)	-0.006(2)
Cl(7)	0.058(2)	0.048(2)	0.057(2)	0.003(1)	0.018(1)	-0.014(1)
Cl(8)	0.063(2)	0.102(3)	0.049(2)	-0.016(2)	0.019(1)	-0.039(2)
Cl(9)	0.046(2)	0.077(2)	0.058(2)	-0.026(2)	0.012(1)	-0.037(2)
Cl(10)	0.047(2)	0.060(2)	0.054(2)	-0.005(1)	0.010(1)	-0.010(1)
Cl(11)	0.062(2)	0.034(1)	0.034(1)	0.009(1)	-0.005(1)	-0.019(1)
Cl(12)	0.047(2)	0.052(2)	0.0318(5)	-0.012(1)	0.013(1)	-0.019(1)
O(1)	0.0944	0.0944	0.0944	-0.0066	-0.0002	-0.0459
N(1)	0.0619	0.0619	0.0619	-0.0043	-0.0001	-0.0301

The general temperature factor expression:

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

Intramolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	atom	atom	distance
Te(1)	Cl(1)	2.50(1)	O(2)	O(3)	2.17(6)
Te(1)	Cl(2)	2.49(1)	O(3)	O(4)	1.19(9)
Te(1)	C(1)	2.11(4)	N(1)	C(19)	1.30(4)
Te(1)	C(9)	2.13(4)	N(1)	C(20)	1.43(8)
Te(2)	Cl(3)	2.45(1)	N(1)	C(21)	1.41(7)
Te(2)	Cl(4)	2.58(1)	C(1)	C(2)	1.58(5)
Te(2)	C(3)	2.10(5)	C(1)	C(3)	2.52(6)
Te(2)	C(4)	2.26(4)	C(2)	C(3)	1.49(6)
Te(3)	Cl(5)	2.50(1)	C(4)	C(5)	1.40(6)
Te(3)	Cl(6)	2.50(1)	C(4)	C(6)	2.37(6)
Te(3)	C(6)	2.15(4)	C(5)	C(6)	1.50(6)
Te(3)	C(7)	2.17(4)	C(7)	C(8)	1.52(5)
Te(4)	Cl(7)	2.50(1)	C(7)	C(9)	2.46(6)
Te(4)	Cl(8)	2.49(1)	C(8)	C(9)	1.45(5)
Te(4)	C(10)	2.13(5)	C(10)	C(11)	1.49(6)
Te(4)	C(18)	2.18(4)	C(10)	C(12)	2.54(6)
Te(5)	Cl(9)	2.51(1)	C(11)	C(12)	1.46(5)
Te(5)	Cl(10)	2.50(1)	C(13)	C(14)	1.54(5)
Te(5)	C(12)	2.04(5)	C(13)	C(15)	2.45(5)
Te(5)	C(13)	2.19(4)	C(14)	C(15)	1.48(5)
Te(6)	Cl(11)	2.582(9)	C(16)	C(17)	1.52(7)
Te(6)	Cl(12)	2.44(1)	C(16)	C(18)	2.46(7)
Te(6)	C(15)	2.12(4)	C(17)	C(18)	1.48(6)
Te(6)	C(16)	2.22(5)	C(19)	C(20)	2.43(9)
O(1)	N(1)	2.2433(1)	C(19)	C(21)	2.44(7)
O(1)	C(19)	1.16(4)	C(20)	C(21)	2.3(1)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	Te(1)	Cl(2)	178.2(4)	Cl(9)	Te(5)	C(13)	87(1)
Cl(1)	Te(1)	C(1)	87(1)	Cl(10)	Te(5)	C(12)	87(1)
Cl(1)	Te(1)	C(9)	90(1)	Cl(10)	Te(5)	C(13)	92(1)
Cl(2)	Te(1)	C(1)	92(1)	C(12)	Te(5)	C(13)	102(2)
Cl(2)	Te(1)	C(9)	89(1)	Cl(11)	Te(6)	Cl(12)	176.4(4)
C(1)	Te(1)	C(9)	101(1)	Cl(11)	Te(6)	C(15)	86(1)
Cl(3)	Te(2)	Cl(4)	176.1(4)	Cl(11)	Te(6)	C(16)	86(1)
Cl(3)	Te(2)	C(3)	91(1)	Cl(12)	Te(6)	C(15)	91(1)
Cl(3)	Te(2)	C(4)	91(1)	Cl(12)	Te(6)	C(16)	92(1)
Cl(4)	Te(2)	C(3)	86(1)	C(15)	Te(6)	C(16)	99(2)
Cl(4)	Te(2)	C(4)	86(1)	N(1)	O(1)	C(19)	26(2)
C(3)	Te(2)	C(4)	96(2)	O(2)	O(3)	O(4)	108(5)
Cl(5)	Te(3)	Cl(6)	173.5(5)	O(1)	N(1)	C(19)	23(2)
Cl(5)	Te(3)	C(6)	88(1)	O(1)	N(1)	C(20)	147(3)
Cl(5)	Te(3)	C(7)	90(1)	O(1)	N(1)	C(21)	106(3)
Cl(6)	Te(3)	C(6)	89(1)	C(19)	N(1)	C(20)	126(4)
Cl(6)	Te(3)	C(7)	86(1)	C(19)	N(1)	C(21)	128(3)
C(6)	Te(3)	C(7)	107(2)	C(20)	N(1)	C(21)	107(4)
Cl(7)	Te(4)	Cl(8)	173.4(5)	Te(1)	C(1)	C(2)	116(2)
Cl(7)	Te(4)	C(10)	86(1)	Te(1)	C(1)	C(3)	149(2)
Cl(7)	Te(4)	C(18)	86(1)	C(2)	C(1)	C(3)	34(2)
Cl(8)	Te(4)	C(10)	89(1)	C(1)	C(2)	C(3)	110(3)
Cl(8)	Te(4)	C(18)	91(1)	Te(2)	C(3)	C(1)	155(2)
C(10)	Te(4)	C(18)	106(2)	Te(2)	C(3)	C(2)	123(3)
Cl(9)	Te(5)	Cl(10)	177.6(4)	C(1)	C(3)	C(2)	36(2)
Cl(9)	Te(5)	C(12)	91(1)	Te(2)	C(4)	C(5)	114(3)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
Te(2)	C(4)	C(6)	150(2)	C(13)	C(15)	C(14)	37(2)
C(5)	C(4)	C(6)	37(2)	Te(6)	C(16)	C(17)	112(3)
C(4)	C(5)	C(6)	109(4)	Te(6)	C(16)	C(18)	145(3)
Te(3)	C(6)	C(4)	150(2)	C(17)	C(16)	C(18)	34(2)
Te(3)	C(6)	C(5)	116(3)	C(16)	C(17)	C(18)	110(4)
C(4)	C(6)	C(5)	34(2)	Te(4)	C(18)	C(16)	149(2)
Te(3)	C(7)	C(8)	120(3)	Te(4)	C(18)	C(17)	114(3)
Te(3)	C(7)	C(9)	153(2)	C(16)	C(18)	C(17)	35(2)
C(8)	C(7)	C(9)	33(2)	O(1)	C(19)	N(1)	131(4)
C(7)	C(8)	C(9)	111(3)	O(1)	C(19)	C(20)	157(4)
Te(1)	C(9)	C(7)	153(2)	O(1)	C(19)	C(21)	105(3)
Te(1)	C(9)	C(8)	119(3)	N(1)	C(19)	C(20)	29(2)
C(7)	C(9)	C(8)	35(2)	N(1)	C(19)	C(21)	27(2)
Te(4)	C(10)	C(11)	128(3)	C(20)	C(19)	C(21)	56(3)
Te(4)	C(10)	C(12)	157(2)	N(1)	C(20)	C(19)	26(2)
C(11)	C(10)	C(12)	30(2)	N(1)	C(20)	C(21)	36(3)
C(10)	C(11)	C(12)	119(3)	C(19)	C(20)	C(21)	62(3)
Te(5)	C(12)	C(10)	153(2)	N(1)	C(21)	C(19)	25(2)
Te(5)	C(12)	C(11)	123(3)	N(1)	C(21)	C(20)	37(2)
C(10)	C(12)	C(11)	31(2)	C(19)	C(21)	C(20)	62(3)
Te(5)	C(13)	C(14)	113(3)				
Te(5)	C(13)	C(15)	148(2)				
C(14)	C(13)	C(15)	35(2)				
C(13)	C(14)	C(15)	108(3)				
Te(6)	C(15)	C(13)	157(2)				
Te(6)	C(15)	C(14)	122(2)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Torsion or Conformation Angles

(1)	(2)	(3)	(4)	angle
Te(1)	C(1)	C(2)	C(3)	172(3)
Te(1)	C(1)	C(3)	Te(2)	27(8)
Te(1)	C(1)	C(3)	C(2)	-14(5)
Te(1)	C(9)	C(7)	Te(3)	-19(9)
Te(1)	C(9)	C(7)	C(8)	-16(5)
Te(1)	C(9)	C(8)	C(7)	172(3)
Te(2)	C(3)	C(1)	C(2)	41(5)
Te(2)	C(3)	C(2)	C(1)	-161(3)
Te(2)	C(4)	C(5)	C(6)	173(3)
Te(2)	C(4)	C(6)	Te(3)	-7(8)
Te(2)	C(4)	C(6)	C(5)	-14(5)
Te(3)	C(6)	C(4)	C(5)	7(5)
Te(3)	C(6)	C(5)	C(4)	-176(3)
Te(3)	C(7)	C(8)	C(9)	179(3)
Te(3)	C(7)	C(9)	C(8)	-3(5)
Te(4)	C(10)	C(11)	C(12)	167(3)
Te(4)	C(10)	C(12)	Te(5)	-8(11)
Te(4)	C(10)	C(12)	C(11)	-26(6)
Te(4)	C(18)	C(16)	Te(6)	31(8)
Te(4)	C(18)	C(16)	C(17)	11(5)
Te(4)	C(18)	C(17)	C(16)	-174(3)
Te(5)	C(12)	C(10)	C(11)	18(6)
Te(5)	C(12)	C(11)	C(10)	-170(3)
Te(5)	C(13)	C(14)	C(15)	-172(2)
Te(5)	C(13)	C(15)	Te(6)	-16(8)
Te(5)	C(13)	C(15)	C(14)	14(4)
Te(6)	C(15)	C(13)	C(14)	-30(5)
Te(6)	C(15)	C(14)	C(13)	166(2)
Te(6)	C(16)	C(17)	C(18)	-168(3)
Te(6)	C(16)	C(18)	C(17)	20(5)
Cl(1)	Te(1)	C(1)	C(2)	-145(2)
Cl(1)	Te(1)	C(1)	C(3)	-137(4)
Cl(1)	Te(1)	C(9)	C(7)	74(5)
Cl(1)	Te(1)	C(9)	C(8)	63(3)
Cl(2)	Te(1)	C(1)	C(2)	33(2)
Cl(2)	Te(1)	C(1)	C(3)	42(4)
Cl(2)	Te(1)	C(9)	C(7)	-105(5)
Cl(2)	Te(1)	C(9)	C(8)	-116(3)
Cl(3)	Te(2)	C(3)	C(1)	-37(5)
Cl(3)	Te(2)	C(3)	C(2)	-9(3)
Cl(3)	Te(2)	C(4)	C(5)	28(3)
Cl(3)	Te(2)	C(4)	C(6)	37(4)
Cl(4)	Te(2)	C(3)	C(1)	141(6)
Cl(4)	Te(2)	C(3)	C(2)	168(3)
Cl(4)	Te(2)	C(4)	C(5)	-148(3)
Cl(4)	Te(2)	C(4)	C(6)	-140(4)
Cl(5)	Te(3)	C(6)	C(4)	112(4)
Cl(5)	Te(3)	C(6)	C(5)	117(3)
Cl(5)	Te(3)	C(7)	C(8)	-50(3)
Cl(5)	Te(3)	C(7)	C(9)	-48(5)
Cl(6)	Te(3)	C(6)	C(4)	-62(4)
Cl(6)	Te(3)	C(6)	C(5)	-58(3)

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.

Torsion or Conformation Angles cont

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
Cl(6)	Te(3)	C(7)	C(8)	126(3)	O(1)	N(1)	C(19)	C(20)	-162(5)
Cl(6)	Te(3)	C(7)	C(9)	127(5)	O(1)	N(1)	C(19)	C(21)	17(6)
Cl(7)	Te(4)	C(10)	C(11)	48(4)	O(1)	N(1)	C(20)	C(19)	13(3)
Cl(7)	Te(4)	C(10)	C(12)	64(6)	O(1)	N(1)	C(20)	C(21)	-166(6)
Cl(7)	Te(4)	C(18)	C(16)	-125(5)	O(1)	N(1)	C(21)	C(19)	-7(3)
Cl(7)	Te(4)	C(18)	C(17)	-118(3)	O(1)	N(1)	C(21)	C(20)	172(4)
Cl(8)	Te(4)	C(10)	C(11)	-128(4)	O(1)	C(19)	N(1)	C(20)	162(5)
Cl(8)	Te(4)	C(10)	C(12)	-111(6)	O(1)	C(19)	N(1)	C(21)	-17(6)
Cl(8)	Te(4)	C(18)	C(16)	50(4)	O(1)	C(19)	C(20)	N(1)	-37(9)
Cl(8)	Te(4)	C(18)	C(17)	57(3)	O(1)	C(19)	C(20)	C(21)	-37(9)
Cl(9)	Te(5)	C(12)	C(10)	-61(5)	O(1)	C(19)	C(21)	N(1)	167(5)
Cl(9)	Te(5)	C(12)	C(11)	-51(3)	O(1)	C(19)	C(21)	C(20)	166(4)
Cl(9)	Te(5)	C(13)	C(14)	139(3)	N(1)	O(1)	C(19)	C(20)	23(6)
Cl(9)	Te(5)	C(13)	C(15)	130(4)	N(1)	O(1)	C(19)	C(21)	-8(3)
Cl(10	Te(5)	C(12)	C(10)	117(5)	N(1)	C(19)	C(20)	C(21)	1(3)
Cl(10	Te(5)	C(12)	C(11)	128(3)	N(1)	C(19)	C(21)	C(20)	-1(3)
Cl(10	Te(5)	C(13)	C(14)	-38(3)	N(1)	C(20)	C(19)	C(21)	-1(3)
Cl(10	Te(5)	C(13)	C(15)	-47(4)	N(1)	C(20)	C(21)	C(19)	0(2)
Cl(11	Te(6)	C(15)	C(13)	-147(5)	N(1)	C(21)	C(19)	C(20)	1(3)
Cl(11	Te(6)	C(15)	C(14)	-167(3)	N(1)	C(21)	C(20)	C(19)	0(2)
Cl(11	Te(6)	C(16)	C(17)	139(3)	C(1)	Te(1)	C(9)	C(7)	-13(5)
Cl(11	Te(6)	C(16)	C(18)	127(4)	C(1)	Te(1)	C(9)	C(8)	-23(3)
Cl(12	Te(6)	C(15)	C(13)	31(5)	C(1)	C(3)	Te(2)	C(4)	55(6)
Cl(12	Te(6)	C(15)	C(14)	10(3)	C(2)	C(1)	Te(1)	C(9)	-56(3)
Cl(12	Te(6)	C(16)	C(17)	-38(3)	C(2)	C(3)	Te(2)	C(4)	82(4)
Cl(12	Te(6)	C(16)	C(18)	-50(4)	C(3)	Te(2)	C(4)	C(5)	-63(4)

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.

Torsion or Conformation Angles cont

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
C(3)	Te(2)	C(4)	C(6)	-54(5)					
C(3)	C(1)	Te(1)	C(9)	-48(4)					
C(4)	C(6)	Te(3)	C(7)	23(5)					
C(5)	C(6)	Te(3)	C(7)	27(3)					
C(6)	Te(3)	C(7)	C(8)	38(3)					
C(6)	Te(3)	C(7)	C(9)	40(5)					
C(10)	Te(4)	C(18)	C(16)	-40(5)					
C(10)	Te(4)	C(18)	C(17)	-33(4)					
C(10)	C(12)	Te(5)	C(13)	26(6)					
C(11)	C(10)	Te(4)	C(18)	-37(4)					
C(11)	C(12)	Te(5)	C(13)	36(4)					
C(12)	Te(5)	C(13)	C(14)	49(3)					
C(12)	Te(5)	C(13)	C(15)	40(4)					
C(12)	C(10)	Te(4)	C(18)	-21(7)					
C(13)	C(15)	Te(6)	C(16)	-61(5)					
C(14)	C(15)	Te(6)	C(16)	-82(3)					
C(15)	Te(6)	C(16)	C(17)	54(4)					
C(15)	Te(6)	C(16)	C(18)	42(5)					
C(19)	O(1)	N(1)	C(20)	-28(7)					
C(19)	O(1)	N(1)	C(21)	166(5)					
C(19)	N(1)	C(20)	C(21)	-179(5)					
C(19)	N(1)	C(21)	C(20)	179(5)					
C(19)	C(20)	N(1)	C(21)	179(5)					
C(19)	C(21)	N(1)	C(20)	-179(5)					
C(20)	N(1)	C(19)	C(21)	179(6)					
C(20)	C(19)	N(1)	C(21)	-179(6)					

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.

Intermolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
Te(1)	Cl(10)	3.62(1)	55601	Cl(9)	C(6)	3.75(4)	45501
Te(1)	Cl(11)	3.81(1)	56501	Cl(10)	C(9)	3.58(4)	55401
Te(2)	Cl(5)	3.36(1)	65501	Cl(10)	C(20)	3.61(8)	55601
Te(2)	Cl(1)	3.48(1)	65501	Cl(11)	C(1)	3.59(4)	54501
Te(3)	Cl(11)	3.628(9)	1	Cl(11)	C(6)	3.68(4)	1
Te(3)	Cl(8)	3.76(1)	55601	Cl(12)	C(7)	3.41(4)	55401
Te(4)	Cl(4)	3.61(1)	44501	Cl(12)	C(9)	3.49(4)	55401
Te(4)	Cl(6)	3.77(1)	45401	Cl(12)	C(11)	3.66(3)	65501
Te(5)	Cl(2)	3.64(1)	45401	O(1)	C(3)	3.33(5)	55401
Te(6)	Cl(7)	3.36(1)	65501	O(1)	C(1)	3.39(4)	55401
Te(6)	Cl(9)	3.48(1)	65501	O(1)	C(4)	3.53(4)	55401
Cl(1)	C(16)	3.65(5)	56501	O(1)	C(5)	3.54(5)	55401
Cl(1)	C(18)	3.70(4)	56501	O(1)	C(2)	3.68(4)	55401
Cl(1)	C(3)	3.79(5)	45501	O(1)	C(6)	3.72(4)	55401
Cl(2)	C(12)	3.60(5)	65601	O(1)	C(8)	3.76(3)	55401
Cl(3)	C(12)	3.52(5)	65601	O(2)	O(3)	2.17(6)	1
Cl(3)	C(10)	3.53(5)	65601	O(2)	O(4)	2.8(1)	1
Cl(4)	C(13)	3.57(4)	65501	O(2)	C(15)	3.34(6)	65501
Cl(4)	C(18)	3.67(4)	66501	O(2)	C(13)	3.42(6)	65501
Cl(5)	C(15)	3.53(4)	1	O(2)	C(17)	3.51(7)	65501
Cl(5)	C(4)	3.80(5)	45501	O(2)	C(14)	3.65(6)	65501
Cl(6)	C(10)	3.76(5)	65601	O(2)	C(18)	3.67(6)	65501
Cl(7)	C(3)	3.55(5)	44501	O(2)	C(16)	3.71(7)	65501
Cl(7)	C(16)	3.64(6)	45501	O(2)	C(11)	3.81(6)	65501
Cl(8)	C(7)	3.76(4)	55401	C(1)	C(16)	3.78(6)	56501
Cl(9)	C(4)	3.62(4)	45501				

Contacts out to 3.82 angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one-digit numbers and one two-digit number: TA (first digit) + TB (second digit) + TC (third digit) + SN (last two digits). TA, TB and TC are the crystal lattice translation digits along cell edges a, b and c. A translation digit of 5 indicates the origin unit cell. If TA = 4, this indicates a translation of one unit cell length along the a-axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus ± 4 lattice translations from the origin (TA=5, TB=5, TC=5) can be represented.

The SN, or symmetry operator number, refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always 55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of the atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through symmetry operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (eg. cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

(1) X, Y, Z