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The Crystal Structures of $AuTe_2Cl$ and $AuTe_2I$*

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The structures of $AuTe_2Cl$ and $AuTe_2I$ have been determined. Both compounds are orthorhombic: for $AuTe_2Cl$, $a = 4.020$ Å, $b = 11.867$ Å, $c = 8.773$ Å, $Z = 4$, space group *Cmcm*; for $AuTe_2I$, $a = 4.056$ Å, $b = 12.579$ Å, $c = 4.741$ Å, $Z = 2$, *Pmmb*. Intensities were measured on an automatic diffractometer, and the structures were refined, with anisotropic temperature factors, to $R = 2.1\%$ and $R = 3.5\%$, respectively. The structures consist essentially of corrugated two-dimensional nets of gold and tellurium atoms, with interleaving halogen atoms. The tellurium atoms form pairs coordinated to four gold atoms, and each gold atom is coordinated to four tellurium atoms.

Introduction

The preparation and some properties of four gold tellurium halides have been reported (*1*). Basic crystallographic properties of AuTeI and $AuTe_2X$ (X = Cl, Br, I) were given, and these indicated that $AuTe_2Cl$ and $AuTe_2Br$ were isotypes. The crystal structures of $AuTe_2Cl$ and $AuTe_2I$ have now been determined.

Experimental

Both compounds had been prepared by hydrothermal synthesis in hydrohalic acid. The crystals are silvery white, the chloride crystallizing in a square shape, the iodide as spears. Oscillation, Weissenberg, and precession photographs confirmed the orthorhombic symmetry, approximate cell dimensions, and cell contents previously reported (*1*) for both compounds. Improved lattice parameters were obtained by a least-squares fit of angle measurements, made on a diffractometer at room temperature, with copper radiation. The pertinent data are summarized in Table I.

Intensity measurements were made on a Siemens-type automatic diffractometer, with paper tape control, using Nb-filtered Mo$K\alpha$ radiation. The instrument was run in the 5-value $\theta/2\theta$ scanning mode, the maximum measuring time being 1.2 sec/0.01° in θ. Reflections were measured to an upper limit of $2\theta = 70°$ ($(\sin\theta)/\lambda \sim 0.8$ Å^{-1}). Intensities were checked against standard reflections; scaling remained constant during both sets of measurements.

Structure Determination and Refinement

Reflections with net negative intensities were set to zero, otherwise no distinction was made between observed and "less than" reflections. The standard deviations were assigned values of $\sigma_I = \sqrt{(\sigma_I)^2 + (0.02I)^2}$ and $\sigma_F = \sqrt{F^2 + \sigma_F^2} - F$. The atomic scattering

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TABLE I

CRYSTALLOGRAPHIC DATA

	$AuTe_2Cl$	$AuTe_2I$
Symmetry	orthorhombic	orthorhombic
Cell dimensions	$a = 4.0199(3)$ Å	$a = 4.056(1)$ Å
	$b = 11.8666(7)$ Å	$b = 12.579(2)$ Å
	$c = 8.7728(7)$ Å	$c = 4.741(1)$ Å
Cell volume	418.48 Å^3	241.9 Å^3
Formula weight	487.62	579.07
Z	4	2
Density (measured)	7.72	7.98
Density (X-ray)	7.738	7.949
Absorption coefficient[a], μ	507.6 cm^{-1}	498.2 cm^{-1}
Systematic absences	hkl: $h + k = 2n + 1$	$hk0$: $k = 2n + 1$
	$h0l$: $l = 2n + 1$	
Possible space groups	$Cmc2_1$	$Pm2_1b$ ($Pmc2_1$)[b]
	$C2cm$ ($Ama2$)	$P2mb$ ($Pma2$)
	$Cmcm$	$Pmmb$ ($Pmma$)
Final space group	$Cmcm$	$Pmmb$

[a] For molybdenum $K\alpha$ radiation.

[b] Symbols in parentheses are the conventional ones.

factors used were those of Cromer and Mann (*2*). A dispersion correction was made for all atoms, using Templeton-type factors (*3*). The intensities were corrected for absorption, using the Gaussian grid method. The program and its application were checked by the method suggested by Cahen and Ibers (*4*). In the full-matrix least-squares refinement, the function minimized is $\sum w(|F_o| - 1/k|F_c|)^2$; $w = (1/\sigma_F)^2$. Residuals quoted are

$$R = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}$$

and

$$Rw = \left[\frac{\sum w(|F_o| - |F_c|)^2}{\sum w|F_o|^2}\right]^{1/2}.$$

TABLE II

ATOMIC PARAMETERS

Atom	x[a]	y	z	U_{11}[b]	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
				$AuTe_2Cl$					
Au	0.00	0.08659(3)	0.25	0.0074(1)	0.0155(1)	0.0104(1)	0.0	0.0	0.0
Te	0.50	0.11077(3)	0.05161(4)	0.0081(2)	0.0152(2)	0.0101(2)	0.0	0.0	0.0001(1)
Cl	0.00	−0.16090(18)	0.25	0.0227(10)	0.0151(8)	0.0214(9)	0.0	0.0	0.0
				$AuTe_2I$					
Au	0.00	0.00	0.50	0.0115(2)	0.0268(3)	0.0117(2)	0.0	0.0	0.0027(2)
Te	0.50	0.08158(5)	0.19745(12)	0.0128(3)	0.0190(3)	0.0134(2)	0.0	0.0	0.0020(2)
I	0.00	0.25	0.73103(21)	0.0241(5)	0.0185(4)	0.0294(4)	0.0	0.0	0.0

[a] Values given in fractions of the lattice translations. Estimated standard deviations are in parentheses.

[b] The expression for the temperature factor is of the form: $\exp[-2\pi^2(U_{11}h^2a^{*2} + 2U_{23}klb^*c^* + \cdots)]$ with U_{ij} in Å^2.

Atomic coordinates and structure amplitude comparisons are given in Tables II and III.

$AuTe_2Cl$

The crystal of $AuTe_2Cl$ used for the intensity measurements was $0.040 \times 0.042 \times 0.120$ mm in size, mounted with the *a*-axis as the rotation (ϕ) axis, parallel to the longest dimension. No measurements were rejected during data reduction, and 544 independent reflections were available for the calculations. The absorption correction was based on a $9 \times 9 \times 27 = 2187$ grid. The value of A^* in the expression $I_{corr} = I_{obs} \cdot A^*$ varied from 4.84 to 7.59. The structure was completely determined by an analysis of the Patterson function, with the atoms in the following locations of the space group *Cmcm*:

Au and Cl in 4*c*	*mm*	0	*y*	1/4,
Te in 8*f*	*m*	1/2	*y*	*z*.

Three cycles of refinement, with anisotropic temperature factors, gave an *R* factor of 4.9% and a weighted *R* factor (*Rw*) of 6.0%. Six additional cycles, including an isotropic correction for extinction, after the method of Larson (*5*), further reduced *R* to 2.1% and *Rw* to 2.3%. The initial extinction coefficient of 0.0 converged at 3.56(6) on refinement. An additional set of three cycles, with a variation in the $\Delta f''$ term for gold, initially 10.1, had no influence on the *R* factors, with $\Delta f''$ converging at 10.8(2).

$AuTe_2I$

The $AuTe_2I$ crystal was $0.03 \times 0.05 \times 0.12$ mm in size. The *a*-axis was again taken as the rotation (ϕ) axis, parallel to the longest dimension. Five reflections were eliminated during data reduction because of poor agreement between duplicate measurements, and 622 independent reflections remained. The absorption correction was based on a $6 \times 10 \times 24 = 1440$ grid, and A^* varied from 3.76 to 9.32. The structure was first postulated by reference to the chloride structure, the lattice constant relations between the two compounds, and space group considerations. All details were then substantiated by a complete solution of the Patterson function. The setting *Pmmb* of the space group adopted was better suited to comparison of the structures than was the conventional one (*Pmma*). The atoms are in the following locations:

Au in 2*c*	2/*m*	0	0	1/2
Te in 4*j*	*m*	1/2	*y*	*z*
I in 2*e*	*mm*	0	1/4	*z*.

Three cycles of refinement, with isotropic temperature factors, gave $R = 10.4\%$, $Rw = 11.6\%$. This was followed by three cycles, with anisotropic temperature factors, reducing *R* to 5.0% and *Rw* to 5.5%. Two additional cycles, with an added extinction correction, gave $R = 3.5\%$ and $Rw = 3.6\%$. The initial estimated extinction coefficient of 3.0 converged at 2.90(8).

Discussion

The two structures bear a marked similarity to each other. Each consists essentially of corrugated two-dimensional nets of gold and tellurium atoms, with interleaving halogen atoms. The tellurium atoms form pairs, joined to successive gold atoms in a –Au–Te–Te–Au– sequence. Each gold atom is coordinated to four tellurium atoms, and each tellurium pair is likewise coordinated to four gold atoms. These considerations, and the unusually long gold–halogen distances, suggest that structurally the compounds might conceivably be represented as

$$[Au^{III}(Te_2)_{4/4}]^{(+)}X^{(-)},$$

in which the fourfold gold coordination is exactly planar in the iodide but distorted in the chloride.

The doubling of the *c*-axis in the chloride, as compared to the iodide, is associated with an alternating up-and-down arrangement of tellurium pairs within the nets. The gold atoms are consequently also alternately disposed in the chloride, but not in the iodide, in which the iodine atoms are equidistant from adjacent nets. We have no satisfactory explanation to offer for these fundamental structural differences, nor do the structures suggest any obvious explanation for the observed metallic

TABLE III

COMPARISON OF OBSERVED AND CALCULATED STRUCTURE AMPLITUDES (VALUES MULTIPLIED BY 10)

$AuTe_2Cl$

	0,0,L			8 514 516		0,14,L			4 109 118			7 1283 1277			5 741 738			6 1543 1560			2,14,L		
2 609 553			9 395 395			0 961 943			5 274 320			8 1177 1177			6 856 842			7 935 924			0 865 853		
4 2901 2858			10 1625 1613			1 753 750			6 0 32			9 1055 1049						8 477 494			1 712 702		
6 2604 2744			11 518 515			2 1155 1160			7 2726 2672			10 1005 1013			2,0,L			9 362 361			2 1060 1058		
8 249 282			12 455 438			3 1145 1134			8 1058 1036			11 863 865			0 3885 3861			10 1496 1494			3 1065 1054		
10 2731 2727			13 641 624			4 190 81			9 1026 1028			12 705 711			2 497 468			11 475 475			4 48 73		
12 263 316						5 401 455			10 466 478						4 2723 2619			12 398 415			5 433 434		
14 986 1021			0,8,L			6 190 156			11 634 642			1,11,L			6 2542 2402						6 86 145		
			0 986 1017			7 924 922			12 563 565			0 1054 1042			8 242 273			2,8,L			7 870 863		
0,2,L			1 2300 2307			8 892 903			13 1567 1576			1 720 711			10 2499 2510			0 856 875			8 840 837		
0 1598 1465			2 1919 1941			9 543 565						2 1556 1557			12 265 293			1 2034 2070					
1 2308 2290			3 753 774						1,5,L			3 1074 1092						2 1712 1723			2,16,L		
2 556 552			4 208 247			0,16,L			0 767 771			4 1135 1153			2,2,L			3 702 691			0 580 584		
3 824 799			5 2034 2675			0 646 641			1 1482 1512			5 1539 1533			0 1336 1353			4 219 225			1 297 300		
4 1045 1036			6 197 107			1 307 327			2 2990 3143			6 1023 1017			1 2165 2288			5 2386 2435			2 812 793		
5 3292 3301			7 653 661			2 885 867			3 466 473			7 763 766			2 492 505			6 75 103			3 1256 1261		
6 944 920			8 1386 1385			3 1385 1368			4 1080 1080			8 1145 1137			3 584 545			7 594 604			4 634 624		
7 328 369			9 1389 1369			4 688 682			5 1692 1674			9 397 379			4 926 906			8 1263 1258			5 302 320		
8 381 365			10 575 507			5 348 341			6 800 773			10 629 622			5 3149 3080			9 1261 1252			6 545 547		
9 1436 1426			11 1230 1232			6 587 596			7 384 371			11 498 486			6 850 818			10 464 465					
10 780 782			12 851 829			7 1083 1085			8 2421 2394						7 287 309			11 1139 1135			2,16,L		
11 1394 1396									9 786 776			1,13,L			8 340 341			12 779 769			0 274 265		
12 274 276			0,10,L			0,18,L			10 308 323			0 2168 2138			9 1297 1311						1 193 185		
13 239 253			0 2193 2230			0 318 289			11 732 694			1 587 572			10 705 718			2,10,L			2 1106 1082		
14 435 368			1 652 649			1 210 194			12 1502 1510			2 142 134			11 1307 1295			0 1969 1996					
			2 343 373			2 1180 1157			13 170 142			3 1102 1074			12 241 262			1 592 599			3,1,L		
0,4,L			3 1786 1817			3 105 156						4 1186 1183			13 200 234			2 315 311			0 233 222		
0 3235 3229			4 1135 1129			4 331 335			1,7,L			5 257 238						3 1627 1649			1 341 325		
1 2284 2335			5 193 217						0 1638 1643			6 1165 1157			2,4,L			4 1016 1029			2 2820 2750		
2 644 643			6 1096 1110			1,11,L			1 686 693			7 849 862			0 2889 3113			5 141 190			3 1841 1783		
3 1335 1347			7 1406 1401			0 268 249			2 989 998			8 93 143			1 2007 2091			6 1015 1019			4 1181 1147		
4 1925 1962			8 255 275			1 298 303			3 2757 2790			9 425 425			2 544 543			7 1294 1288			5 573 585		
5 2427 2447			9 516 515			2 3237 3158			4 1246 1254			10 1306 1300			3 1118 1142			8 276 242			6 989 893		
6 1083 1060			10 1309 1304			3 2333 2193			5 783 782						4 1717 1719			9 466 482			7 1356 1347		
7 1031 1002			11 338 320			4 1557 1486			6 1138 1139			1,15,L			5 2187 2197			10 1216 1213			8 2040 2047		
8 480 476			12 103 128			5 868 843			7 2151 2140			0 177 171			6 1675 1655			11 303 303			9 290 321		
9 1377 1350						6 1159 1109			8 693 691			1 1126 1108			7 912 901						10 186 169		
10 2028 2017			1,12,L			7 1701 1646			9 560 535			2 844 855			8 421 419			2,12,L			11 221 159		
11 1154 1159			0 739 735			8 2513 2457			10 940 930			3 156 170			9 1215 1227			0 659 670			12 1297 1305		
12 193 187			1 833 837			9 361 356			11 250 237			4 246 234			10 1844 1846			1 751 749					
13 475 476			2 1919 1928			10 189 181			12 501 504			5 1536 1518			11 1039 1063			2 1747 1752			3,3,L		
			3 695 668			11 165 160			13 1246 1262			6 176 166			12 199 178			3 612 615			0 738 742		
0,6,L			4 1136 1142			12 1503 1525						7 188 172			13 437 440			4 1044 1038			1 1156 1186		
0 4693 2699			5 1404 1446			13 942 955			1,9,L			8 645 645						5 1311 1350			2 1171 1180		
1 927 936			6 965 980			14 579 598			0 1898 1894						2,6,L			6 974 876			3 2831 2848		
2 714 739			7 476 483						1 1665 1655			1,17,L			0 2443 2501			7 430 444			4 82 54		
3 1537 1553			8 1440 1427			1,3,L			2 1578 1580			0 1414 1388			1 809 798			8 1299 1313			5 191 256		
4 1828 1848			9 489 447			0 950 949			3 1579 1609			1 442 437			2 663 687			9 387 410			6 85 42		
5 1886 1930			10 442 428			1 1521 1515			4 441 438			2 261 268			3 1311 1341			10 393 394			7 2265 2242		
6 1713 1714			11 494 499			2 1675 1662			5 1406 1407			3 208 229			4 1641 1668						8 831 818		
7 1051 1045						3 3305 3317			6 501 520			4 887 862			5 1709 1716						9 849 875		

			10 426 411			4 970 969			1 1497 1496			5 1048 1046			6 671 715								
	3,15,L		11 519 557			5 1282 1291			2 335 350			6 669 679			7 1272 1277								
0 1778 1787			12 453 470			6 860 862			3 842 819														
1 511 498						7 626 622			4 1258 1235			4,14,L			5,9,L								
2 146 124			3,5,L			8 960 971			5 1654 1632			0 660 661			0 997 988								
3 906 915			0 567 516			9 313 339			6 1245 1221			1 589 584			1 949 963								
4 983 985			1 1094 1112						7 682 684			2 838 830			2 904 918								
5 950 973			2 2580 2667			3,13,L			8 343 314			3 850 860			3 940 948								
6 758 748			3 342 343			0 1778 1787			9 951 945			4 123 59			4 235 194								
7 148 137			4 675 683			1 511 498			10 1454 1450						5 829 847								
			5 1291 1313			2 146 124						5,1,L			6 249 260								
3,15,L			6 651 661			3 906 915			4,6,L			0 101 194											
1 957 955			7 309 297			4 983 985			0 1888 1914			1 302 277			5,11,L								
2 727 710			8 2028 2021			5 950 973			1 578 557			2 1939 1910			0 646 634								
3 131 161			9 633 634			6 758 748			2 580 577			3 1232 1227			1 443 457								
4 252 187			10 262 266			7 148 137			3 921 926			4 812 793			2 921 943								
5 1321 1315			11 587 579						4 1284 1283			5 340 339			3 587 583								
			12 1265 1309			3,15,L			5 1298 1261			6 627 634			4 702 712								
3,17,L						1 957 955			6 1220 1222			7 996 977											
0 1187 1196			3,7,L			2 727 710			7 705 678			8 1467 1480			6,0,L								
			0 1318 1329			3 131 161			8 416 426			9 212 262			0 2167 2125								
4,0,L			1 551 537			4 252 187			9 0 285						2 265 271								
0 3313 3152			2 810 824			5 1321 1315						5,3,L			4 1321 1283								
2 408 365			3 2242 2291						4,8,L			0 491 485											
4 1996 1952			4 1038 1033			3,17,L			0 569 601			1 806 841			6,2,L								
6 1890 1882			5 578 600			0 1187 1196			1 1552 1540			2 709 726			0 696 629								
8 254 240			6 951 956						2 1256 1259			3 2026 2028			1 1178 1151								
10 1970 1982			7 1757 1776			4,0,L			3 522 524			4 79 11			2 282 280								
			8 598 601			0 3313 3152			4 182 177			5 267 207			3 248 204								
4,0,L			9 451 447			2 408 365			5 1836 1863			6 161 54			4 466 455								
0 1460 1480			10 796 805			4 1996 1952			6 124 89			7 1633 1634			5 1697 1663								
1 1328 1351			11 210 200			6 1890 1882			8 981 976			8 553 556											
2 1202 1277						8 254 240			9 966 976						6,4,L								
3 1203 1322			3,9,L			10 1970 1982						5,5,L			0 1556 1560								
4 355 321			0 1460 1480						4,10,L			0 273 297			1 968 966								
5 1145 1169			1 1328 1351			4,2,L			0 1549 1536			1 681 719			2 191 232								
6 391 399			2 1202 1277			0 1027 949			1 559 490			2 1855 1897			3 535 534								
7 1069 1074			3 1203 1322			1 1705 1703			2 203 202			3 174 225			4 834 802								
8 984 1002			4 355 321			2 368 385			3 1278 1278			4 634 653											
9 874 893			5 1145 1169			3 362 334			4 813 811			5 873 886			6,6,L								
10 832 852			6 391 399			4 697 663			5 127 148			6 495 504			0 1332 1320								
			7 1069 1074			5 2424 2399			6 807 813			7 212 198			1 386 368								
3,11,L			8 984 1002			6 637 619			7 1028 1026			8 1501 1498			2 430 441								
0 856 871			9 874 893			7 205 215			8 179 184						3 594 596								
1 583 597			10 832 852			8 297 283						5,7,L											
2 1272 1295						9 1043 1044			4,12,L			0 940 953											
3 892 857			4,4,L			10 578 573			0 520 514			1 352 373											
			0 2300 2373			11 1062 1049			1 559 561			2 509 614											
									2 1350 1347			3 1501 1601											
									3 484 474			4 754 761											
									4 812 798			5 421 421											

$AuTe_2I$

	0,K,0		19 99 71	11 153 156	10 758 726	1 281 280	4 457 463	17 221 210		2,K,6		1 221 192	1 169 139	2 651 633	8 620 617	10 214 237
2 1413 1092				12 164 82	11 853 842	2 366 356	5 125 117	18 599 603	0 575 582			2 1490 1510	2 700 708	3 405 386	9 121 87	
4 1259 1171		0,K,3		13 112 130	12 614 609	3 1031 1030	6 719 716		1 340 346	3	661 659	3 179 180	4 611 610		5,K,4	
6 983 975	0 1571 1680			14 10 59	13 566 575	4 1132 1138	7 116 6	2,K,3	2 702 706	4	131 110	4 337 344	5 307 310	0 427 428		
8 808 800	1 175 176			15 9 48	14 523 512	5 322 321		0 1469 1486	3 380 387	5	211 200	5 111 124	4,K,5	1 147 157		
10 599 614	2 1516 1569				15 243 237	6 584 581		1 145 128	4 270 273	6	574 587	6 177 169	0 449 450	2 253 252		
12 1060 1024	3 1000 1112				16 303 306	7 143 139	0 2498 2431	2 1398 1372	5 350 353	7	145 134	7 112 110	1 250 244	3 489 492		
14 488 507	4 328 332	0,K,5	0 621 657	17 458 471	8 887 901	1 2189 1083	3 926 934	6 340 340	8	87 95	8 241 226	2 531 517	4 578 559		
16 408 422	5 125 124		1 386 393	18 113 104	9 768 719	4 1658 1003	4 308 306	7 250 242	9	502 501	9 165 178	5,K,0	5 178 181		
18 339 336	6 176 166		2 780 789	19 244 255	10 188 191	6 791 782	5 84 86	8 175 168	10	945 956	10 431 433	0 151 186	6 346 358		
20 166 135	7 206 187		3 423 426		11 181 195	8 688 677	6 157 153	9 262 258	11	109 184	11 72 30	1 203 182	7 91 90		
	8 152 152		4 300 293	1,K,2	12 457 457	10 556 560	7 147 144	10 464 435	12	624 599	12 700 689	2 93 88		
	0,K,1		5 400 399	0 1454 1472	13 119 108	12 1375 1436	8 154 151	11 225 218	13	63 31		3 237 242	0,K,6	
0 908 868	9 738 758		6 362 381	1 279 263	14 126 129	14 457 469	9 632 645		14	723 714	3,K,6	4 15 186 183	8 823 873	0 1032 1019	
1 77 60	10 905 923		7 283 275	2 1913 1953	15 486 471	16 358 369	10 814 816	2,K,7	15	258 264	0 108 106		10 63 66	2 563 514	
2 908 903	11 139 119		8 184 177	3 922 934	16 448 428	18 313 295	11 126 92	0 607 615	16	25 46	1 108 122	4,K,5	12 118 82	4 359 339	
3 1730 1625	12 864 872		9 274 280	4 131 122	17 193 171		12 790 785	1 208 196	17	121 91	2 414 421	0 1069 1056		6 226 191	
4 1328 1359	13 46 74		10 495 486	5 257 268		2,K,1	13 43 54	2 601 603			3 471 479	1 88 45	5,K,1	8 220 233	
5 120 15	14 743 723		11 284 285	6 523 541		1 40 12	14 670 647	3 212 191		3,K,5	4 361 385	2 961 949	0 761 773		
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7 105 96	16 94 122			8 167 164	1 205 200	3 1581 1625	16 122 115	5 200 192	1	545 544	6 627 615	4 249 250	2 602 620	0 323 297	
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9 1454 1394	18 6 48		0 661 671	10 1225 1242	3 254 252	5 61 42		3,K,0	3	150 131	8 149 124	4 422 458	2 330 326		
10 502 538			1 211 221	11 246 230	4 446 432	6 1113 1122	2,K,4	0 356 331	4	658 657		5 472 492	3 545 551		
11 64 60	0,K,4		2 647 600	12 736 716	5 185 176	7 6 56	0 1171 1196	2 214 196	5	484 487	4,K,0	6 262 281	4 448 472		
12 372 366	0 1301 1369		3 203 208	13 68 33	6 243 234	8 981 961	1 549 543	4 1575 1591	6	1270 1277	0 1802 1773	7 388 389	5 47 84		
13 158 113	1 634 640		4 192 171	14 913 902	7 150 153	9 1242 1203	2 540 533	6 1175 1196	7	460 459	2 877 767	8 357 345	6 463 476		
14 269 288	2 589 583		5 208 215	15 340 334	8 291 282	10 493 479	3 629 624	8 1341 1399	8	749 765	4 666 631	9 357 387	7 38 44		
15 750 765	3 707 714		6 148 156	16 62 63	9 249 236	11 53 74	4 846 833	10 101 98	9	124 129	6 439 423	10 367 387			
16 392 402	4 957 957		7 207 193	17 55 107	10 518 516	12 326 327	5 513 517	12 156 148	10	355 360	8 434 434	11 353 363			
17 9 34	5 606 604		8 128 120	18 125 122	11 63 51	13 58 85	6 187 200	14 184 183	11	376 377	10 439 444	12 396 426			
18 329 334	6 208 200			19 0 24	12 843 841	14 240 245	7 440 432	16 558 572	12	135 112	12 961 1014		0,K,2		
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20 249 261	8 777 781	0 540 511	1,K,3		14 428 422	16 348 360	9 502 503		14	190 141	16 266 253	0 820 827	2 354 347		
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0,K,2	10 386 370	2 2647 1927	1 782 789			18 298 306	11 435 432	0 1262 1248	16	265 265	4,K,1	2 413 421	4 113 128		
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7 391 387		10 450 455	9 143 133	6 762 758	4 624 617	1 219 219	8 531 526	5	271 258	7 0 11	10 287 281				
8 739 764	0,K,5	11 497 507	10 450 455	7 151 137	5 487 497	2 141 150	9 374 354	6	492 490	8 677 670	11 292 307				
9 423 444	0 77 117		11 497 507	8 434 420	6 1786 1841	3 104 118	10 595 575	7	163 118	9 817 789	12 490 470				
10 761 767	1 257 261	1,K,1		9 526 517	7 321 322	4 962 958	11 616 616	8	690 705	10 365 354		5,K,3			
11 372 370	2 153 150	0 1645 1611	12 153 156	10 402 397	8 685 687	5 251 242	12 641 640	9	546 558	11 79 88		0 92 84			
12 369 376	3 179 146	1 1405 1362	13 342 337	11 163 159	9 391 385	6 984 964	13 420 424	10	163 186	12 214 242	4,K,5	1 290 294			
13 231 224	4 1072 1078	2 1331 1361	14 196 175	12 99 82	10 662 661	7 139 124	14 407 418	11	194 164	13 25 30	0 6 89	2 300 309			
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15 263 265	6 1074 1068	4 951 984	16 318 314	1,K,7	12 329 309	10 118 122	16 241 250	13	116 95	15 456 466	2 145 136	4 578 573			
16 263 262	7 151 150	5 1238 1275	17 253 241	0 78 75	13 222 194	11 156 135	17 361 367	14	153 122		3 75 63	5 269 268			
17 234 235	8 949 941	6 509 521	18 524 511	1 85 74	14 362 356	12 106 58				4,K,2	4 682 694	6 808 830			
18 238 229	9 159 164	7 1116 1014		2 332 333	15 243 240	13 121 119	3,K,2				5 172 156	7 258 260			
19 671 672	10 126 126	8 708 665	1,K,4	3 384 378	16 225 218	14 67 54	0 1170 1158	0 1160 1181			0 286 248	8 739 727			
				9 452 431	0 881 898						1 310 299	9 109 72			

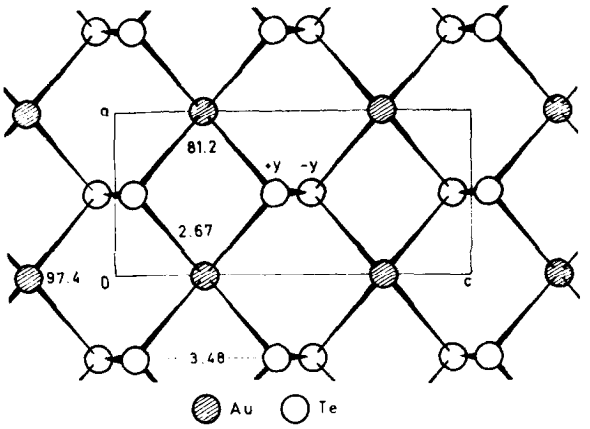

FIG. 1. $AuTe_2Cl$: Au–Te_2 net shown perpendicular to *b*-axis.

conductivity (*1*) of these compounds, in view of the long gold–gold distances (~4 Å).

$AuTe_2Cl$

The pertinent distances and angles are listed in Table IV. Figure 1 shows the gold–tellurium net, in which the tellurium–tellurium distance is 2.78 Å. This can be compared to the corresponding distance in ditellurides with pyrite and marcasite structures, in which the concept of tellurium pairs is commonly used. The gold–tellurium distance is 2.67 Å. In krennerite and calaverite, two forms of $AuTe_2$, the shortest reported gold–tellurium distances are 2.624 and 2.680 Å, respectively (*6*). A side view of the net planes is shown in Fig. 2, illustrating the distortion of the square planar coordination about gold. The chlorine atom is at a distance of 2.94 Å, considerably greater than the approximately 2.3 Å observed in

TABLE IV

BOND DISTANCES AND BOND ANGELS

	$AuTe_2Cl$		$AuTe_2I$	
Au–Te	2.6742(3) Å	4[a]	2.6876(6) Å	4[a]
Au–X	2.9369(22)	1	3.3300(6)	2
Te–Te	2.7805(5)	1	2.7781(6)	1
Te–Au–Te	81.21(1)°	2	82.03(2)°	2
	97.46(1)	2	97.98(2)	2
	167.68(2)	2	180.00(2)	2
Te–Au–X	96.16(1)	4	79.34(2)	4
	—		100.66(2)	4
X–Au–X	—		180.00	1
Au–Te–Au	97.46(1)	1	97.98(2)	1
Au–Te–Te	96.35(1)	2	94.45(2)	2
Au–X–Au	—		141.59(3)	1

[a] Number of equivalent distances from the first atom or of equivalent angles at the central atom.

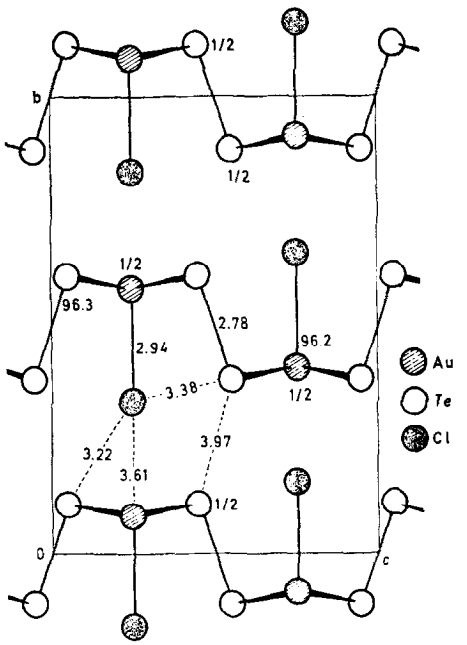

FIG. 2. $AuTe_2Cl$: Side view of structure perpendicular to *a*-axis.

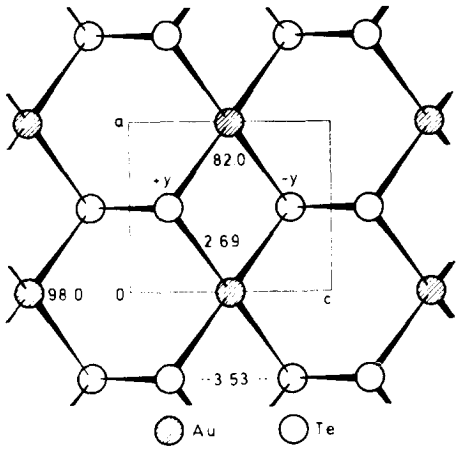

FIG. 3. $AuTe_2I$: $Au-Te_2$ net shown perpendicular to *b*-axis.

gold (III) chloride (*7*) and in rubidium tetrachloroaurate (*8*), in which chlorine is one of the four ligands of the square planar configuration. There is thus, in $AuTe_2Cl$, a pyramidal structure about the gold, with the apical atom (chlorine) at a distance greater than the equal distances (2.67 Å) of the four tellurium atoms.

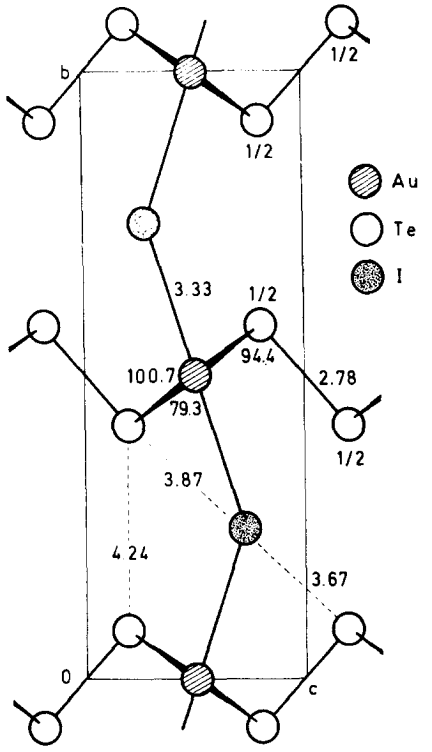

FIG. 4. $AuTe_2I$: Side view of structure perpendicular to *a*-axis.

$AuTe_2I$

Distances and angles are also listed in Table IV, and structural details are shown in Figs. 3 and 4. The tellurium–tellurium bonds in a net point in the same direction, the Te–Te distance again being 2.78 Å. The coordination of tellurium around the gold is perfectly planar, with a gold–tellurium distance of 2.69 Å. Neighboring layers are related by a symmetry plane passing through the interleaving halogen atoms, here equidistant from two gold atoms at what is again a relatively long distance of 3.33 Å, compared with 2.62 Å in the complex anion $[Au(CN)_2I_2]^-$ (*9*).

Acknowledgments

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References

1. A. RABENAU, H. RAU, AND G. ROSENSTEIN, *J. Less Common Metals* **21**, 395–401 (1970).
2. D. T. CROMER AND J. B. MANN, *Acta Cryst.* **A24**, 321–324 (1968).
3. "International Tables for X-Ray Crystallography," Vol. III, p. 216, Kynoch Press, Birmingham (1962).
4. D. CAHEN AND J. A. IBERS, *J. Appl. Cryst.* **5**, 298–299 (1972).
5. A. C. LARSON, *in* "Crystallographic Computing" (F. R. Ahmed, Ed.), pp. 291–294, Munksgaard, Copenhagen (1970).
6. R. V. BARANOVA, R. M. IMAMOV, AND Z. G. PINSKER *Kristallografiya* **16**, 127–137 (1971); *Sov. Phys. Crystallogr.* **16**, 99–106 (1971).
7. E. S. CLARK, D. H. TEMPLETON, AND C. H. MACGILLAVRY, *Acta Cryst.* **11**, 284–288 (1958).
8. J. STRÄHLE AND H. BÄRNIGHAUSEN, *Z. Naturforsch.* **25B**, 1186–1187 (1970).
9. C. BERTINOTTI AND A. BERTINOTTI, *Acta Cryst.* **B28**, 2635–2639 (1972)
10. K.-R. ALBRAND, Dissertation, Technische Universität Braunschweig, (1972).
11. The X-Ray System—Version of June 1972, Technical Report TR-192 of the Computer Science Center, University of Maryland, June 1972.