some bearing on the solution pmr studies. Close counterion approach to within 6.6–8.0 Å is achieved from four different directions and is to be compared with the 9.0 Å estimate made from solution studies. While none of the cations approaches exactly along the "C_3" axis of the anion, the two closest, A and B, do approach from the side opposite the triphenylphosphine. Cations C and D come almost as close *via* a sidewise approach. This latter mode of ion-pair contact was not considered in the analysis of the solution data. It is to be noted that close approach from the triphenylphosphine end of the anion does not occur.

While the factors which affect the structures of ion pairs in solution (counterion attraction and solvation considerations) and solid-state structure (Madelung energy and favorable packing) are by no means identical, the present results indicate that some caution must be exercised when interpreting solution-state pmr results in terms of quantitative interionic distance estimates. The assumption that the sole mode of counterion approach is along the "C_3" axis of the anion is particularly questionable. However, it is not unreasonable that this is perhaps the dominant situation in ion pairs in solution. A reevaluation of the solution-state data in terms of alternative modes of approach would not be fruitful in view of the additional unknown parameters involved.

Acknowledgments.—R. P. T. and W. D. H. wish to thank the Lawrence Radiation Laboratory for its hospitality during the course of this work. We are indebted to Mr. B. G. DeBoer, Dr. M. G. B. Drew, and Mrs. H. Ruben for considerable help and useful discussion involving all aspects of this work.

CONTRIBUTION FROM THE DEPARTMENT OF CHEMISTRY,
NORTHWESTERN UNIVERSITY, EVANSTON, ILLINOIS 60201

The Crystal and Molecular Structure of Chlorotriphenylphosphonium Bis(*cis*-1,2-bis(trifluoromethyl)ethene-1,2-dithiolato)gold, $[PCl(C_6H_5)_3][Au(S_2C_2(CF_3)_2)_2]$

BY JOHN H. ENEMARK AND JAMES A. IBERS

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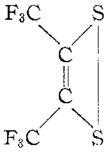
An X-ray diffraction study has shown that the product of the reaction between *cis*-bis(trifluoromethyl)-1,2-dithietene, $S_2C_2(CF_3)_2$, and chlorotriphenylphosphinegold, $(C_6H_5)_3PAuCl$, is the unexpected compound chlorotriphenylphosphonium bis(*cis*-1,2-bis(trifluoromethyl)ethene-1,2-dithiolato)gold, $[PCl(C_6H_5)_3][Au(S_2C_2(CF_3)_2)_2]$. The compound crystallizes in space group C_{2h}^5-$P2_1/n$ of the monoclinic system with four molecules in a cell of dimensions a = 13.166 (10), b = 11.623 (9), c = 20.486 (15) Å, and β = 91.21 (2)°. The calculated and observed densities are 2.01 and 2.03 (2) g cm^{-3}. Least-squares refinement of the structure has led to a final value of the conventional R factor of 0.070 for the 1858 reflections, observed by counter methods, for which $F_o^2 > 3\sigma(F_o^2)$. The structure consists of well-separated ions. The coordination about the Au atom of the anion is square planar, with the four independent Au–S distances ranging from 2.282 (8) to 2.296 (8) Å. The S–Au–S angles range from 89.6 (3) to 90.6 (3)°. The S···S intra- and interligand distances, which range from 3.225 (11) to 3.254 (11) Å, are considerably longer than those previously observed in square-planar dithiolate complexes. The chlorotriphenylphosphonium cation has nearly tetrahedral geometry; the P–Cl distance is 1.98 (1) Å and the three P–C distances are in the range 1.76–1.77 (2) Å.

Introduction

Because of a general interest in five-coordinate transition metal compounds and in *cis*-1,2-disubstituted ethene-1,2-dithiolato complexes (hereafter called dithiolate complexes), we were intrigued by the report of a novel five-coordinate gold complex $[(C_6H_5)_3P\cdot Au(S_2C_2(CF_3)_2)_2]Cl$. This compound was prepared by Davison, Howe, and Shawl[1] from the reaction of bis(trifluoromethyl)-1,2-dithietene (I) with chlorotriphenylphosphinegold, $(C_6H_5)_3PAuCl$. The results, reported here, of an X-ray diffraction study of this compound indicate that it does not contain five-coordinate gold but that an unusual reaction has occurred to yield the chlorotriphenylphosphonium cation and the square-planar bis(*cis*-1,2-bis(trifluoromethyl)ethene-1,2-dithiolato)gold anion.[2]



I

Collection and Reduction of the X-Ray Data

Pale green crystals of what proved to be $[PCl(C_6H_5)_3][Au(S_2C_2(CF_3)_2)_2]$ were kindly supplied by Professor A. Davison and were used without further recrystallization. Preliminary precession photographs taken with Cu Kα radiation indicated that the crystals

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[1] A. Davison, D. V. Howe, and E. T. Shawl, *Inorg. Chem.*, **6**, 458 (1967).

[2] This nomenclature follows that previously used (R. Eisenberg and J. A. Ibers, *ibid.*, **5**, 411 (1966), particularly footnote 20), and it is not meant to imply a particular valence bond description of the complex.

are monoclinic. The systematic absences $h0l$ when $h + l \neq 2n$ and $0k0$ when $k \neq 2n$ are consistent with the space group C_{2h}^5-$P2_1/n$. (The equivalent positions of this alternative setting of $P2_1/c$ are: $\pm(x, y, z)$; $\pm(^1/_2 - x, ^1/_2 + y, ^1/_2 - z)$.) At 22 ± 1° the cell constants are a = 13.166 (10), b = 11.623 (9), c = 20.486 (15) Å, β = 91.21 (2)°. These parameters were determined from least-squares refinement of the setting angles of 13 reflections that had been accurately centered on a Picker four-circle automatic diffractometer, as previously described.[3] In this refinement the wavelength of Mo Kα_1 radiation was taken as 0.70930 Å. The crystal density, determined as 2.03 (2) g cm^{-3} by flotation in diiodomethane–xylene mixtures, is in good agreement with that of 2.01 g cm^{-3} calculated for four formula units in the cell. Thus no crystallographic symmetry conditions need be imposed on the cation or anion.

For data collection, a crystal of dimensions 0.06 × 0.13 × 0.36 mm was sealed in a thin-walled glass capillary. The long axis of the crystal (the reciprocal vector (103)) was approximately coincident with the ϕ axis of the Picker four-circle diffractometer. The mosaicity of the crystal was checked from ω scans at a take-off angle of 0.5° on several independent reflections. All scans had peak widths at half-height of 0.15° or less. The intensities were recorded by procedures similar to those previously described.[3,4] Mo Kα radiation was used; the diffracted beams were filtered through 3.0 mils of Nb foil. The take-off angle was set to 1.2°; at this angle the intensity of the diffracted beam was about 75% of the maximum intensity as a function of take-off angle. The scintillation counter had an aperture of 4 × 4 mm and was 31 cm from the crystal. The pulse-height analyzer was set to admit about 90% of the Mo Kα peak. No attenuators were required as no reflections exceeded 7000 counts/sec during a scan. An asymmetric scan range was used to allow for Kα_1–Kα_2 dispersion at high angles. The scan was taken from −0.60° from the 2θ value calculated for Mo Kα_1 (0.70930 Å) radiation to +0.60° from the 2θ value calculated for a wavelength of 0.71496 Å. This latter value was determined empirically from several test scans. The scan rate was 1.0°/min and stationary crystal, stationary counter background counts of 10 sec each were taken at each end of the scan range. It was apparent from the chart tracings that there were few reflections of significant intensity beyond 2θ of 40°. Accordingly, the 2940 independent observations with $2\theta \leq 40°$ were gathered; these were reduced to values of F_o^2 and $\sigma(F_o^2)$ by methods previously described.[3,4] The value of p of 0.04 was chosen. Of the 2940 observations, 1082 had $F_o^2 < 3\sigma(F_o^2)$. During the data collection the intensities of four standard reflections in diverse regions of reciprocal space were monitored at least once a day. None of the four showed any significant variation in intensity during the 7 days required to collect the data.

Absorption is an important effect in the chosen crystal. The linear absorption coefficient for Mo Kα radiation is calculated to be 53.4 cm^{-1}. Therefore, the crystal was carefully measured by using a microscope equipped with a screw-micrometer eyepiece. The major faces of the crystal were identified by optical goniometry; these are: $\{010\}$ (plate faces); $\{10\bar{1}\}$, (103), and $(\bar{1}\bar{1}\bar{3})$. The magnitude of the absorption correction ranged from 1.4 to 1.9.[5] Secondary extinction is not a problem in this crystal (see Table I) and no extinction correction was made.

Solution of the Structure

The positions of the Au atom and the four S atoms were readily deduced from a three-dimensional Patterson function. Least-squares refinement of these positions as well as individual isotropic thermal parameters and an over-all scale factor was followed by a difference electron density map. The positions of the remaining nonhydrogen atoms were clearly visible on this map. At this point it was readily apparent that the compound did not contain the five-coordinate cationic gold complex $[(C_6H_5)_3P\cdot Au(S_2C_2(CF_3)_2)_2]Cl$ that had been proposed originally,[1] but rather the compound is correctly formulated as an anionic square-planar gold complex $[PCl(C_6H_5)_3][Au(S_2C_2(CF_3)_2)_2]$. Although five-coordination is now a reasonably common phenomenon in inorganic chemistry, this present case provides yet another example[6] of the dangers of deducing coordination number from indirect chemical and physical evidence. Since square-planar gold is certainly not a novelty in structural inorganic chemistry and since the refinement of this many-variable problem (45 nonhydrogen atoms) involves considerable computing, the following refinement sequence was carried out in an attempt to minimize computing time concomitant with the determination of structural parameters of interest.

Refinement was based on $|F_o|$, the quantity minimized being $\Sigma w(|F_o| - |F_c|)^2$, with the weights w taken as $4F_o^2/\sigma^2(F_o^2)$. The atomic scattering factors for Cl, P, S, F, and C were from the usual tabulation;[7] those for Au were from the calculations of Cromer and Waber.[8] The hydrogen scattering factors were those of Stewart, *et al.*[9] The effects of anomalous scattering were included in F_c;[10] the values of $\Delta f'$ and $\Delta f''$ calculated by Cromer[11] were used for Au, Cl, S, and P. The initial structure factor calculation based on all 45 nonhydrogen atoms gave $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o| = 0.31$ and $R_2 = (\Sigma w(|F_o| - |F_c|)^2/\Sigma w\cdot F_o^2)^{1/2} = 0.34$ for the 1858 reflections with $F_o^2 > 3\sigma$-

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(3) P. W. R. Corfield, R. J. Doedens, and J. A. Ibers, *Inorg. Chem.*, **6**, 197 (1967).

(4) R. J. Doedens and J. A. Ibers, *ibid.*, **6**, 204 (1967).

(5) GONO, Hamilton's general absorption program, was used for this calculation. Other programs used included local versions of Zalkin's FORDAP Fourier summation program, Busing and Levy's ORFFE bond distance and angle program, Johnson's ORTEP plotting program, and various local programs for data processing and least-squares refinement.

(6) H. C. Clark, P. W. R. Corfield, K. R. Dixon, and J. A. Ibers, *J. Am. Chem. Soc.*, **89**, 3360 (1967).

(7) J. A. Ibers, "International Tables for X-ray Crystallography," Vol. 3, The Kynoch Press, Birmingham, England, 1962, Table 3.3.1A.

(8) D. T. Cromer and J. T. Waber, *Acta Cryst.*, **18**, 104 (1965).

(9) R. F. Stewart, E. R. Davidson, and W. T. Simpson, *J. Chem. Phys.*, **42**, 3175 (1965).

(10) J. A. Ibers and W. C. Hamilton, *Acta Cryst.*, **17**, 781 (1964).

(11) D. T. Cromer, *ibid.*, **18**, 17 (1965).

TABLE I

VALUES OF $|F_o|$ AND $|F_c|$ (IN ELECTRONS) FOR $[P(Cl)(C_6H_5)_3][Au(S_2C_2(CF_3)_2)_2]$

K	L	FO	FC
***** H = 0 *****			
0	0		1816
0	2	337	295
0	4	180	180
0	6	196	210
0	8	63	63
0	10	51	63
0	12	84	87
0	14	110	105
0	16	121	112
0	18	113	119
1	1	220	203
1	2	31	29
1	3	153	150
1	4	179	192
1	5	116	106
1	6	193	193
1	7	67	66
1	8	207	221
1	9	79	69
1	10	215	211
1	11	5	6
1	12	179	179
1	13	46	47
1	14	176	182
1	15	60	63
1	16	84	90
1	17	51	48
1	18	49	45
1	19	40	51
2	0	376	376
2	1	129	120
2	2	234	235
2	3	168	173
2	4	323	337
2	5	223	220
2	6	97	86
2	7	175	163
2	8	27	15
2	9	120	125
2	10	16	0
2	11	169	164
2	12	59	57
2	13	122	116
2	14	41	27
2	15	84	76
2	16	41	42
2	17	18	7
2	18	85	88
2	19	31	17
3	1	270	264
3	2	80	74
3	3	258	260
3	4	128	120
3	5	141	145
3	6	77	83
3	7	98	106
3	8	100	89
3	9	77	75
3	10	45	46
3	11	25	17
3	12	11	28
3	13	74	63
3	14	69	67
3	15	67	65
3	16	48	47
3	17	119	113
3	18	38	36
3	19	116	119
4	0	88	90
4	1	93	36
4	2	17	33
4	3	113	107
4	4	66	52
4	5	133	139
4	6	38	62
4	7	243	221
4	8	36	37
4	9	147	126
4	10	0	5
4	11	88	102
4	12	54	46
4	13	89	81
4	14	42	41
4	15	93	90
4	16	0	26
4	17	53	41
4	18	0	5
5	1	104	104
5	2	27	27
5	3	115	105
5	4	32	42
5	5	110	106
5	6	220	219
5	7	108	120
5	8	26	35
5	9	23	27
5	10	27	35
5	11	40	23
5	12	59	48
5	13	34	24
5	14	22	9
5	15	65	61
5	16	56	54
5	17	86	94
6	0	67	67
6	1	44	39
6	2	149	151
6	3	86	72
6	4	125	120
6	5	67	59
6	6	0	14
6	7	27	42
6	8	19	11
6	9	49	46
6	10	53	60
6	11	66	65
6	12	37	22
6	13	30	26
6	14	53	47
6	15	32	36
6	16	53	57
7	1	15	5
7	2	64	68
7	3	51	60
7	4	37	52
7	5	21	19
7	6	79	76
7	7	0	11
7	8	66	59
7	9	11	22
7	10	68	74
7	11	43	38
7	12	88	98
7	13	0	21
7	14	65	67
7	15	11	25
8	0	110	95
8	1	26	11
8	2	122	129
8	3	0	4
8	4	87	96
8	5	0	9
8	6	19	28
8	7	23	25
8	8	55	46
8	9	20	14
8	10	25	32
8	11	17	19
8	12	0	11
8	13	9	20
9	1	64	61
9	2	46	45
9	3	60	48
9	4	34	32
9	5	38	29
9	6	34	32
9	7	26	7
9	8	38	54
9	9	23	22
9	10	76	70
9	11	0	7
10	0	0	19
10	1	0	12
10	2	59	62
10	3	38	47
10	4	50	45
10	5	46	47
10	6	0	5
10	7	59	54
10	8	23	12
11	1	55	60
11	2	7	5
11	3	65	65
***** H = 1 *****			
0	-19	95	99
0	-17	44	54
0	-15	110	97
0	-13	39	29
0	-11	92	90
0	-9	109	100
0	-7	166	167
0	-5	238	230
0	-3	75	76
0	-1	279	262
0	1	293	258
0	3	357	358
0	5	146	137
0	7	48	50
0	9	18	23
0	11	214	216
0	13	115	123
0	15	111	121
0	17	126	133
0	19	44	60
1	-19	39	45
1	-18	29	21
1	-17	104	104
1	-16	42	32
1	-15	188	186
1	-14	81	83
1	-13	233	230
1	-12	32	17
1	-11	224	220
1	-10	149	153
1	-9	276	263
1	-8	99	99
1	-7	86	91
1	-6	26	35
1	-5	73	67
1	-4	82	74
1	-3	15	29
1	-2	85	82
1	-1	9	14
1	0	151	138
1	1	208	194
1	2	134	126
1	3	336	339
1	4	122	116
1	5	225	234
1	6	7	5
1	7	199	204
1	8	45	48
1	9	150	178
1	10	41	55
1	11	170	180
1	12	57	45
1	13	147	150
1	14	55	61
1	15	22	41
1	16	59	56
1	17	46	47
1	18	20	29
1	19	23	11
2	-19	91	85
2	-18	67	66
2	-17	44	40
2	-16	101	99
2	-15	31	33
2	-14	131	127
2	-13	29	10
2	-12	123	134
2	-11	52	39
2	-10	153	140
2	-9	0	30
2	-8	143	155
2	-7	53	62
2	-6	19	17
2	-5	129	121
2	-4	24	25
2	-3	67	60
2	-2	73	64
2	-1	241	234
2	0	2	12
2	1	118	122
2	2	182	200
2	3	358	384
2	4	432	461
2	5	187	215
2	6	199	212
2	7	7	10
2	8	97	104
2	9	23	4
2	10	162	167
2	11	77	66
2	12	114	120
2	13	20	51
2	14	29	40
2	15	38	52
2	16	41	40
2	17	61	65
2	18	19	15
2	19	53	54
3	-19	0	15
3	-18	89	83
3	-17	30	31
3	-16	71	69
3	-15	35	51
3	-14	63	55
3	-13	54	50
3	-12	12	15
3	-11	75	84
3	-10	91	89
3	-9	92	91
3	-8	220	210
3	-7	137	133
3	-6	240	232
3	-5	114	125
3	-4	142	149
3	-3	56	68
3	-2	398	400
3	-1	8	14
3	0	38	45
3	1	125	125
3	2	129	121
3	3	12	8
3	4	67	68
3	5	13	19
3	6	98	84
3	7	119	124
3	8	30	28
3	9	69	71
3	10	95	93
3	11	18	32
3	12	66	75
3	13	73	76
3	14	68	69
3	15	36	24
3	16	95	103
3	17	77	69
3	18	88	95
4	-18	74	66
4	-17	0	6
4	-16	132	129
4	-15	28	9
4	-14	103	110
4	-13	28	2
4	-12	121	119
4	-11	0	21
4	-10	135	150
4	-9	71	70
4	-8	156	159
4	-7	77	75
4	-6	145	141
4	-5	0	17
4	-4	33	41
4	-3	85	80
4	-2	12	10
4	-1	0	10
4	0	58	56
4	1	50	64
4	2	107	113
4	3	56	53
4	4	190	196
4	5	60	80
4	6	274	274
4	7	36	39
4	8	246	264
4	9	116	113
4	10	149	151
4	11	33	20
4	12	82	71
4	13	46	42
4	14	59	63
4	15	17	10
4	16	29	32
4	17	31	17
4	18	0	3
5	-17	66	65
5	-16	66	58
5	-15	58	44
5	-14	18	16
5	-13	81	82
5	-12	0	22
5	-11	39	25
5	-10	42	29
5	-9	51	44
5	-8	45	53
5	-7	92	88
5	-6	182	187
5	-5	91	56
5	-4	119	128
5	-3	17	4
5	-2	176	173
5	-1	26	41
5	0	111	114
5	1	45	61
5	2	124	146
5	3	53	55
5	4	58	65
5	5	160	154
5	6	69	69
5	7	45	45
5	8	24	5
5	9	85	86
5	10	31	12
5	11	36	51
5	12	57	43
5	13	0	16
5	14	53	42
5	15	28	10
5	16	70	77
5	17	16	6
6	-16	22	21
6	-15	0	13
6	-14	51	55
6	-13	8	11
6	-12	92	86
6	-11	13	5
6	-10	52	45
6	-9	50	65
6	-8	20	11
6	-7	22	47
6	-6	62	70
6	-5	108	104
6	-4	29	29
6	-3	137	142
6	-2	63	51
6	-1	97	107
6	0	23	23
6	1	104	113
6	2	92	93
6	3	118	123
6	4	53	56
6	5	86	92
6	6	127	118
6	7	25	33
6	8	105	103
6	9	57	64
6	10	87	90
6	11	34	36
6	12	36	41
6	13	84	76
6	14	41	30
6	15	61	73
6	16	28	6
7	-15	52	60
7	-14	19	14
7	-13	117	113
7	-12	24	17
7	-11	99	91
7	-10	0	9
7	-9	63	70
7	-8	43	36
7	-7	51	56
7	-6	0	24
7	-5	31	19
7	-4	25	18
7	-3	13	26
7	-2	0	9
7	-1	68	59
7	0	58	44
7	1	101	86
7	2	34	8
7	3	72	58
7	4	14	22
7	5	131	140
7	6	0	27
7	7	86	95
7	8	25	23
7	9	144	135
7	10	63	60
7	11	83	81
7	12	31	17
7	13	60	62
7	14	50	39
7	15	51	46
8	-13	0	14
8	-12	34	24
8	-11	0	5
8	-10	0	9
8	-9	50	57
8	-8	63	56
8	-7	39	31
8	-6	31	9
8	-5	80	64
8	-4	21	21
8	-3	74	83
8	-2	29	17
8	-1	107	119
8	0	26	6
8	1	167	170
8	2	0	2
8	3	80	69
8	4	40	26
8	5	21	24
8	6	5	8
8	7	39	26
8	8	33	30
8	9	26	39
8	10	0	14
8	11	38	38
8	12	12	25
8	13	92	77
9	-11	54	61
9	-10	45	42
9	-9	57	60
9	-8	12	15
9	-7	21	21
9	-6	36	31
9	-5	11	5
9	-4	37	41
9	-3	27	5
9	-2	55	50
9	-1	51	50
9	0	78	79
9	1	87	76
9	2	47	47
9	3	23	36
9	4	0	29
9	5	79	82
9	6	31	24
9	7	57	73
9	8	34	8
9	9	71	79
9	10	15	13
9	11	31	36
10	-8	50	43
10	-7	9	13
10	-6	26	37
10	-5	52	57
10	-4	49	39
10	-3	54	42
10	-2	0	7
10	-1	37	20
10	0	33	24
10	1	57	53
10	2	44	49
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1	5	21	29
1	6	110	101
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1	8	132	117
1	9	17	23
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1	11	13	16
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3	11	29	5
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5	12	59	59
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6	8	48	63
6	9	60	68
6	10	15	15
7	-9	24	8
7	-8	93	93
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7	-2	49	44
7	-1	31	29
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7	4	39	48
7	5	21	12
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7	7	18	2
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8	5	30	11
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0	5	61	70
0	7	20	15
0	9	22	9
0	11	58	61
0	13	37	32
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1	-10	32	25
1	-9	70	68
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1	-6	82	73
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1	-2	35	29
1	-1	26	20
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2	-8	57	64
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2	-5	60	76
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2	8	74	72
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2	12	45	44
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3	-10	29	23
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3	7	0	26
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3	10	33	41
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6	4	65	61
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6	6	63	60
6	7	52	46
6	8	72	68
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7	-5	36	32
7	-4	33	38
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7	4	0	4
7	5	115	114
7	6	28	14
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0	6	15	11
0	8	56	61
0	10	82	82
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2	10	56	62
2	11	22	28
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3	-9	89	79
3	-8	17	25
3	-7	62	56
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3	-5	62	66
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4	3	127	133
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4	9	73	70
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5	4	82	79
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6	-4	91	92
6	-3	32	44
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6	-1	48	64
6	0	86	98
6	1	79	77
6	2	36	34
6	3	51	56
6	4	31	4
6	5	58	61
***** H = 11 *****			
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0	-7	115	101
0	-5	127	128
0	-3	114	119
0	-1	42	40
0	1	28	21
0	3	21	5
0	5	30	22
0	7	117	112
0	9	135	122
1	-10	34	22
1	-9	12	10
1	-8	41	31
1	-7	25	13
1	-6	61	59
1	-5	57	60
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1	-1	72	74
1	0	34	26
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1	2	41	39
1	3	74	78
1	4	36	26
1	5	131	121
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1	7	89	81
1	8	44	42
1	9	76	65
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2	-4	32	40
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2	1	4	14
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2	3	61	52
2	4	97	95
2	5	57	60
2	6	76	74
2	7	64	64
2	8	82	78
3	-8	96	85
3	-7	0	28
3	-6	84	81
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3	-4	71	87
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3	-2	51	60
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3	0	71	57
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3	2	30	22
3	3	18	23
3	4	18	12
3	5	27	27
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3	7	17	7
4	-7	19	6
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4	-4	40	38
4	-3	18	28
4	-2	73	70
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4	2	101	104
4	3	32	40
4	4	106	111
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4	6	63	68
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5	2	13	9
5	3	55	57
5	4	0	24
***** H = 12 *****			
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0	2	25	14
0	4	56	54
0	6	90	110
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1	-5	39	47
1	-4	75	80
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1	-1	18	3
1	0	114	109
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1	2	83	94
1	3	14	3
1	4	74	85
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2	-4	35	34
2	-3	65	60
2	-2	20	26
2	-1	93	102
2	0	30	14
2	1	71	79
2	2	33	44
2	3	95	90
2	4	54	59
2	5	52	63
3	-4	26	29
3	-3	32	33
3	-2	38	35
3	-1	16	20
3	0	30	30
3	1	0	10
3	2	44	36
3	3	33	28

(F_o^2). (These reflections, which we describe as being above background, were the only ones employed in the refinements.) In a subsequent refinement the phenyl rings were treated as rigid groups[12] (C–C = 1.397 Å, D_{6h} symmetry) with each ring assigned a single isotropic thermal parameter; all nongroup atoms were allowed to vibrate isotropically. Three cycles of full-matrix refinement resulted in convergence of this isotropic model to values of R_1 and R_2 of 0.091 and 0.100, respectively. A disturbing feature of the results was the large vibration of the F atoms. Thermal parameters on the F atoms ranged from 7 to 15 Å^2, corresponding to root-mean-square (rms) amplitudes of vibration of 0.30–0.44 Å. A difference electron density map was computed from the signs obtained from a structure factor calculation from which the 12 F atoms had been omitted. (Phenyl hydrogen atoms (C–H = 1.08 Å) were included at this point as fixed contributions.) From this map it is apparent that the CF_3 groups are undergoing hindered rotation about the C–C bonds: the F atoms reappear in this map at their original positions with peak heights of 3–5 e/Å^3, but the peaks themselves are very diffuse and there are regions of electron density as high as 1.8 e/Å^3 between the F atoms. This map also contained residual electron density of the order of 4–5 e/Å^3 near the gold atom, as is expected if the gold atom is undergoing vibrations that are significantly anisotropic.

Despite the inadequacy of describing the thermal motions of each F atom by a single isotropic thermal parameter, refinement was continued from the original model with the addition of anisotropic thermal parameters for the Au and four S atoms. Two more cycles of least-squares refinement (155 variable parameters) resulted in convergence to values of R_1 and R_2 of 0.070 and 0.080, respectively. A difference electron density map, with the contributions of all atoms subtracted out, was again calculated; the largest residual was 1.8 (1) e/Å^3 and the 11 largest peaks (all of height greater than 1.2 e/Å^3) could be interpreted as residuals of the CF_3 groups. On this same scale the F atoms in their assumed positions had heights of about 6 e/Å^3.

Obviously, the model is unsuitable for a description of the scattering of the F atoms, because of the complex thermal motions of the CF_3 groups. A proper model would treat these CF_3 groups as coupled, hindered rotors. Such a model would lead to extensive and expensive calculation that would not result in an appreciably better description of those parts of the structure of chemical interest, namely, the inner parts of the anion and the cation. Thus we leave a complete description of the thermal motions of the CF_3 groups as an exercise for the wealthy reader and justify this procedure by noting that the difference map is very clean in the region of the Au and S atoms and that, with the exception of the C–F distances, chemically equivalent distances agree with one another to well within the estimated standard deviations. The values of $|F_o|$ and $|F_c|$ (in

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(12) S. J. La Placa and J. A. Ibers, *Acta. Cryst.*, **18**, 511 (1965); R. Eisenberg and J. A. Ibers, *Inorg. Chem.*, **4**, 773 (1965).

electrons) for all 2940 observations are included in Table I. The 1082 data which were not included in the least-squares refinements ($F_o^2 < 3\sigma(F_o^2)$) generally have $|F_o| < 30$. A final structure factor calculation on all 2940 reflections gives $R_1 = 0.116$ and $R_2 = 0.088$.

The standard deviation of an observation of unit weight for the 1858 reflections used in the refinement is 2.00. Analysis of this quantity as a function of $|F_o|$ and of scattering angle shows a range of 1.5–2.7, with the value decreasing with increasing scattering angle. In view of the improper treatment of the CF_3 scattering, this dependence is not surprising. We believe that the data, including the weighting scheme, are better than the model used in the refinement.

The final structural parameters are given in Table II and the derived fractional coordinates of the phenyl carbon atoms are given in Table III.

Table II

Final Atomic and Group Parameters for $[PCl(C_6H_5)_3][Au(S_2C_2(CF_3)_2)_2]$

Atom	x[a]	y	z	B, Å^2
Au	0.06202 (8)	0.18316 (11)	0.02465 (5)	[b]
S_1	0.1151 (5)	0.3126 (9)	−0.0519 (4)	[b]
S_2	0.2229 (6)	0.1108 (8)	0.0325 (4)	[b]
S_3	0.0097 (6)	0.0589 (8)	0.1043 (4)	[b]
S_4	−0.0991 (6)	0.2551 (8)	0.0155 (4)	[b]
P	0.2019 (6)	0.2531 (8)	0.3017 (4)	3.6 (2)
Cl	0.2276 (7)	0.3652 (8)	0.3731 (4)	5.8 (2)
C_1	0.241 (2)	0.275 (2)	−0.062 (1)	3.1 (6)
C_2	0.288 (2)	0.195 (3)	−0.025 (1)	3.9 (6)
C_3	−0.117 (2)	0.102 (3)	0.113 (1)	3.7 (7)
C_4	−0.161 (2)	0.178 (3)	0.078 (1)	2.9 (5)
C_5	0.291 (4)	0.355 (4)	−0.107 (2)	7.9 (12)
C_6	0.395 (3)	0.163 (4)	−0.029 (2)	8.0 (11)
C_7	−0.167 (3)	0.038 (4)	0.164 (2)	7.3 (10)
C_8	−0.273 (4)	0.229 (5)	0.087 (3)	9.5 (14)
F_1	0.237 (2)	0.425 (3)	−0.140 (1)	12.0 (8)
F_2	0.304 (2)	0.281 (3)	−0.165 (2)	13.6 (9)
F_3	0.383 (3)	0.367 (3)	−0.106 (2)	15.3 (11)
F	0.427 (2)	0.127 (2)	−0.087 (1)	7.5 (5)
F_5	0.457 (2)	0.238 (3)	−0.010 (1)	12.9 (9)
F_6	0.424 (2)	0.077 (3)	0.009 (1)	12.0 (8)
F_7	−0.119 (2)	−0.060 (3)	0.182 (1)	13.1 (9)
F_8	−0.168 (2)	0.087 (3)	0.221 (2)	13.1 (9)
F_9	−0.253 (2)	0.000 (2)	0.157 (1)	10.9 (7)
F_{10}	−0.290 (2)	0.319 (3)	0.051 (1)	12.7 (8)
F_{11}	−0.290 (2)	0.255 (2)	0.145 (1)	9.7 (7)
F_{12}	−0.335 (2)	0.151 (3)	0.073 (2)	13.8 (10)

Atom	$10^4\beta_{11}$[c]	$10^4\beta_{22}$	$10^4\beta_{33}$	$10^4\beta_{12}$	$10^4\beta_{13}$	$10^4\beta_{23}$
Au	41.5 (7)	81.6 (12)	16.4 (3)	12.2 (11)	−0.5 (3)	0.8 (7)
S_1	54 (5)	103 (9)	30 (2)	16 (7)	7 (3)	25 (5)
S_2	52 (6)	109 (10)	31 (3)	27 (6)	−3 (3)	14 (4)
S_3	51 (6)	93 (9)	27 (2)	8 (6)	2 (3)	12 (4)
S_4	49 (5)	128 (10)	19 (2)	14 (6)	−3 (3)	15 (4)

Group[d]	x_c	y_c	z_c
R_1	0.0541 (10)	0.3699 (12)	0.1985 (6)
R_2	0.4136 (10)	0.1807 (11)	0.2446 (6)
R_3	0.1090 (9)	0.0280 (13)	0.3632 (7)

δ	ϵ	η	B, Å^2
−1.24 (1)	2.54 (1)	−2.26 (2)	4.5 (3)
−0.89 (2)	−2.24 (1)	−0.65 (2)	4.7 (3)
−1.15 (2)	−2.10 (1)	0.91 (3)	5.3 (3)

[a] x, y, and z are in fractional monoclinic coordinates. The standard deviation of the least significant digits is given in parentheses. [b] Atom refined anisotropically. [c] Anisotropic thermal parameters are in the form: $\exp[-(h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23})]$. [d] x_c, y_c, and z_c are the fractional coordinates of the group centers. The angles δ, ϵ, and η (in radians) which bring about alignment (except for translation) of an internal coordinate system within the ring with a fixed external coordinate system are those previously described.[12] B is the isotropic thermal parameter of the group.

Table III

Derived Parameters for Group Carbon Atoms[a]

	x	y	z
		R_1	
C_1	0.120 (1)	0.315 (2)	0.2428 (9)
C_2	0.015 (1)	0.315 (2)	0.2532 (8)
C_3	−0.050 (1)	0.370 (2)	0.2089 (10)
C_4	−0.012 (1)	0.425 (2)	0.1543 (9)
C_5	0.093 (2)	0.425 (2)	0.1439 (8)
C_6	0.159 (1)	0.370 (2)	0.1881 (10)
		R_2	
C_1	0.321 (1)	0.219 (3)	0.2691 (10)
C_2	0.323 (1)	0.159 (2)	0.2101 (9)
C_3	0.415 (2)	0.121 (2)	0.1856 (7)
C_4	0.506 (1)	0.143 (3)	0.2201 (10)
C_5	0.504 (1)	0.203 (2)	0.2790 (9)
C_6	0.412 (2)	0.241 (2)	0.3035 (7)
		R_3	
C_1	0.148 (3)	0.129 (2)	0.3365 (10)
C_2	0.086 (2)	0.057 (2)	0.2985 (7)
C_3	0.047 (2)	−0.044 (2)	0.3252 (10)
C_4	0.070 (3)	−0.073 (2)	0.3900 (10)
C_5	0.132 (2)	−0.001 (2)	0.4280 (7)
C_6	0.171 (2)	0.100 (2)	0.4013 (10)

[a] The rings are numbered so that C_1 is attached to P; C_4 is *para* to C_1. The estimated standard deviations were derived from those of the group parameters and are meant to be used in error analyses on inter-ring distances. Intra-ring C–C = 1.397 Å.

Description and Discussion

Figures 1 and 2 show the numbering schemes of the $Au(S_2C_2(CF_3)_2)_2^-$ and the $PCl(C_6H_5)_3^+$ ions, respectively. In these drawings the sizes and shapes of the atoms are determined by the probability ellipsoids associated with their thermal motions and by the perspective view. The rms amplitudes of vibration for the Au and S atoms are given in Table IV, and the directions of the principal axes of vibration can be deduced in part from Figure 1. Interatomic distances and angles computed from the final parameters of Table II are given in Tables V and VI, respectively. The estimated standard deviations of the distances and angles were derived from the inverse least-squares matrix of the final refinement. Selected distances and angles are also shown in Figures 1 and 2.

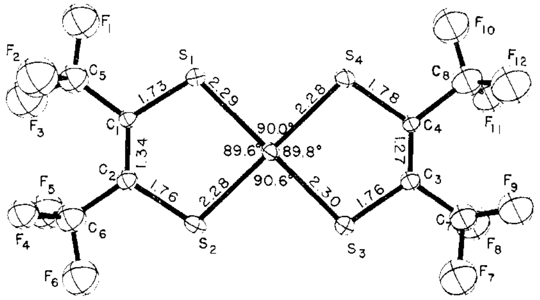

Figure 1.—View of the $Au(S_2C_2(CF_3)_2)_2^-$ ion. The size and shape of the atoms are determined by their final thermal parameters. The ellipsoids are drawn to enclose 20% of the probability distribution.

As we have indicated, the compound originally formu-

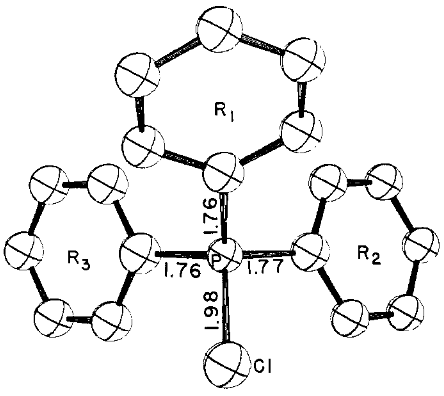

Figure 2.—Perspective view of the $PCl(C_6H_5)_3^+$ ion. The ellipsoids are drawn to include 40% of the probability distribution. Hydrogen atoms are not shown.

TABLE IV

ROOT-MEAN-SQUARE AMPLITUDES OF VIBRATION (Å)

Atom	Min	Intermed	Max
Au	0.178 (2)	0.189 (2)	0.244 (2)
S_1	0.191 (16)	0.209 (11)	0.318 (13)
S_2	0.173 (14)	0.251 (11)	0.304 (12)
S_3	0.206 (13)	0.217 (12)	0.277 (12)
S_4	0.172 (13)	0.215 (12)	0.309 (11)

TABLE V

INTERATOMIC DISTANCES (Å)

Atoms	Distance	Atoms	Distance
$Au-S_1$	2.292 (8)	C_4-C_8	1.61 (5)
$Au-S_2$	2.282 (8)	C_5-F_1	1.27 (4)[b]
$Au-S_3$	2.296 (8)	C_5-F_2	1.49 (5)
$Au-S_4$	2.285 (8)	C_5-F_3	1.21 (4)
S_1-S_2	3.225 (12)	C_6-F_4	1.34 (4)
S_1-S_4	3.236 (11)	C_6-F_5	1.25 (4)
S_2-S_3	3.254 (11)	C_6-F_6	1.32 (4)
S_3-S_4	3.233 (11)	C_7-F_7	1.35 (4)
S_1-C_1	1.73 (3)	C_7-F_8	1.29 (4)
S_2-C_2	1.76 (3)	C_7-F_9	1.23 (4)
S_3-C_3	1.76 (3)	C_8-F_{10}	1.30 (5)
S_4-C_4	1.78 (3)	C_8-F_{11}	1.26 (5)
C_1-C_2	1.34 (4)	C_8-F_{12}	1.25 (5)
C_3-C_4	1.27 (4)	P–Cl	1.98 (1)
C_1-C_5	1.47 (5)[b]	$P-R_1C_1$[a]	1.76 (2)
C_2-C_6	1.47 (4)	$P-R_2C_1$	1.77 (2)
C_3-C_7	1.45 (4)	$P-R_3C_1$	1.76 (3)

[a] R_1C_1 means atom C_1 of group R_1. [b] See footnote 16.

TABLE VI

BOND ANGLES (DEG)

Atoms	Angle	Atoms	Angle
S_1-Au-S_2	89.6 (3)	$C_3-C_4-C_8$	127 (3)
S_1-Au-S_4	90.0 (3)	$F_1-C_5-F_2$	90 (3)[a]
S_2-Au-S_3	90.6 (3)	$F_1-C_5-F_3$	119 (5)
S_3-Au-S_4	89.8 (3)	$F_2-C_5-F_3$	88 (4)
$Au-S_1-C_1$	102.8 (10)	$F_4-C_6-F_5$	106 (4)
$Au-S_2-C_2$	102.2 (10)	$F_4-C_6-F_6$	102 (4)
$Au-S_3-C_3$	101.2 (11)	$F_5-C_6-F_6$	100 (4)
$Au-S_4-C_4$	101.2 (9)	$F_7-C_7-F_8$	98 (4)
$S_1-C_1-C_2$	123 (2)	$F_7-C_7-F_9$	98 (4)
$S_2-C_2-C_1$	123 (2)	$F_8-C_7-F_9$	103 (4)
$S_3-C_3-C_4$	124 (2)	$F_{10}-C_8-F_{11}$	108 (5)
$S_4-C_4-C_3$	124 (2)	$F_{10}-C_8-F_{12}$	110 (5)
$S_1-C_1-C_5$	111 (3)	$F_{11}-C_8-F_{12}$	106 (5)
$S_2-C_2-C_6$	112 (3)	$Cl-P-R_1C_1$	109 (1)
$S_3-C_3-C_7$	112 (3)	$Cl-P-R_2C_1$	107 (1)
$S_4-C_4-C_8$	109 (3)	$Cl-P-R_3C_1$	108 (1)
$C_2-C_1-C_5$	126 (3)	$R_1C_1-P-R_2C_1$	112 (1)
$C_1-C_2-C_6$	125 (3)	$R_1C_1-P-R_3C_1$	111 (1)
$C_4-C_3-C_7$	124 (3)	$R_2C_1-P-R_3C_1$	110 (1)

[a] See footnote 16.

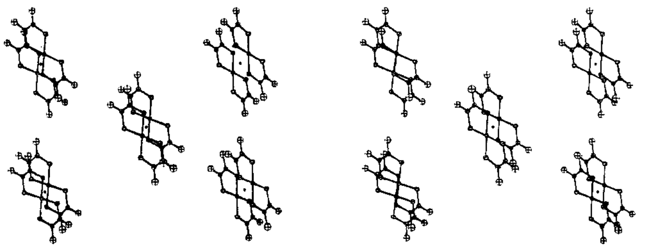

Figure 3.—Stereoscopic view of the packing of the $Au(S_2C_2(CF_3)_2)_2^-$ ions in the unit cell; *a* is up, *c* is to the right, and *b* is coming out of the page.

lated as $[(C_6H_5)_3PAu(S_2C_2(CF_3)_2)_2]Cl$ is correctly formulated as $[PCl(C_6H_5)_3][Au(S_2C_2(CF_3)_2)_2]$. The structure consists of well-separated cations and anions. The anions pack about the symmetry centers at 0, 0, 0 and $^1/_2$, $^1/_2$, $^1/_2$ as can be seen in the stereoscopic view down the *b* axis (Figure 3). The Au···Au distance is 4.66 Å, the minimum interionic Au···S distance is 3.96 Å, and the minimum interionic S···S contact is 4.55 Å. This arrangement of anions is different from the structures found for $Cu(S_2C_2(CN)_2)_2^-$ [13] and $Ni(S_2C_2(CN)_2)_2^-$.[14] The latter two structures have similar metal–metal distances (4.03 and 4.40 Å, respectively) but consist of strings of anions stacked in a staggered manner. The $PCl(C_6H_5)_3^+$ cations fit into channels along the twofold screw axes at $^1/_4$, 0, $^1/_4$ and $^3/_4$, 0, $^3/_4$. The shortest cation–anion interactions are H···F van der Waals contacts.

From Figure 1 it is readily apparent that the coordination geometry about the Au atom is square planar. The four independent S–Au–S angles average 90.0 (3)° and do not differ significantly from one another. The four independent Au—S distances average 2.291 (8) Å and are equivalent. The C=C distances in the chelate rings are 1.34 (4) and 1.27 (4) Å. These are not significantly different from those observed for other square-planar complexes of *cis*-1,2-disubstituted ethene-1,2-dithiolates.[15] The S—C distances range from 1.73 to 1.78 Å and average 1.76 (3) Å. This is toward the long end of the range of known S—C distances in related compounds.[15]

The distances and angles involving the atoms of the CF_3 groups vary considerably (Tables V and VI), presumably because the scattering of these atoms has been improperly accounted for in the assumed model. On the assumption that these groups are chemically equiv-

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[13] J. D. Forrester, A. Zalkin, and D. H. Templeton, *Inorg. Chem.*, **3**, 1507 (1964).

[14] C. J. Fritchie, *Acta Cryst.*, **20**, 107 (1966).

[15] For a complete list of references to the structures of *cis*-1,2-disubstituted ethene-1,2-dithiolates as well as a tabulation of the S—C and C=C distances in these compounds see M. R. Churchill and J. P. Fennessey, *Inorg. Chem.*, **7**, 1123 (1968).

alent, the average C–CF_3 distance of 1.50 (7) Å[16] may be compared with that of 1.51 (1) Å found in $[Co(S_2C_2(CF_3)_2)_2]_2$,[17] where the CF_3 groups are well behaved. Similarly, the average C–F distance of 1.30 (7) Å may be compared with the value of 1.30 (2) Å found previously. The average F–C–F angle is 102 (8)°.

The AuS_4 fragment deviates slightly from planarity. The dihedral angle between the planes S_1–Au–S_2 and S_3–Au–S_4 is 2.3 (3)°. A weighted, best least-squares plane[18] through the four S atoms has the equation $2.73x + 7.81y + 14.48z - 1.97 = 0$ (monoclinic coordinates), and S_1 and S_3 are 0.02 and 0.03 Å above the plane while S_2 and S_4 are 0.03 and 0.02 Å (all ±0.01 Å) below the plane (closer to the origin). The Au atom is 0.016 Å below the plane. The equation of the weighted, best least-squares plane through all nine atoms of the $Au(S_2C_2)_2$ chelate system is $2.82x + 7.83y + 14.39z - 1.97 = 0$. Atoms S_1, C_3, and C_4 are 0.06 (1), 0.13 (3), and 0.10 (3) Å above the plane and all other atoms are within 0.025 Å of the plane.

The S···S distances in bis- and tris-dithiolate complexes usually are about 3.05 Å. Gray, Eisenberg, and Stiefel[19] have suggested that this ubiquitous S···S distance is an indication of S–S interligand bonding which, in turn, they employ to account for the unusual trigonal-prismatic coordination displayed by highly oxidized tris complexes, such as $Re(S_2C_2(C_6H_5)_2)_3$.[2] However, the square-planar dithiolate derivatives whose structures have been previously reported[15] have all contained first-row transition metals. If interligand S–S bonding is important in these compounds, then one would expect the intraligand S···S distance to increase more than the interligand S···S contact upon introduction of a large third-row metal atom, such as Au. In $Au(S_2C_2(CF_3)_2)_2^-$, however, the intraligand S···S contacts of 3.22 and 3.23 (1) Å are essentially identical with the interligand contacts of 3.24 and 3.25 (1) Å. Thus, the ligands have moved further apart, the chelate bite has increased, and the square-planar coordination has been maintained. The S···S contacts found here are about 0.45 Å less than the sum of the van der Waals radius for S. Interligand S–S bonding may well be an important factor in the bonding of dithiolate complexes, but such bonding certainly appears to be much weaker in the present anion than in the structures reported previously.[15]

The chlorotriphenylphosphonium ion has been identified previously,[20] but this appears to be the first determination of its structure. As can be seen from Figure 2, the ion has the expected tetrahedral geometry. The effective symmetry of the cation, including the phenyl groups, is very nearly m. However, there is undoubtedly considerable flexibility about the P–C bonds so that such symmetry is not expected to be the rule, any more than is a specific symmetry expected for triphenylphosphine ligands themselves. The P–Cl distance of 1.98 (1) Å agrees well with the less certain values of 1.97 and 1.98 Å previously found for PCl_4^+,[21,22] while the average P–C distance of 1.76 (1) Å is distinctly shorter, as expected, than a typical value of 1.83 Å for triphenylphosphine ligands.

Finally it is of interest to review the chemical reactions leading to this unexpected product. Davison, Howe, and Shawl[1] allowed $(CF_3)_2C_2S_2$ to react with an excess of $(C_6H_5)_3PAuCl$ in refluxing benzene. The solution turned orange and then deep green. After removing the solvent, they recrystallized the green solid from dichloromethane. The compound, though insoluble in nonpolar solvents, dissolved in dichloromethane to give a conducting solution and appeared to decompose into $(C_6H_5)_3P$, Cl^-, and $Au(S_2C_2(CF_3)_2)_2^-$ in solvents containing O or N functional groups. On this basis, together with analytical data, the authors proposed the formulation $[(C_6H_5)_3PAu(S_2C_2(CF_3)_2)_2]Cl$. Note that the correct formulation given here, namely, $[PCl(C_6H_5)_3][Au(S_2C_2(CF_3)_2)_2]$, though totally unexpected, is equally consistent with the analytical and conductivity data that Davison, Howe, and Shawl had accumulated. Chlorophosphonium ions are readily hydrolyzed by even trace amounts of water.[23] Thus, the observed decomposition in an ethanol–water solution was actually hydrolysis of the $PCl(C_6H_5)_3^+$ cation and not reduction of the postulated gold complex.

Although the isolation of the $Au(S_2C_2(CF_3)_2)_2^-$ ion from the reaction is reasonable, the formation of the chlorotriphenylphosphonium ion is totally unexpected. Because a green solution and green solid were formed prior to recrystallization from dichloromethane, it seems reasonable to suppose that the source of Cl for the cation was the original reaction mixture, rather than the dichloromethane. The use of dry benzene and dry dichloromethane prevented the hydrolysis of the unstable $PCl(C_6H_5)_3^+$ cation. In the solid state this cation has been stabilized by the large counteranion $Au(S_2C_2(CF_3)_2)_2^-$.[24]

Acknowledgments.—We thank Professor A. Davison for providing the sample. Financial support by the National Science Foundation is gratefully acknowledged.

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(16) It is reasonable to assume that the CF_3 groups should be chemically equivalent in this compound. This implies that for the individual atoms of the CF_3 groups, the standard deviations obtained from the inverse least-squares matrix are too small. Therefore, $\bar{x}$ and $\sigma(x)$ were calculated by

$$\bar{x} = \left(\sum_{i=1}^{N} x_i\right)/N \text{ and } \sigma(x) = \left(\sum_{i=1}^{N} (x_i - \bar{x})^2/(N-1)\right)^{1/2}$$

where x_i is the value of an individual observation and N is the number observations. The values for $\sigma(x)$ obtained for distances and angles involving the CF_3 groups and quoted in the text are 2–3 times the individual standard deviations given in Tables V and VI. However, the individual standard deviations of distances and angles in the $Au(S_2C_2)_2$ chelate rings and in the cation are probably correct because $\sigma(x)$ for these quantities is always less than or equal to the individual standard deviations of the presumed chemically equivalent distances or angles.

(17) J. H. Enemark and W. N. Lipscomb, *Inorg. Chem.*, **4**, 1729 (1965).

(18) W. C. Hamilton, *Acta Cryst.*, **14**, 185 (1961).

(19) H. B. Gray, R. Eisenberg, and E. I. Stiefel in "Werner Centennial," Advances in Chemistry Series, No. 62, American Chemical Society, Washington, D. C., 1967, pp 641–649.

(20) See, for example, J. K. Ruff, *Inorg. Chem.*, **2**, 813 (1963).

(21) D. Clark, H. M. Powell, and A. F. Wells, *J. Chem. Soc.*, 642 (1942).

(22) W. F. Zelezny and N. C. Baenziger, *J. Am. Chem. Soc.*, **74**, 6151 (1952).

(23) H. N. Rydon and B. L. Tonge, *J. Chem. Soc.*, 3043 (1956).

(24) K. N. Raymond and F. Basolo, *Inorg. Chem.*, **5**, 949 (1966).