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Crystal Structures of Two Isomeric Forms of Bis[μ-((*p*-ethoxyphenyl)tellurio)]-bis(cyclopentadienylcarbonyliron)

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The crystal structures of two isomeric modifications of bis[μ-((*p*-ethoxyphenyl)tellurio)]-bis(cyclopentadienylcarbonyliron) have been determined. Isomer I, $C_{28}H_{28}Fe_2Fe_2O_4$, crystallizes in the orthorhomibc space group *Pbcn* with a = 18.150 (9) Å, b = 7.651 (4) Å, c = 19.929 (14) Å, V = 2767.6 Å^3, and Z = 4. Isomer II, $C_{28}H_{28}Fe_2Te_2O_4{\cdot}0.8C_6H_{12}$, crystallizes in the monoclinic space group $P2_1/c$ with a = 13.617 (4) Å, b = 14.491 (3) Å, c = 19.016 (6) Å, β = 112.03 (2)°, V = 3478.4 Å^3, and Z = 4. Both isomers contain an –Fe–Te–Fe–Te– macrocyclic ring which is slightly puckered about the axis joining the Fe atoms. The Fe and Te atoms in both compounds are found to have very similar coordination environments. Each Fe atom lies at the center of a distorted tetrahedron (82.78 (5)–128.6(8)°), four-coordination being completed by a carbonyl and a cyclopentadienyl ligand, while each Te atom lies at the apex of an irregular trigonal pyramid (93.80 (6)–108.9 (2)°), three-coordination being completed by σ bonding to a *p*-ethoxyphenyl ligand. The isomerism exhibited by these compounds is geometric. Isomer I has its two Cp ligands cis disposed with respect to one another and the puckering of the Fe_2Te_2 ring, while on the opposite side of the ring are found both pairs of *p*-ethoxyphenyl and carbonyl ligands, also cis with respect to one another. Isomer II has each pair of carbonyl, cyclopentadienyl, and *p*-ethoxyphenyl ligands approximately trans. The ^{125}Te and ^{57}Fe Mössbauer parameters of both isomers are discussed.

Introduction

The reaction of $[Fe(\eta\text{-}C_5H_5)(CO)_2]_2$ with a diaryl disulfide, diselenide, or ditelluride, R_2E_2, yields $Fe(\eta\text{-}C_5H_5)(CO)_2ER$, which then dimerizes to produce the compound $[Fe(\eta\text{-}C_5H_5)(CO)ER]_2$.[1-4] While there are several possible isomers for this product,[4] as illustrated in Figure 1, in general only two are formed in any appreciable yield. For $[Fe(\eta\text{-}C_5H_5)(CO)SPh]_2$ it was found that one isomer is formed in much greater yield than the other, and the X-ray crystal structure[1] of the more abundant isomer showed it to have the structure *cis*-I of Figure 1. In this isomer the CO groups are cis disposed with respect to the puckered Fe_2S_2 ring while the SPh groups lie on the same side of the ring as the carbonyl groups. The structure of the second isomer, which forms in only very small yield, has not been determined. On the basis of NMR data, Dekker et al.[2] proposed that the second isomer has the structure *cis*-III of Figure 1. In subsequent work, Haines et al.[4] reinterpreted the NMR data in the light of similar work on $[Fe(\eta\text{-}C_5H_5)(CO)E(CH_3)_2]_2$, E = P or As, and concluded that the second isomer has the structure *trans*-I.

Schermer and Baddley[3] have prepared the selenium and tellurium analogues of the above compound, $[Fe(\eta\text{-}C_5H_5)(CO)EPh]_2$, E = Se or Te, and again observed that two isomers are formed in each case. They were able to separate the two isomers of the selenium compound but were unsuccessful in the case of tellurium. They also observed that the ratio of the two isomers formed in each case, as identified by IR spectroscopy, changed in such a way that the less abundant isomer for sulfur becomes the more abundant isomer for tellurium.

In the present work we have synthesized the compound $[Fe(\eta\text{-}C_5H_5)(CO)Te(C_6H_4OC_2H_5\text{-}p)]_2$ and have separated the two isomers manually. The crystal structures of both isomers have been determined, and the results are presented here together with a brief discussion of the ^{57}Fe and ^{125}Te Mössbauer spectra of these isomers.

Experimental Section

In the preparation of $[Fe(\eta\text{-}C_5H_5)(CO)Te(C_6H_4OC_2H_5\text{-}p)]_2$, $(p\text{-}C_2H_5OC_6H_4Te)_2$ (4.96 g, 10 mmol) and $[C_5H_5Fe(CO)_2]_2$ (2.8 g, 7 mmol) were refluxed in benzene (150 mL) for 3 h. The filtered solution was taken to dryness under reduced pressure and the resulting dark brown solid recrystallized from dichloromethane/hexane. The product consisted of a mixture of two crystal modifications, denoted as I, mp 102–103 °C, and II, mp 99–101 °C, which were separated manually. Anal. Calcd: C, 42.32; H, 3.52. Found: C, 41.96; H, 2.92. Type I crystals consisted of short needles and formed approximately 5% of the isomer mixture. Type II crystals, which made up the bulk of the product, were not suitable for crystallographic study. However, because of the large yield of this product, we were able to produce satisfactory crystals by recrystallization from dichloromethane/cyclohexane.

Table I. Crystal Data

	isomer I	isomer II
fw	795.45	862.78
formula	$C_{28}H_{28}Fe_2Te_2O_4$	$C_{28}H_{28}Fe_2Te_2O_4{\cdot}0.8C_6H_{12}$
space group	*Pbcn*	$P2_1/c$
a, A	18.150 (9)	13.617 (4)
b, A	7.651 (4)	14.491 (3)
c, A	19.929 (14)	19.016 (6)
β, deg		112.03 (2)
vol, A^3	2767.6	3478.4
Z	4	4
D_O, g cm^{-3}	1.90	1.67
D_C, g cm^{-3}	1.909	1.647
μ, cm^{-1}	32.50	25.95

Table II. Data Collection Parameters

	isomer I	isomer II
no. of reflctns used in accurate cell determination	11	18
takeoff angle, deg	3	3
scan type	θ–2θ	θ–2θ[a]
scan speed, deg/min	2	2
scan width, deg	(1.4 + 0.692 tan θ) for 2θ ≤ 15° and (1.1 + 0.692 tan θ) for 15 ≤ 2θ ≤ 40°	(1.4 + 0.692 tan θ)
bkgd, s	20	10% of total scan
2θ range, deg	3–40	3.2–45
no. of independent reflctns	1271	4588
no. of obsd reflctns	890 ($I > 2.3\sigma(I)$)[b]	2914 ($I > 3.0\sigma(I)$)

[a] Each reflection was analyzed by the peak profile method of ref 6. [b] $\sigma(I)$ is the standard deviation derived from counting statistics.

The ^{57}Fe and ^{125}Te Mössbauer spectra of the two isomers were determined, and the experimental details of the Mössbauer spec-

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(2) Dekker, M.; Knox, G. R.; Robinson, C. G. *J. Organomet. Chem.* **1969**, *18*, 161.

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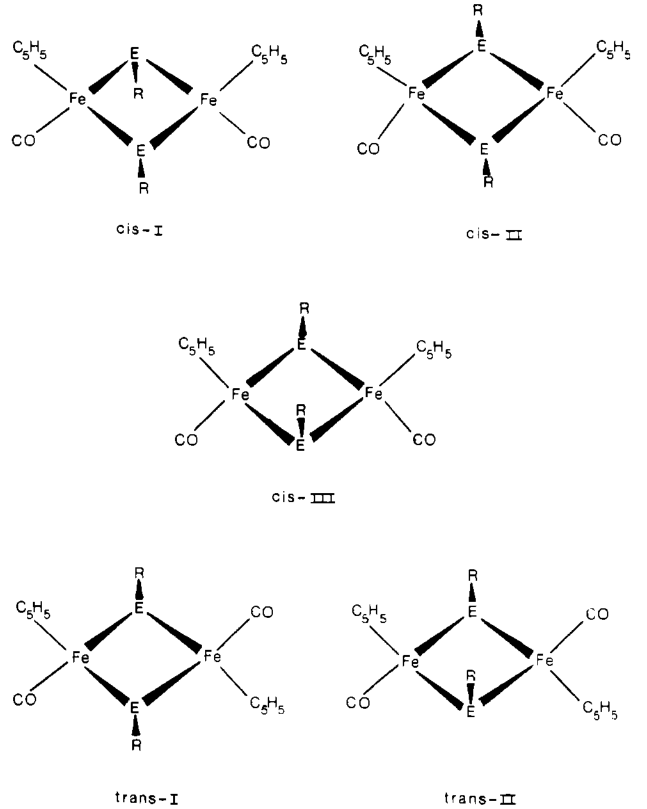

cis-I cis-II cis-III trans-I trans-II

Figure 1. Isomers of $[\mathrm{Fe}(\eta\text{-}C_5H_5)(CO)ER]_2$, with use of the nomenclature of ref 4.

trometer and the general methods used[5] have been given previously. Infrared spectra were recorded on a Perkin-Elmer 457.

X-ray Data Collection

Crystal data and data collection parameters may be found in Tables I and II, respectively. Precession and Weissenberg photograhs were used to determine space groups and approximate unit cell dimensions. Accurate unit cell dimensions were determined by least-squares refinement of accurately centered reflections (2θ = 25–33°, Mo Kα radiation).

Data were collected at 20 °C with use of a Picker FACS-I four-circle diffratometer [λ(Mo Kα) = 0.709 26 Å] with a graphite monochromator and scinillation counter with pulse height discrimination. Intensity measurement of two standards every 70 reflections showed no evidence of crystal deterioration in either compound.

Lorentz and polarization corrections have been applied to both data sets. An absorption correction has only been made for the crystal of isomer II, which was in the shape of a rectangular block with dimensions 0.06 × 0.08 × 0.07 mm.

Structure Determination and Refinement

Isomer I. The structure was solved by Patterson and Fourier methods and indicated molecules of $[\mathrm{Fe}(\eta\text{-}C_5H_5)(CO)\mathrm{Te}(C_6H_4OC_2H_5)]_2$ with crystallographic 2-fold symmetry. Hydrogen atom positions were determined from subsequent difference electron density maps. Full-matrix least-squares refinement with anisotropic temperature parameters for the nonhydrogen atoms converged at R = 0.040.

Isomer II. The tellurium and iron atoms were located by direct methods and all other nonhydrogen atoms by subsequent difference syntheses. After location of all the nonhydrogen atoms of the molecule under investigation, the subsequent difference map revealed the presence of cyclohexane of recrystallization in nonstoichiometric proportions. Reasonable isotropic temperature factors and agreement were achieved by using an occupancy of 80%. Hydrogen atoms were included in their calculated positions. Block-diagonal least-squares refinement with anisotropic temperature factors for tellurium and iron atoms and isotropic temperature factors for all other atoms gave final agreement of R = 0.047.

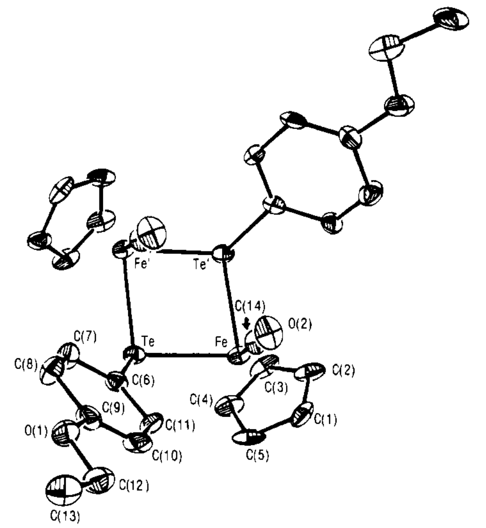

Figure 2. Molecular geometry and labeling for "isomer I" (ORTEP diagram; 50% probability contours for all atoms).

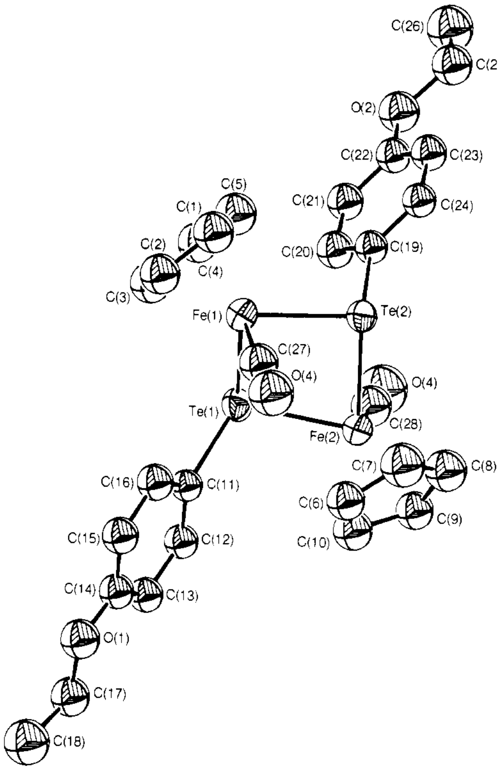

Figure 3. Molecular geometry and labeling for "isomer II" (ORTEP diagram; 50% probability contours for all atoms).

Weighting schemes have been applied to both data sets: for I $w = 1/(\sigma(F_o))^2$ and for II $w = [1/\sigma(F_o^2) + 0.0004F_o^2]^{-1}$. The agreement factors quoted are of the form $R = \sum||F_o| - |F_c||/\sum|F_o|$. Atomic scattering factors and anomalous dispersion corrections were taken from ref 7. For isomer I dispersion corrections were applied to only the Fe and Te atoms, while for isomer II all nonhydrogen atoms were corrected. The computer programs used for the structure solution of isomer I have been cited elsewhere[8] while those used for the structure solution of isomer II are contained in the "The NSERC PDP-8e Crystal Structure System".[9]

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(8) Einstein, F. W. B.; Jones, R. D. G. *Inorg. Chem.* **1972**, *11*, 395.

Table III. Atomic Coordinates ($\times 10^5$ for Te, Fe; $\times 10^4$ for C, O; $\times 10^3$ for H) for Isomer I

	x	*y*	*z*		*x*	*y*	*z*
Te	4399 (5)	18275 (11)	17574 (5)	C(13)	1690 (7)	−7664 (24)	159 (8)
Fe	9161 (10)	14963 (23)	29486 (10)	C(14)	850 (8)	−764 (23)	2927 (8)
O(1)	1140 (5)	−5090 (15)	206 (5)	H(1)[a]	219	35	349
O(2)	814 (6)	−2235 (13)	2931 (5)	H(2)	134	200	423
C(1)	1927 (9)	1419 (22)	3422 (10)	H(3)	85	461	365
C(2)	1441 (9)	2369 (29)	3817 (9)	H(4)	139	469	254
C(3)	1165 (9)	3796 (22)	3473 (12)	H(5)	229	212	243
C(4)	1508 (10)	3828 (22)	2872 (11)	H(7)	−21	−57	71
C(5)	1986 (8)	2400 (24)	2808 (10)	H(8)	3	−316	14
C(6)	728 (8)	−533 (18)	1249 (7)	H(10)	196	−364	114
C(7)	240 (8)	−1205 (19)	774 (7)	H(11)	170	−103	174
C(8)	377 (9)	−2684 (20)	448 (8)	H(12)	218	−550	18
C(9)	1056 (9)	−3573 (23)	591 (8)	H(12′)	178	−657	73
C(10)	1521 (8)	−2969 (23)	1041 (8)	H(13)	120	−833	−3
C(11)	1365 (7)	−1456 (21)	1389 (7)	H(13′)	211	−838	−14
C(12)	1740 (8)	−6070 (22)	291 (8)	H(13″)	165	−725	−63

[a] Hydrogen atoms are numbered corresponding to the carbon atoms to which they are attached in isomers I and II.

Table IV. Atomic Coordinates ($\times 10^5$ for Te, Fe; $\times 10^4$ for C, O; $\times 10^3$ for H) for Isomer II

	x	*y*	*z*		*x*	*y*	*z*
Te(1)	3738 (6)	16139 (5)	15325 (4)	CS(3)	5585 (25)	490 (21)	6904 (17)
Te(2)	1891 (6)	35797 (5)	24208 (4)	CS(4)	4762 (22)	−118 (19)	6808 (15)
Fe(1)	15169 (13)	22535 (11)	28224 (9)	CS(5)	3857 (22)	2 (20)	6105 (15)
Fe(2)	−4623 (13)	31678 (10)	10172 (9)	CS(6)	3700 (30)	773 (22)	5714 (19)
O(1)	3290 (6)	345 (5)	−195 (5)	H(1)	296	283	427
O(2)	−3370 (6)	2594 (6)	3648 (5)	H(2)	352	142	361
O(3)	2896 (8)	3357 (6)	2342 (6)	H(3)	184	33	296
O(4)	−2559 (8)	2602 (7)	864 (6)	H(4)	25	106	334
C(1)	2473 (10)	2271 (9)	3985 (7)	H(5)	98	260	410
C(2)	2758 (10)	1528 (9)	3627 (8)	H(6)	145	181	572
C(3)	1879 (10)	950 (9)	3296 (7)	H(7)	94	30	629
C(4)	1032 (10)	1329 (9)	3473 (7)	H(8)	−116	500	58
C(5)	1429 (10)	2137 (9)	3890 (7)	H(9)	−186	366	−43
C(6)	669 (12)	3499 (8)	557 (7)	H(10)	−34	254	−37
C(7)	390 (10)	4286 (10)	838 (8)	H(12)	6	88	−6
C(8)	−716 (11)	4446 (9)	469 (8)	H(13)	117	36	−77
C(9)	−1144 (10)	3737 (8)	−63 (7)	H(15)	396	98	113
C(10)	−273 (10)	3148 (9)	−22 (7)	H(16)	287	147	186
C(11)	1369 (8)	1239 (7)	939 (6)	H(17)	233	−64	−94
C(12)	914 (9)	904 (7)	207 (6)	H(17′)	232	46	−134
C(13)	1528 (9)	611 (8)	−203 (6)	H(20)	−135	186	233
C(14)	2615 (9)	649 (8)	138 (6)	H(21)	−270	152	289
C(15)	3108 (9)	954 (8)	871 (7)	H(23)	−223	417	392
C(16)	2487 (9)	1244 (8)	1288 (7)	H(24)	−89	452	336
C(17)	2840 (10)	−50 (9)	−933 (7)	H(25)	−307	344	461
C(18)	3742 (12)	−335 (10)	−1181 (9)	H(25′)	−394	392	375
C(19)	−1008 (8)	3207 (7)	2844 (6)	H(51)	479	126	531
C(20)	−1544 (9)	2364 (8)	2680 (7)	H(51′)	429	211	575
C(21)	−2303 (9)	2187 (8)	2983 (7)	H(52)	549	185	687
C(22)	−2567 (9)	2853 (8)	3401 (6)	H(52′)	618	133	636
C(23)	−2053 (9)	3670 (8)	3562 (7)	H(53)	623	7	684
C(24)	−1270 (9)	3859 (8)	3270 (6)	H(53′)	590	69	752
C(25)	−3705 (10)	3282 (9)	4074 (7)	H(54)	505	−82	683
C(26)	−4630 (11)	2841 (11)	4203 (9)	H(54′)	451	−3	730
C(27)	2301 (10)	2892 (9)	2500 (7)	H(55)	313	−11	625
C(28)	−1702 (10)	2816 (9)	925 (7)	H(55′)	386	−54	573
CS(1)	4497 (23)	1399 (20)	5802 (18)	H(56)	326	61	511
CS(2)	5485 (24)	1267 (21)	6490 (17)	H(56′)	308	120	586

Final positional parameters for isomers I and II are given in Tables III and IV, respectively.

Description of Structures

Bond parameters for isomer I are given in Table V. The molecule has crystallographic 2-fold symmetry (Figure 2), the axis passing through the center of a Fe–Te–Fe–Te– ring and perpendicular to the plane through the ring. The iron atom is also bonded to a carbonyl and cyclopentadienyl ligand, which together with the two Te contacts yield a distorted tetrahedral environment (82.88 (6)–128.6 (8)°) about Fe. On the other hand, the tellurium atom is also bonded to a *p*-ethoxyphenyl ligand, which, together with the two iron contacts, gives rise to a distorted trigonal-pyramidal arrangement (95.98 (7)–106.0 (4)°) in which Te lies at the apex of the pyramid. Each pair of ligands in the molecule are cis disposed with respect to one another, the *p*-ethoxyphenyl and carbonyl ligands lying on the same side of the ring to each other but on the opposite side from the two cyclopentadienyl ligands. The cyclopentadienyl ligands are also cis disposed with respect to the puckering of the Fe_2Te_2 ring. Thus the structure of this molecule is similar to that of $[Fe(\eta\text{-}C_5H_5)(CO)SPh]_2$ and corresponds to the *cis*-I structure of Figure 1.

Bond parameters for isomer II are given in Table VI. in this isomer, Figure 1, the cyclopentadienyl ligands on the iron

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Table V. Bond Parameters for Isomer I[a]

	(a) Bond Lengths, A		
Te-Fe	2.539 (2)	Fe-Cp[b]	1.71
Te-Fe′	2.543 (2)	C(14)-O(2)	1.13 (2)
Te-C(6)	2.14 (1)	C(1)-C(2)	1.39 (2)
Fe-C(1)	2.06 (1)	C(1)-C(5)	1.44 (2)
Fe-C(2)	2.09 (2)	C(2)-C(3)	1.38 (2)
Fe-C(3)	2.10 (1)	C(3)-C(4)	1.35 (2)
Fe-C(4)	2.09 (1)	C(4)-C(5)	1.40 (2)
Fe-C(5)	2.08 (1)	C(6)-C(7)	1.39 (2)
Fe-C(14)	1.73 (1)	C(6)-(11)	1.38 (2)
	(b) Bond Angles, Deg		
Fe-Te-Fe′	95.98 (6)	Fe-C(14)-O(2)	178.(2)
Fe-Te-C(6)	106.0 (4)	C(2)-C(1)-C(5)	105 (2)
Fe′-Te-C(6)	105.2 (4)	C(1)-C(2)-C(3)	111 (2)
Te(1)-Fe(1)-Cp(1)	123.4	C(2)-C(3)-C(4)	107 (1)
Te(1′)-Fe(1)-Cp(1)	124.2	C(3)-C(4)-C(5)	111 (2)
C(14)-Fe(1)-Cp(1)	128.6	C(1)-C(5)-C(4)	106 (1)
Te-Fe-C(14)	93.0 (5)	Te-C(6)-C(7)	119 (1)
Te′-Fe-C(14)	92.2 (5)	Te-C(6)-C(11)	123 (1)
Te-Fe-Te′	82.88 (6)		

[a] Bond parameters for the phenyl substituents have been deposited as supplementary material. [b] Cp denotes the centroid of a cyclopentadienyl ring.

Table VI. Bond Parameters for Isomer II

	Bond Distances, A		
Te(1)-Fe(1)	2.536 (2)	Te(2)-Fe(1)	2.551 (2)
Te(1)-Fe(2)	2.548 (2)	Te(2)-Fe(2)	2.548 (2)
Te(1)-C(11)	2.13 (1)	Te(2)-C(19)	2.14 (1)
Fe(1)-C(1)	2.10 (1)	Fe(2)-C(6)	2.09 (1)
Fe(1)-C(2)	2.09 (1)	Fe(2)-C(7)	2.09 (1)
Fe(1)-C(3)	2.07 (1)	Fe(2)-C(8)	2.08 (1)
Fe(1)-C(4)	2.09 (1)	Fe(2)-C(9)	2.08 (1)
Fe(1)-C(5)	2.08 (1)	Fe(2)-C(10)	2.09 (1)
Fe(1)-C(27)	1.69 (1)	Fe(2)-C(28)	1.71 (1)
Fe(1)-Cp(1)[a]	1.71	Fe(2)-Cp(2)	1.71
C(27)-O(3)	1.18 (2)	C(28)-O(4)	1.17 (2)
Te(1)---Te(2)	3.369 (1)	Fe(1)---Fe(2)	3.723 (2)
C(1)-C(2)	1.40 (2)	C(6)-C(7)	1.37 (2)
C(2)-C(3)	1.40 (2)	C(7)-C(8)	1.42 (2)
C(3)-C(4)	1.43 (2)	C(8)-C(9)	1.41 (2)
C(4)-C(5)	1.40 (2)	C(9)-C(10)	1.44 (2)
C(5)-C(1)	1.38 (2)	C(10)-C(6)	1.44 (2)
	Angles, Deg		
Fe(1)-Te(1)-Fe(2)	94.16 (6)	Fe(1)-Te(2)-Fe(2)	93.80 (6)
Fe(1)-Te(1)-C(11)	108.9 (3)	Fe(1)-Te(2)-C(19)	104.6 (3)
Fe(2)-Te(1)-C(11)	107.6 (3)	Fe(2)-Te(2)-C(19)	108.7 (3)
Te(1)-Fe(1)-Cp(1)	124.8	Te(1)-Fe(2)-Cp(2)	126.3
Te(2)-Fe(1)-Cp(1)	127.5	Te(2)-Fe(2)-Cp(2)	123.6
C(27)-Fe(1)-Cp(1)	126.4	C(28)-Fe(2)-Cp(2)	123.4
Te(1)-Fe(1)-C(27)	95.2 (4)	Te(1)-Fe(2)-C(28)	96.9
Te(2)-Fe(1)-C(27)	87.3 (4)	Te(2)-Fe(2)-C(28)	93.3
Te(1)-Fe(1)-Te(2)	82.93 (5)	Te(1)-Fe(2)-Te(2)	82.78 (5)
C(1)-C(2)-C(3)	109 (1)	C(6)-C(7)-C(8)	110 (1)
C(2)-C(3)-C(4)	107 (1)	C(7)-C(8)-C(9)	108 (1)
C(3)-C(4)-C(5)	106 (1)	C(8)-C(9)-C(10)	107 (1)
C(14)-C(5)-C(1)	111 (1)	C(9)-C(10)-C(6)	108 (1)
C(5)-C(1)-C(2)	107 (1)	C(10)-C(6)-C(7)	107 (1)
Fe(1)-C(27)-O(3)	178 (1)	Fe(2)-C(28)-O(4)	174 (1)
Te(1)-C(11)-C(12)	119.2 (8)	Te(2)-C(19)-C(20)	123.0 (8)
Te(1)-C(11)-C(16)	122.4 (8)	Te(2)-C(19)-C(24)	116.8 (8)

[a] Cp denotes the centroid of a cyclopentadienyl ring.

Table VII

Least-Squares Plane Calculations[a] for Isomer II

plane no.	equation[b]
1	$0.9250x + 0.1823y - 0.3333z + 1.0143 = 0$
2	$0.7982x + 0.5929y - 0.1062z - 1.4496 = 0$
3	$0.7825x + 0.4685y - 0.4100z + 0.4690 = 0$
4	$0.9494x + 0.3123y - 0.0316z - 0.0907 = 0$

Deviations from the Planes (A)

	plane no.			
atom	1	2	3	4
Te(1)	0.0		0.0	0.0
Te(2)		0.0	0.0	0.0
Fe(1)	0.0	0.0	0.0	
Fe(2)	0.0	0.0		0.0
C(11)	1.89 (1)[c]			
C(19)		−1.94 (1)[c]		
C(27)			1.68 (1)[c]	
C(28)				1.69 (1)[c]
Cp(1)			−1.05[c]	
Cp(2)				1.10[c]

[a] The equations of the planes are referred to orthogonal axes *a*, *b*′, and c*. [b] $X^2 = 0.00$. [c] These atoms have not been included in the mean planes calculations.

atoms are trans disposed with respect to each other and the *p*-ethoxyphenyl ligands on the tellurium atoms are also in a trans configuration. Thus, this isomer has the *trans*-I structure of Figure 1, as initially proposed by Haines et al.[4] for the sulfur analogue.

The Fe_2Te_2 ring of this second isomer is unsymmetrical, and the two iron atoms are inequivalent as are the two tellurium atoms. The coordinaton geometries of Te and Fe in isomer II are however very similar to those of isomer I, the tellurium atoms being in a distorted trigonal environment (93.80 (6)–108.9 (2)°) and the iron atoms in a distorted tetrahedral (82.78 (5)–127.5 (5)°). The extent of the deviation from the perfectly symmetric trans configuration is indicated by the mean plane data given in Table VII.

Apart from the difference in these two structures as a result of their geometric isomerism, many bond parameters are found to be similar (Tables V and VI). The four-membered Fe_2Te_2 macrocycle in both cis and trans isomers is folded 17 and 28°, respectively, about a line joining the Fe atoms. This situation is analogous of the ring puckering in $[Fe(\eta\text{-}C_5H_5)(CO)SPh]_2$ (**1**), where the angles are 16 and 19° for the two independent molecules of the asymmetric unit. The mean Fe–Te bond distance in the cis isomer is 2.541 (2) Å and in the trans isomer 2.546 (2) Å. These values are slightly larger than the shortest bond of 2.508 (8) Å observed in the marcasite modification of iron telluride, where each Fe and atom is coordinated octahedrally to six atoms.[10] There are few Fe–Te bonds for comparison, but the difference of 0.28 Å between the Fe–Te and Fe–S shortest bond distance in the marcasite structures[10] is in excellent agreement with the differences between mean Fe–Te distances in the present structures and the mean Fe–S distances in related compounds: 0.28 Å for $[Fe(\eta\text{-}C_5H_5)(CO)SPh]_2$ (**1**), 0.28 Å for $[CH_3CH_2SFe(CO)_3]_2$,[11] and 0.27 Å for $[C_6H_5SFe(CO)_3]_2$.[12] The internal ring angles in cis and trans isomers range from 93.80 (6) to 95.98 (6)° for Fe–Te–Fe and from 82.78 (6) to 82.92 (6)° for Te–Fe–Te. The intramolecular distances across the ring in both compounds are also very close viz., 3.363 Å (cis) and 3.369 Å (trans) for Te---Te and 3.776 Å (cis) and 3.723 Å (trans) for Fe---Fe.

The Fe–C (carbonyl) distance of 1.73 (1) Å for the cis isomer and 1.69 (1)–1.71 (1) Å for the trans isomer and the Fe–C (π-C_5H_5) distances of 2.06 (1)–2.14 (1) Å in both compounds are comparable with distances in similar iron compounds. The carbonyl groups in both isomers are very close to linear. The C–C (η-C_5H_5) distances in both isomers are normal and lie in the ragne 1.37 (2)–1.44 (2) Å. Tellurium–carbon (phenyl) distances, of 2.14 (1) Å for the cis isomer and of 2.07 (1) and 2.10 (1) Å for the trans isomer, compare favorably with other Te–C distances, e.g., 2.136 (8)

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Table VIII. IR Spectroscopic Data

compd[a]	C-O str, cm^{-1}	solvent	ref
cis-$[FeCp(CO)SPh]_2$	1983 (s), 1974 (sh)[b]	cyclohexane	4
cis-$[FeCp(CO)SPh]_2$	1983 (sh),[b] 1974 (s)	cyclohexane	4
trans-$[FeCp(CO)SPh]_2$	1953 (ms), 1938 (s)	cyclohexane	4
cis-$[FeCp(CO)SePh]_2$	1975 (s)	cyclohexane	3
trans-$[FeCp(CO)SePh]_2$	1947 (s), 1931 (s)	cyclohexane	3
$[FeCp(CO)Te(PhOEt\text{-}p)]_2$ (I)	1943 (s)	CS_2	this work
$[FeCp(CO)Te(PhOEt\text{-}p)]_2$ (II)	1934 (m), 1920 (s)	CS_2	this work

[a] The nomenclature, cis and trans, used by Haines et al.[4] has been adopted rather than that used in ref 2 and 3. [b] Possible contaminant.

Table IX. Mössbauer Parameters

compd	δ, mm s^{-1}		Δ, mm s^{-1}		ref
	^{57}Fe[a]	^{125}Te[b]	^{57}Fe	^{125}Te	
cis-$[FeCp(CO)SPh]_2$	0.605		1.670		11
trans-$[FeCp(CO)SPh]_2$	0.611		1.720		11
cis-$[FeCp(CO)SMe]_2$	0.569		1.634		11
$[FeCp(CO)Te(PhOEt\text{-}p)]_2$ (I)	0.66 (01)	0.06 (08)	1.64 (01)	6.2 (1)	this work[c]
$[FeCp(CO)Te(PhOEt\text{-}p)]_2$ (II)	0.64 (01)	0.01 (08)	1.68 (01)	6.1 (1)	this work[c]

[a] ^{57}Fe spectra recorded in ref 11 and this work, with the source ($^{57}Co/Pd$) at room temperature and the absorbers at 77 K; δ given with respect to $Na_2[Fe(CN)_5NO]\cdot 2H_2O$. [b] ^{125}Te spectra recorded with the source ($^{125}Sb/Cu$) and absorbers at 4.2 K; δ given with respect to I/Cu. [c] Errors are given in parentheses.

Å in 2-biphenyltellurium tribromide.[13] The geometries of the phenyl rings in both compounds are typical, and the planes defined by the two carbon atoms and oxygen atom of the *p*-ethoxy groups are tilted slightly with respect to the phenyl ring planes, viz., 1° for the cis isomer and 4 and 5° for the trans isomer. A similar small deviation from planarity (3°) is observed in the structure of *p*-ethoxybenzoic acid.[14] Least-squares planes for selected groupings have been deposited.

IR Data

The separation of $[Fe(\eta\text{-}C_5H_5)(CO)Te(C_6H_4OC_2H_5\text{-}p)]_2$ into its two isomers was monitored by IR spectroscopy (Table VIII). The C–O stretching frequencies correlate with those of the corresponding isomers of the sulfur and selenium analogues, and the frequencies are lower for the tellurium compounds.

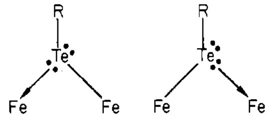
In the preparation of $[Fe(\eta\text{-}C_5H_5)(CO)SPh]_2$, by UV irradiation of a solution of $[Fe(\eta\text{-}C_5H_5)(CO)_2]_2$ and $(C_6H_5)_2S_2$ in benzene, Haines et al.[4] obtained a mixture that contained three isomers. Two were identified as cis isomers with C–O stretching frequencies of 1983 and 1974 cm^{-1}, and these were thought to correspond to two of the cis I–III isomers of Figure 1. In the present experiments, conducted under a variety of conditions including irradiation with UV light, no evidence was found for any additional isomers other than two identified here.

Mössbauer Data

The ^{57}Fe and ^{125}Te Mössbauer parameters of the two isomers are reported in Table IX.

The Mössbauer spectra were consistent with the presence of only one iron site in each isomer, the two sites in the trans isomer being so similar as to appear identical within the resolution of this method. The two isomers have the same ^{57}Fe parameters within the errors, and this is to be expected, given the similarity in the coordination about the iron atoms. A similar observation has previously been reported[15] for the two isomers of $[Fe(\eta\text{-}C_5H_5)(CO)SPh]_2$. Indeed, the Mössbauer isomer shifts, δ, and quadrupole splittings, Δ, for the two tellurium isomers are very similar to those of $[Fe(\eta\text{-}C_5H_5)(CO)SPh]_2$ and $[Fe(\eta\text{-}C_5H_5)(CO)SMe]_2$. Any differences in the donor character of the SPh, SMe, and $Te(C_6H_4OC_2H_5\text{-}p)$ ligands are not sufficient to lead to any measurable differences in δ and Δ. The bonds to cyclopentadienyl and carbonyl ligands appear to be dominant in determining the ^{57}Fe Mössbauer parameters in these complexes.

The ^{125}Te Mössbauer spectra of the two isomers again indicate the presence of only one tellurium site in each, and the Mössbauer parameters for the two isomers are the same within the errors. The environment about the tellurium is trigonal, and the magnitude of the quadrupole splitting, Δ, is comparable with that observed in other compounds where there is a similar trigonal coordination about the tellurium; cf. $Ph_3Te^+Cl^-$ $\Delta = 5.8$ mm s^{-1}). The ^{125}Te quadrupole splitting in the two isomers may arise from some stereochemical activity of the lone pair on the tellurium and from inequivalence of the tellurium p-orbital occupancies of the Te–Fe and Te–C bonds. In the two isomers the tellurium may be viewed as donating three electrons to form the two Fe–Te bonds:



Such a bonding scheme would suggest that there is a relatively large electron density on tellurium, and the small Mössbauer isomer shift is consistent with that proposal.

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Registry No. I, 79329-14-9; II, 79389-89-2; $[C_5H_5Fe(CO)_2]_2$, 12154-95-9; $(p\text{-}C_2H_5OC_6H_4Te)_2$, 35684-38-9.

Supplementary Material Available: Lists of structure factors, thermal parameters, selected mean plane calculations, and bond parameters for the phenyl substitutents (38 pages). Ordering information is given on any current masthead page.

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