Reaction of $Fe_3(CO)_{12}$ with Tellurium−Nitrogen Heterocycles: A Source of Novel Organoiron Compounds

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Heterocyclic tellurium compounds containing both tellurium and nitrogen in the heterocyclic ring are shown to be useful precursors for the synthesis of novel organoiron compounds. Thus, reaction of $Fe_3(CO)_{12}$ with benzoisotellurazole yields $(C_6H_4CHNTe)_2Fe_3(CO)_7$, **5**. The structure of **5** was established by X-ray crystallography; it is based on a nonlinear chain of three iron atoms, Fe1−Fe2−Fe3 133.4(1)°, with Fe1−Fe2, 2.472(2) Å doubly-bridged by nitrogen and Fe2−Fe3, 2.683(2) Å, doubly-bridged by tellurium. The reaction of $Fe_3(CO)_{12}$ with 2-methylbenzotellurazole results in two new crystalline products $C_{18}H_7NFe_3O_{10}$, **6**, and $C_{14}H_7NFe_2O_6$, **7**, involving detelluration of the heterocycle. X-ray crystallography shows that **6** contains a triangular arrangement of iron atoms, two edges of which are bridged respectively by the nitrogen and carbon atoms of the NC formal double bond and the latter edge is also bridged by a carbonyl in an almost symmetrical manner. The third edge of the iron triangle is not directly bridged, and at 2.647(1) Å, it is the longest edge of the triangle. In **7**, one iron atom forms part of a benzoferrazole system, and the second iron is π-bonded to the C−C−N═C residue of the ferrazole with a relatively short Fe−Fe contact of 2.498(1) Å.

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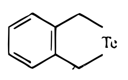
Introduction

The possibility of removing sulfur from thiophene by reaction with a metal carbonyl, e.g., $Fe_3(CO)_{12}$, was illustrated as long as 37 years ago.[1] However, reactions of more condensed thiophenes, e.g., benzo- and dibenzothiophene, with $Fe_3(CO)_{12}$ do not proceed to the desulfurization stage.[2,3] By contrast, related tellurium heterocyclic compounds do undergo detelluration reactions relatively readily, thus providing a route to some novel organometallic compounds.[4]

A chemically interesting result was obtained when detelluration of 2-telluraindane **(1)** was achieved[4] using $Fe_3(CO)_{12}$; thus, an organic fragment **(2)** formed by the unsymmetric dimerization of two C_8H_8 fragments derived from **(1)** was stabilized by coordination to a Fe(CO)$_3$ unit. The above observation led to the expectation that the relatively facile detelluration of heterocyclic organotellurium compounds could enable these materials to be used as precursors for novel organometallic compounds; in particular, it was speculated that if the tellurium heterocycle contained an additional heteroatom, such as nitrogen (e.g., **3** and **4**), access to new areas of organometallic chemistry should be possible. In this paper, evidence is presented to support this contention.



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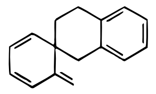

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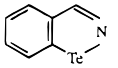

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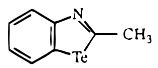

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Experimental Section

Synthesis. (1) Reaction of Benzisotellurazole[5] (3) with Triiron Dodecacarbonyl. Benzoisotellurazole (0.2 g, 0.87 mmol) and triiron dodecacarbonyl (0.44 g, 0.87 mmol) were dissolved in 35 cm^3 of dry toluene under an atmosphere of argon, and the reaction mixture was refluxed for 3 h. After the reaction mixture was cooled, it was filtered to remove a black residue and the filtrate was concentrated under vacuum, yielding a dark brown solid. The solid was chromatographed on a silica gel column (2 × 12 cm) with hexane/CH_2Cl_2 (2:1) as the eluting solvent, thus, revealing a purple band succeeded by a green band. Collection of the two fractions followed by evaporation of the solvent yielded dark purple crystals from the first eluate (15 mg), which were shown to be the cluster compound $Fe_3Te_2(CO)_9$, and a dark green solid from the second eluate, shown to be the trimeric (wrt iron) compound $(C_6H_4CHNTe)_2(Fe_3(CO)_7$, **5** (55 mg, 15.3% based on benzoisotellurazole). Anal. Calcd for $C_{21}H_{10}N_2Fe_3Te_2O_7$: C, 30.5; H, 1.20; N, 3.39. Found: C, 30.9; H, 1.35; N, 3.28. IR (Bio-Rad FTS-40A, KBr): ν(CO) 2060, 2021, 2008, 1998, 1985, 1964, 1941, 1922, 1905 cm^{-1}. ^{1}H NMR (Brucker AC 300, 300 MHz, $CDCl_3$, 25 °C): δ (*vs* TMS) 9.12 (m, 1H), 8.09 (m, 1H), 7.51 (m, 1H),

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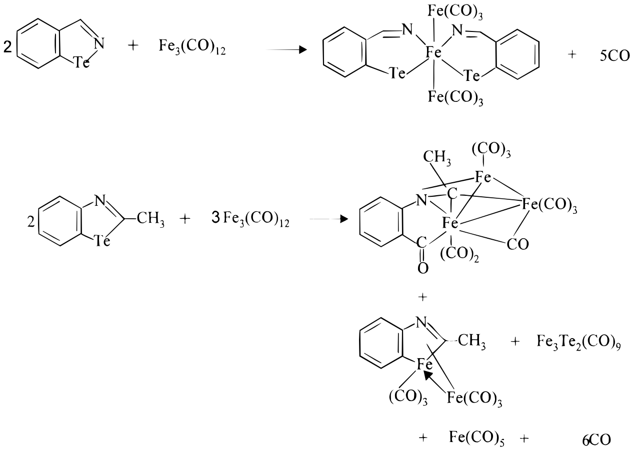
Table 1. Crystallographic Data

	5	6	7
formula	$C_{21}H_{10}N_2Fe_3Te_2O_7 \cdot C_7H_8$	$C_{18}H_7NFe_3O_{10}$	$C_{14}H_7NFe_2O_6$
fw	871.1	564.8	396.9
cryst sys	monoclinic	triclinic	monoclinic
space group	*C*2/*c*	*P*1	*P*2$_1$/*n*
a, Å	21.063(2)	10.587(3)	14.801(3)
b, Å	15.350(1)	11.722(3)	7.148(2)
c, Å	19.000(2)	8.640(2)	15.289(4)
α, deg	90	105.59(2)	90
β, deg	98.49(1)	96.54(2)	109.41(2)
γ, deg	90	90.83(2)	90
V, Å^3	6075.7(9)	1024.9(5)	1525.6(7)
Z	8	2	4
D_c	1.905	1.830	1.728
μ(MoKα), mm^{-1}	3.338	2.152	1.930
size, mm	0.2 × 0.2 × 0.25	0.2 × 0.3 × 0.3	0.25 × 0.25 × 0.35
h,*k*,*l* range	−25 to 25, −18 to 17, −22 to 22	−12 to 12, −13 to 13, −10 to 10	−17 to 17, −7 to 8, −18 to 17
θ range, deg	2−25	2−25	2−25
no. of unique rflns[$I > \sigma(I)$]	5221	3266	2471
no. of variables	332	289	209
Δ/σ(max)	0.001	0.001	0.001
$\Delta\rho$,e Å^{-3}	0.93, −1.67	0.51, −0.55	0.46, −0.67
R, wR2[a]	0.1026, 0.1924	0.0561, 0.1425	0.0719, 0.1832
no. of obsd reflns [$I > 2\sigma(I)$]	3766	3063	2045
R, wR2[a] obsd data	0.0652, 0.1733	0.0520, 0.1386	0.0630, 0.1672
w(*a*,*b*)[b]	0.086, 1.63	0.064, 2.05	0.122, 0

[a] $wR2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$. [b] $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ where $P = (F_o^2 + 2F_c^2)/3$.

Scheme 1. Reactions of Nitrogen-Containing Tellurium Heterocycles with $Fe_3(CO)_{12}$



7.35 (m, 1H), 5.30 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ (*vs* TMS) 104.4, 129.4, 134.1, 137.9, 138.1, 172.3, 207.9, 213.6. Crystals suitable for X-ray crystallography were grown by slowly cooling a concentrated toluene solution of the compound (N.B. the analytical data above are for crystals from hexane/CH_2Cl_2).

(2) Reaction of 2-Methylbenzotellurazole[6] with (Triiron Dodecacarbonyl. 2-Methylbenzotellurazole[5] (0.5 g, 2.04 mmol) and triiron dodecacarbonyl (1.06 g, 2.10 mmol) were dissolved in 50 cm^3 of dry toluene under an atmosphere of argon, and the reaction mixture was refluxed for 3 h. After the reaction mixture was cooled, it was filtered to remove a brown residue and the filtrate was concentrated under vacuum, yielding a dark brown solid. The solid was chromatographed on a silica gel column (2 × 15 cm) with hexane/CH_2Cl_2 (2:1) as the eluting solvent, thereby giving a red band preceded by a brown band and a fast eluting purple band. Collection of the three fractions followed by evaporation of the solvent gave purple crystals from the first eluate, identified as the cluster compound $Fe_3Te_2(CO)_9$ (60 mg, 12.7% based on $Fe_3(CO)_{12}$), a dark purple solid from the second eluate, and a dark red solid from the third. The dark purple solid was shown to have the molecular formula $C_{18}H_7NFe_3O_{10}$, **6** (25 mg, 6.3% based on $Fe_3(CO)_{12}$). Anal. Calcd for $C_{18}H_7NFe_3O_{10}$: C, 38.2; H, 1.24; N, 2.48. Found: C, 38.8; H, 1.30; N, 2.55. IR (KBr): ν(CO) 2083, 2036, 2015, 1978, 1870, 1856, 1690, 1650 cm^{-1}. ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ (*vs* TMS) 7.76 (m, 1H), 7.61 (m, 1H), 7.36 (m, 1H), 7.24 (m, 1H), 2.63 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ (*vs* TMS) 29.7, 33.5, 114.8, 121.3, 122.6, 124.4, 128.7, 134.0, 214.7. FAB-MS (NOBA matrix): M$^+$, 565.8; [M$^+$ − CO], 537.8; [M$^+$ − 3CO], 481.8; [M$^+$ − 6CO], 397.8; [M$^+$ − 8CO], 341.8. Crystals suitable for X-ray crystallography were grown by slowly cooling a concentrated hexane solution of the compound.

The dark red solid obtained from the third eluate was shown to have the molecular formula $C_{14}H_7NFe_2O_6$, **7** (28 mg, 10.1% based on $Fe_3(CO)_{12}$). Anal. Calcd. for $C_{14}H_7NFe_2O_6$: C, 42.3; H, 1.76; N, 3.52. Found: C, 43.4; H, 1.61; N, 3.70. IR (KBr): ν(CO) 2071, 2038, 2015, 1985, 1919, 1881 cm^{-1}. ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ (*vs* TMS) 8.02 (m, 1H), 7.70 (m, 1H), 7.51 (m, 1H), 7.03 (m, 1H), 2.76 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C: δ (*vs* TMS) 36.3, 126.0, 126.3, 133.3, 142.2, 143.9, 149.0, 206.9, 207.7. FAB-MS (NOBA matrix): M$^+$, 397.9; [M$^+$ − 3CO], 313.9; [M$^+$ − 6CO], 229.9. Crystals suitable for X-ray crystallography were grown by slowly cooling a concentrated hexane/CH_2Cl_2 (2:1) solution of the compound. Scheme 1 summarizes the sequence of reactions.

X-ray Crystallography. The structures of compounds **5**, **6**, and **7** were determined, and the crystal parameters are given in Table 1. Data for all three structures were collected on a Rigaku R-axis II area detector diffractometer at 293(2) K using graphite-monochromated Mo Kα radiation, λ = 0.710 69 Å. For **5**, **6**, and **7**, respectively, 60 3°, 24 8°, and 46 4° oscillation exposures were made, with crystal to detector distances of 80 mm.

The structures were determined[7] by direct methods and refined[8] on F^2 by full-matrix least-squares using all data with $I > \sigma(I)$ and anisotropic displacement parameters for the non-hydrogen atoms. H atoms were placed in calculated positions. The relatively high *R* values and large residual electron

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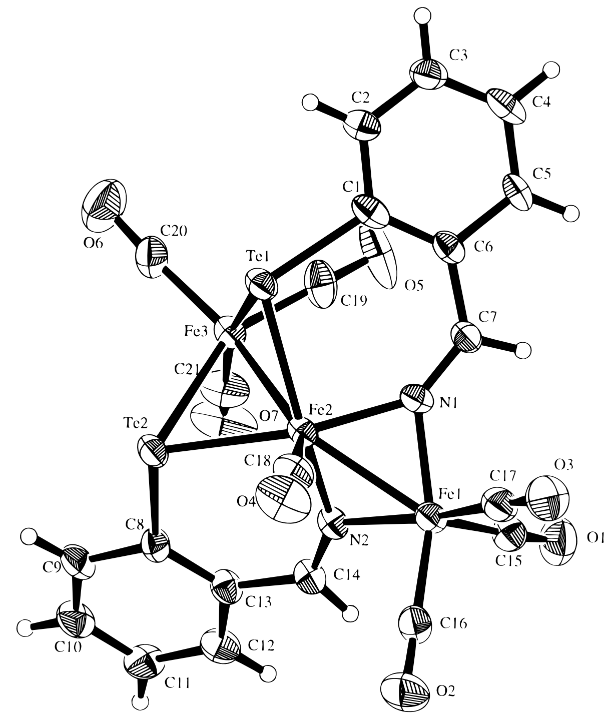

Figure 1.

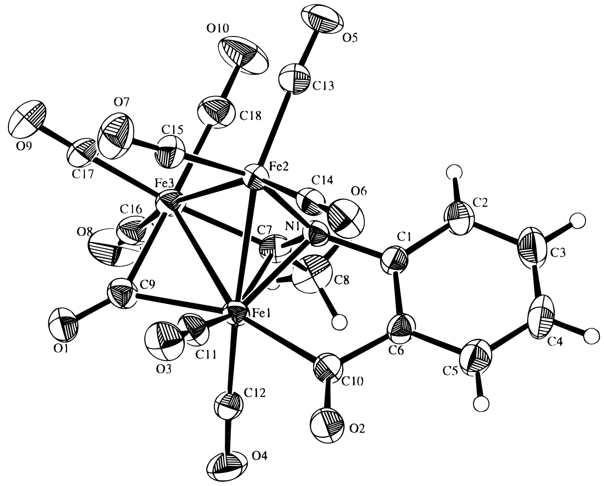

Figure 2.

density for structure **5** are probably due to difficulties in modeling the rather ill-defined toluene solvent of crystallization present in the crystal. The toluene carbon atoms were located from difference maps; however, in the least-squares refinements, the toluene molecule was treated as an idealized rigid group (aromatic C−C 1.39 Å, C(aromatic)−C(methyl) 1.50 Å) with individual isotropic atomic displacement parameters. Refinement of the site occupation factor indicated full site occupancy and rather large atomic displacement parameters.

ORTEP[9] plots of the complexes **5**, **6**, and **7** are shown in Figures 1, 2, and 3. Selected bond lengths and angles are displayed in Tables 2, 3, and 4.

Discussion

The initial aim of the work, namely to demonstrate the potential of heterocyclic Te,N ring compounds as precursors of novel organo transition metal complexes, has been achieved, as evidenced by the isolation of three interesting molecules which have been characterized crystallographically. All spectroscopic data for these new materials (Experimental Section) are consistent with the X-ray determined structures.

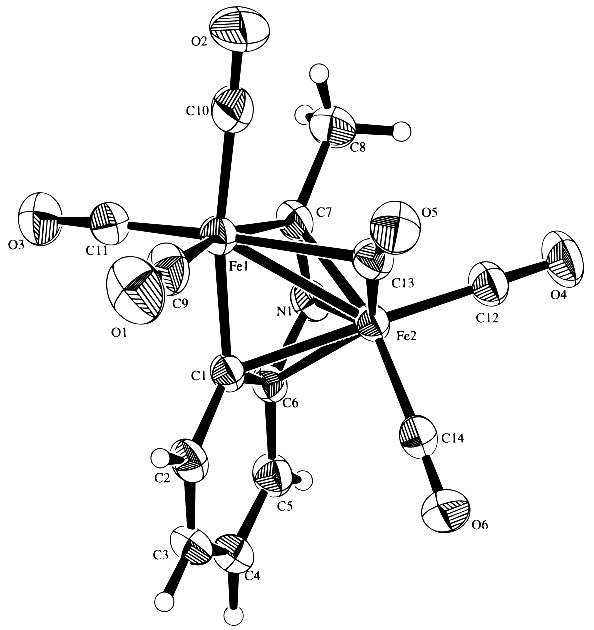

Figure 3.

Table 2. Selected Bond Lengths (Å) and Angles (deg) for 5

Te(1)−C(1)	2.112(12)	Fe(1)−Fe(2)	2.472(2)
Te(1)−Fe(2)	2.507(2)	Fe(2)−C(18)	1.796(14)
Te(1)−Fe(3)	2.553(2)	Fe(2)−N(2)	1.889(9)
Te(2)−C(8)	2.116(11)	Fe(2)−N(1)	1.916(9)
Te(2)−Fe(2)	2.504(2)	Fe(2)−Fe(3)	2.683(2)
Te(2)−Fe(3)	2.543(2)	Fe(3)−C(19)	1.753(14)
Fe(1)−N(1)	1.901(9)	N(1)−C(7)	1.275(13)
Fe(1)−N(2)	1.923(9)	N(2)−C(14)	1.269(14)

C(1)−Te(1)−Fe(2)	105.0(3)	N(1)−Fe(2)−Te(1)	91.1(3)
C(1)−Te(1)−Fe(3)	102.3(3)	Te(2)−Fe(2)−Te(1)	85.3(1)
Fe(2)−Te(1)−Fe(3)	64.0(1)	Fe(1)−Fe(2)−Fe(3)	133.4(1)
C(8)−Te(2)−Fe(2)	103.9(3)	Te(2)−Fe(3)−Te(1)	83.5(1)
C(8)−Te(2)−Fe(3)	100.1(3)	C(7)−N(1)−Fe(1)	133.9(9)
Fe(2)−Te(2)−Fe(3)	64.2(1)	C(7)−N(1)−Fe(2)	144.6(9)
N(1)−Fe(1)−N(2)	83.6(4)	Fe(1)−N(1)−Fe(2)	80.7(3)
N(2)−Fe(2)−N(1)	84.1(4)	C(14)−N(2)−Fe(2)	146.5(9)
N(2)−Fe(2)−Te(2)	90.6(3)	C(14)−N(2)−Fe(1)	131.5(9)
N(1)−Fe(2)−Te(2)	158.1(3)	Fe(2)−N(2)−Fe(1)	80.8(3)
N(2)−Fe(2)−Te(1)	156.3(3)		

Table 3. Selected Bond Lengths (Å) and Angles (deg) for 6

Fe(1)−C(12)	1.801(6)	Fe(2)−Fe(3)	2.647(1)
Fe(1)−C(11)	1.802(6)	Fe(3)−C(9)	1.955(6)
Fe(1)−N(1)	1.999(4)	Fe(3)−C(7)	1.983(6)
Fe(1)−C(10)	2.021(6)	O(1)−C(9)	1.166(7)
Fe(1)−C(9)	2.043(6)	O(2)−C(10)	1.217(7)
Fe(1)−C(7)	2.082(5)	N(1)−C(7)	1.348(7)
Fe(1)−Fe(2)	2.496(1)	N(1)−C(1)	1.435(7)
Fe(1)−Fe(3)	2.589(1)	C(6)−C(10)	1.506(8)
Fe(2)−N(1)	1.936(4)		

N(1)−Fe(1)−C(7)	38.5(2)	Fe(1)−Fe(3)−Fe(2)	56.9(1)
N(1)−Fe(1)−Fe(2)	49.5(1)	C(7)−N(1)−C(1)	122.5(4)
C(7)−Fe(1)−Fe(2)	73.1(2)	C(7)−N(1)−Fe(2)	112.3(3)
N(1)−Fe(1)−Fe(3)	70.6(1)	C(1)−N(1)−Fe(2)	125.2(3)
C(7)−Fe(1)−Fe(3)	48.8(2)	C(7)−N(1)−Fe(1)	74.1(3)
Fe(2)−Fe(1)−Fe(3)	62.7(1)	C(1)−N(1)−Fe(1)	113.8(3)
N(!)−Fe(2)−Fe(1)	51.8(1)	Fe(2)−N(1)−Fe(1)	78.7(2)
N(1)−Fe(2)−Fe(3)	70.1(1)	O(1)−C(9)−Fe(3)	144.1(5)
Fe(1)−Fe(2)−Fe(3)	60.4(1)	O(1)−C(9)−Fe(1)	135.2(5)
C(7)−Fe(3)−Fe(1)	52.2(1)	O(2)−C(10)−Fe(1)	127.1(5)
C(7)−Fe(3)−Fe(2)	71.2(2)		

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Table 4. Selected Bond Lengths (Å) and Angles (deg) for 7

Fe(1)−C(7)	1.974(5)	Fe(2)−C(1)	2.124(4)
Fe(1)−C(1)	1.977(4)	Fe(2)−N(1)	2.132(4)
Fe(1)−C(13)	2.426(5)	Fe(2)−C(6)	2.153(4)
Fe(1)−Fe(2)	2.497(1)	N(1)−C(7)	1.354(6)
Fe(2)−C(13)	1.798(5)	N(1)−C(6)	1.398(6)
Fe(2)−C(7)	2.111(5)	C(1)−C(6)	1.420(6)
C(7)−Fe(1)−C(1)	79.5(2)	C(7)−N(1)−C(6)	111.7(4)
C(7)−Fe(1)−Fe(2)	54.8(1)	C(7)−N(1)−Fe(2)	70.5(3)
C(1)−Fe(1)−Fe(2)	55.2(1)	C(6)−N(1)−Fe(2)	71.7(2)
C(7)−Fe(2)−N(1)	37.2(2)	C(6)−C(1)−Fe(1)	113.2(3)
C(1)−Fe(2)−C(6)	38.8(2)	N(1)−C(6)−C(1)	116.1(4)
N(1)−Fe(2)−C(6)	38.1(2)	N(1)−C(7)−Fe(1)	118.7(3)
C(7)−Fe(2)−Fe(1)	49.9(1)	O(5)−C(13)−Fe(2)	163.5(4)
C(1)−Fe(2)−Fe(1)	49.8(1)	O(5)−C(13)−Fe(1)	125.8(4)

The molecular structure of **5** (Figure 1) contains a nonlinear chain of three iron atoms, Fe1−Fe2−Fe3 133.4(1)°, Fe1−Fe2, 2.472(2) Å, doubly-bridged by nitrogen and Fe2−Fe3, 2.683(2) Å, doubly-bridged by tellurium. Fe1 and Fe3 are six-coordinate, whereas the central iron Fe2 is seven-coordinate. There is no comparable system in the structural literature[10] involving single or double bridging by nitrogen and tellurium of adjacent iron atoms of a three iron chain. In an example of single bridging by tellurium in $Fe_3(CO)_8(\mu_3\text{-}Pr^iP)[\mu_2\text{-}Te(PhMe_3)]_2$,[11] the Fe−Fe distances are 2.666(2) and 2.768(2) Å with Fe−Te in the range 2.527−2.571 Å. Here, however, the Fe−Fe−Fe angle is 94.2°, presumably to allow μ_3-Pr^{i}P coordination. Fe−Fe bonds doubly-bridged by tellurium tend to be somewhat shorter than those found in **5**, e.g., 2.0609 Å in $[Fe_2(CO)_6(\mu\text{-}TeMe)]_2(\mu\text{-}Te_2CH_2)$,[12a] 2.634 Å in $Fe_2(CO)_6(\mu\text{-}TeMe_2)_2$,[12b] 2.633 Å in $Fe_2(CO)_6[\mu\text{-}Te(CH_2)_3Te]$,[12c] and 2.656 Å in $Fe_2(CO)_6(\mu\text{-}TeCHCl_2)_2$.[12d] The Fe−Te distances in these structures are in the range 2.517−2.562 Å, similar to those found in **5**. The N1−C7 and N2−C14 bond lengths (Table 2) correspond to pure double bonds. Only four compounds containing Fe−Fe bonds doubly-bridged by nitrogen, where the nitrogen atoms are double bonded to a carbon atom, have been structurally characterized. The Fe−Fe bonds are again shorter than those in **5**, 2.439 Å in $Fe_2(CO)_6(\mu\text{-}N{=}C_6H_{10})_2$,[13a] 2.403 Å in $Fe_2(CO)_6(\mu\text{-}N{=}CPh_2)_2$,[13b] 2.393 Å in $Fe_2(CO)_6(\mu\text{-}N_2C_{23}H_{18})$,[13c] and 2.415 Å in $Fe_2(CO)_6(\mu\text{-}N{=}CHMe)_2$.[13d] Fe−N distances average 1.935 Å. It is clear that the Fe2 atom has inserted regioselectively into the Te−N bond of the heterocycle, and the resulting *cis* arrangement of the nitrogen and tellurium atoms is of interest. The reaction mimics that in which benzothiophene is the substrate. In this case, it was also the chalcogen S−C bond remote from the benzene ring that underwent attack.[14] The isolation from the reaction mixture of the known cluster compound $Fe_3Te_2(CO)_9$[15] certainly implies detelluration of the heterocyclic tellurium compound, but we failed to isolate from the reaction mixture any material containing detellurated organic moieties. This fact, together with the isolation of $Fe_3Te_2(CO)_9$ from the reaction of **4** with $Fe_3(CO)_{12}$ (*vide infra*) and the isolation of **7** containing only one organic moiety, casts doubt on an otherwise attractive postulate that **5** may be similar to the intermediate from which **2** originated.

The reaction of 2-methylbenzotellurazole with $Fe_3(CO)_{12}$ afforded three isolable pure fractions. One was the purple $Fe_3Te_2(CO)_9$,[13] the second (**6**) was another purple material of complex structure (Figure 2), and the third was the red azaferrole (Figure 3). It is probable that the three compounds can be considered to arise at various stages of a complex parallel reaction sequence involving the detelluration of the heterocycle and the replacement of the tellurium by, interestingly, both an iron atom and an inserted carbonyl group. The structure of **6** (Figure 2) is based on a triangle of iron atoms. The C7−N1 formal double bond at 1.348(7) Å is significantly longer than a pure double bond, and this residue bridges Fe1−Fe2 through the nitrogen atom and Fe1−Fe3 through the carbon atom. In addition, Fe1−Fe3 is bridged by the C9−O1 carbonyl in an almost symmetrical manner (C9−Fe1, Fe3 2.043(6), 1.955(6) Å). The nitrogen-bridged edge of the iron triangle at 2.496(1) Å is the shortest edge of the triangle, and Fe2−Fe3 which is not directly bridged, at 2.647(1) Å, is the longest edge of the triangle. Similar variations in Fe−Fe bond distances have been noted in other Fe_3 triangles.[16,17] Fe1 shows apparent 8-fold coordination, involving two iron atoms, a nitrogen and five carbon atoms (relevant distances in Table 4). Of these, the C7═N1 residue may be considered to be π-bonded whereas the other six atoms are essentially σ-bonded. A seven coordinate iron, *via* five σ-bonds to two iron atoms, a bridging nitrogen and two bridging carbonyls, and two π-bonds to a cyclohexadiene residue, occurs in $Fe_3(\mu_3\text{-}NPh)(\eta^4\text{-}C_6H_8)(CO)_8$.[18]

In **7** (Figure 3), one iron atom, Fe1, forms part of a benzoazaferrole system, and the second iron, Fe2, is π-bonded to the C1−C6−N1−C7 residue of the azaferrole. Here, the C1−C6 aromatic bond is lengthened to 1.420(6) Å, the central C−N single bond is shortened to 1.398(6) Å, and the N1−C7 formal double bond is lengthened to 1.354(6) Å. The Fe−Fe distance is relatively short at 2.498(1) Å. In addition, the Fe2−C13−O5 carbonyl group forms a weak bridge to Fe1 (Fe1−C13 2.426(5) Å, Fe2−C13 1.798(5) Å; O5−C13−Fe1, Fe2 125.8(4)°, 163.5(4)°). If the Fe1−C13 interaction is considered to be significant, Fe1 is seven-coordinate. A search of the CSD[10] indicates no examples of previous X-ray structure determinations of benzoazaferrole systems. However, in two analogous ferrole complexes[19] and a dibenzoferrole,[4] Fe−C(σ) bond lengths

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are in the range 1.921−2.039 Å, mean 1.948(19) Å, Fe−C(π) lengths are in the range 2.035−2.216 Å, mean 2.125(15) Å, and Fe−Fe 2.466(1), 2.567(1), and 2.468(1) Å, similar to the lengths in **7**, and in the 3-ferra-4-pyrrolin-2-one complex $Fe_2(\mu\text{-}CH{=}CHNPhC\{O\})(CO)_6$, Fe−Fe is 2.597 Å.[20]

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Supporting Information Available: Tables of atomic coordinates, bond lengths and angles, anisotropic displacement parameters, and hydrogen coordinates for **5** and **7** and atomic coordinates for **6** (12 pages). Ordering information is given on any current masthead page.

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