ORGANOMETALLICS
Organometallics, 1996, 15(7), 1785-1792, DOI:10.1021/om950806l

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at http://pubs.acs.org/page/copyright/permissions.html

ACS Publications
MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1996 American Chemical Society

©1996 American Chemical Society Organometallics V15 Page 1785 Leung Supplemental Page 1

OM950806L

***α

COMPOUND 1

Got (1)

L1792-1

Table 1. Data collection and processing parameters.

Molecular formula	$C_{24}H_{44}N_2Si_4Fe$ $Fe(C_{12}H_{22}NSi_2)_2$
Molecular weight	528.8
Color and habit	dark-brown inside capillary
Crystal size	0.36 x 0.40 x 0.60 mm^3
Crystal system	monoclinic
Space group	$P2_1/c$ (No. 14)
Unit cell parameters	a = 23.882(5)Å β = 107.32(1)°
	b = 16.820(6) V = 6291(3)Å^3
	c = 16.406(4) Z = 8 $F(000)$ = 2272
Density (calcd)	1.117 g cm^{-3}
Radiation	graphite-monochromatized Mo$K\alpha$, λ = 0.71073 Å
Standard reflections	(4,0,4); (7,7,1)
Intensity variation	±1.1%
R_{int} (from merging of eqiv. reflections)	0.024
Absorption coefficient	0.645 mm^{-1}
Mean μr	0.14
Transmission factors	0.691 to 0.819
Scan type and rate	Wyckoff; 3.08-29.3 deg min^{-1}
Scan range	0.80° below $K\alpha_1$ to 0.80° above $K\alpha_2$
Background counting	stationary counts for one-fifth of scan time at each end of scan range
Collection range	$-28 \le h \le 27$, $-20 \le k \le 0$, $0 \le \ell \le 19$ $9\theta_{max}$ = 50°
Unique data measured	10957
Obs. data with $\|F_o\| \ge 6\sigma(\|F_o\|)$, n	4418
No. of variables, p	559
Weighting scheme	$w = [\sigma^2\|F_o\| + 0.0008\|F_o\|^2]^{-1}$
$R_F = \sum\|\|F_o\| - \|F_o\|\| / \sum\|F_o\|$	0.0411
$wR = [\sum w^2(\|F_o\| - \|F_c\|)^2 / \sum w^2\|F_o\|^2]^{1/2}$	0.0621
$S = [\sum w(\|F_o\| - \|F_c\|)^2/(n-p)]^{1/2}$	1.44
Largest and mean Δ/σ	.003, .000
Residual extrema in final difference map	+0.30 to -0.26 e$Å^{-3}$

L1792-2

Table 2. Atomic coordinates (x 10^5 for Fe; x 10^4 for others) and equivalent isotropic temperature factors* (Å^2 x 10^4 for Fe; x 10^3 for others)

Atom	x	y	z	U_{eq}
Fe(1)	13531(4)	56910(6)	77769(6)	512(4)
Si(1)	2073(1)	6082(1)	6404(1)	60(1)
Si(2)	2337(1)	4433(2)	7363(2)	86(1)
Si(3)	-36(1)	5807(2)	6640(2)	68(1)
Si(4)	402(1)	6908(2)	8300(2)	88(1)
C(1)	2121(3)	5483(4)	7376(4)	52(3)
C(2)	2462(3)	5939(4)	8142(4)	51(3)
C(3)	3067(3)	6031(5)	8448(5)	78(4)
C(4)	3317(3)	6472(5)	9148(6)	82(4)
C(5)	2968(4)	6832(5)	9559(5)	76(4)
C(6)	2367(3)	6706(5)	9248(5)	71(4)
N(1)	2117(2)	6278(3)	8561(4)	53(2)
C(7)	1614(4)	5582(5)	5426(5)	105(5)
C(8)	2814(3)	6293(6)	6265(5)	104(5)
C(9)	1752(3)	7064(5)	6488(5)	88(4)
C(10)	2612(5)	4071(6)	8448(7)	166(8)
C(11)	2949(4)	4243(6)	6924(8)	155(7)
C(12)	1710(4)	3809(5)	6772(7)	131(6)
C(13)	469(3)	5974(4)	7719(4)	54(3)
C(14)	478(4)	5262(6)	8241(5)	75(4)
C(15)	50(4)	4951(7)	8592(7)	118(6)
C(16)	189(8)	4210(10)	9066(10)	179(12)
C(17)	668(7)	3865(12)	9144(11)	177(11)
C(18)	1060(5)	4180(8)	8805(7)	128(7)
N(2)	971(4)	4833(4)	8385(4)	81(4)
C(19)	-820(3)	5754(7)	6546(7)	152(7)
C(20)	137(3)	4836(5)	6218(5)	84(4)
C(21)	28(4)	6581(5)	5882(6)	108(5)
C(22)	790(4)	6776(7)	9460(6)	143(7)
C(23)	-355(4)	7253(6)	8230(8)	165(8)
C(24)	755(4)	7742(5)	7930(7)	118(6)
Fe(2)	38150(4)	43541(6)	27814(6)	432(4)
Si(5)	4863(1)	3003(1)	2764(2)	67(1)
Si(6)	4591(1)	4430(1)	1428(1)	61(1)
Si(7)	2432(1)	4369(2)	1584(1)	65(1)
Si(8)	2832(1)	5701(1)	3017(2)	64(1)
C(25)	4613(3)	4041(4)	2488(4)	47(3)
C(26)	4919(3)	4636(4)	3153(4)	46(3)
C(27)	5518(3)	4787(5)	3450(5)	67(4)
C(28)	5724(3)	5387(6)	4031(6)	81(4)
C(29)	5342(4)	5831(5)	4318(5)	89(4)
C(30)	4758(4)	5664(5)	4023(5)	80(4)
N(3)	4548(2)	5068(3)	3459(3)	51(2)
C(31)	4243(3)	2282(4)	2337(6)	104(5)
C(32)	5130(4)	2827(5)	3942(6)	105(5)
C(33)	5477(4)	2693(5)	2333(7)	120(6)
C(34)	4214(4)	3762(6)	551(5)	110(5)
C(35)	4223(4)	5405(5)	1197(5)	101(5)
C(36)	5342(3)	4618(6)	1292(5)	103(5)
C(37)	2920(3)	4673(4)	2637(4)	43(3)

L1792-3

C(38)	2926(3)	4060(4)	3306(4)	47(3)
C(39)	2496(3)	3925(5)	3731(5)	71(4)
C(40)	2589(4)	3339(5)	4344(5)	87(5)
C(41)	3088(4)	2876(5)	4552(5)	76(4)
C(42)	3489(3)	3028(4)	4132(5)	63(3)
N(4)	3422(2)	3607(3)	3532(3)	47(2)
C(43)	2431(4)	5103(7)	714(5)	141(6)
C(44)	2683(4)	3385(6)	1260(6)	133(6)
C(45)	1653(3)	4179(7)	1553(6)	132(6)
C(46)	3221(4)	5773(5)	4206(5)	109(5)
C(47)	3167(3)	6475(4)	2460(6)	89(4)
C(48)	2050(3)	6022(5)	2884(7)	115(6)

*U_{eq} defined as one third of the trace of the orthogonalized U tensor.

L1792-4

Table 3. Bond lengths (Å) and bond angles (°).

Fe(1)-C(1)	2.154(8)	Fe(1)-N(1)	2.135(5)
Fe(1)-C(13)	2.139(7)	Fe(1)-N(2)	2.111(8)
Si(1)-C(1)	1.861(8)	Si(1)-C(7)	1.853(8)
Si(1)-C(8)	1.885(9)	Si(1)-C(9)	1.842(8)
Si(2)-C(1)	1.841(7)	Si(2)-C(10)	1.810(12)
Si(2)-C(11)	1.841(13)	Si(2)-C(12)	1.849(9)
Si(3)-C(13)	1.843(7)	Si(3)-C(19)	1.835(9)
Si(3)-C(20)	1.866(9)	Si(3)-C(21)	1.838(10)
Si(4)-C(13)	1.869(8)	Si(4)-C(22)	1.866(9)
Si(4)-C(23)	1.869(10)	Si(4)-C(24)	1.830(10)
C(1)-C(2)	1.489(9)	C(2)-C(3)	1.391(10)
C(2)-N(1)	1.347(10)	C(3)-C(4)	1.348(12)
C(4)-C(5)	1.362(14)	C(5)-C(6)	1.389(11)
C(6)-N(1)	1.321(9)	C(13)-C(14)	1.469(12)
C(14)-C(15)	1.413(16)	C(14)-N(2)	1.340(13)
C(15)-C(16)	1.454(20)	C(16)-C(17)	1.256(26)
C(17)-C(18)	1.332(25)	C(18)-N(2)	1.280(15)
Fe(2)-C(25)	2.166(7)	Fe(2)-N(3)	2.141(5)
Fe(2)-C(37)	2.147(6)	Fe(2)-N(4)	2.159(6)
Si(5)-C(25)	1.856(7)	Si(5)-C(31)	1.880(8)
Si(5)-C(32)	1.869(9)	Si(5)-C(33)	1.882(11)
Si(6)-C(25)	1.844(7)	Si(6)-C(34)	1.837(9)
Si(6)-C(35)	1.846(9)	Si(6)-C(36)	1.898(9)
Si(7)-C(37)	1.846(6)	Si(7)-C(43)	1.886(10)
Si(7)-C(44)	1.890(11)	Si(7)-C(45)	1.874(9)
Si(8)-C(37)	1.872(7)	Si(8)-C(46)	1.898(8)
Si(8)-C(47)	1.899(9)	Si(8)-C(48)	1.894(9)
C(25)-C(26)	1.500(9)	C(26)-C(27)	1.391(9)
C(26)-N(3)	1.353(9)	C(27)-C(28)	1.376(12)
C(28)-C(29)	1.364(14)	C(29)-C(30)	1.363(12)
C(30)-N(3)	1.355(10)	C(37)-C(38)	1.502(10)
C(38)-C(39)	1.421(12)	C(38)-N(4)	1.363(8)
C(39)-C(40)	1.379(12)	C(40)-C(41)	1.378(12)
C(41)-C(42)	1.362(13)	C(42)-N(4)	1.360(9)

C(1)-Fe(1)-N(1)	66.8(2)	C(1)-Fe(1)-C(13)	160.4(3)
N(1)-Fe(1)-C(13)	125.4(3)	C(1)-Fe(1)-N(2)	124.1(3)
N(1)-Fe(1)-N(2)	116.3(2)	C(13)-Fe(1)-N(2)	67.2(3)
C(1)-Si(1)-C(7)	111.5(4)	C(1)-Si(1)-C(8)	112.6(3)
C(7)-Si(1)-C(8)	108.4(4)	C(1)-Si(1)-C(9)	110.0(4)
C(7)-Si(1)-C(9)	108.7(4)	C(8)-Si(1)-C(9)	105.5(4)
C(1)-Si(2)-C(10)	109.4(4)	C(1)-Si(2)-C(11)	115.4(4)
C(10)-Si(2)-C(11)	103.2(6)	C(1)-Si(2)-C(12)	111.4(3)
C(10)-Si(2)-C(12)	109.0(5)	C(11)-Si(2)-C(12)	108.0(5)
C(13)-Si(3)-C(19)	116.6(4)	C(13)-Si(3)-C(20)	109.6(3)

L1792-5

C(19)-Si(3)-C(20)	105.0(5)	C(13)-Si(3)-C(21)	112.3(4)
C(19)-Si(3)-C(21)	105.4(5)	C(20)-Si(3)-C(21)	107.3(4)
C(13)-Si(4)-C(22)	109.1(4)	C(13)-Si(4)-C(23)	117.2(4)
C(22)-Si(4)-C(23)	106.0(5)	C(13)-Si(4)-C(24)	111.0(4)
C(22)-Si(4)-C(24)	107.0(4)	C(23)-Si(4)-C(24)	106.0(5)
Fe(1)-C(1)-Si(1)	109.4(3)	Fe(1)-C(1)-Si(2)	115.2(4)
Si(1)-C(1)-Si(2)	117.1(4)	Fe(1)-C(1)-C(2)	87.7(5)
Si(1)-C(1)-C(2)	108.9(5)	Si(2)-C(1)-C(2)	114.8(4)
C(1)-C(2)-C(3)	127.6(7)	C(1)-C(2)-N(1)	112.7(6)
C(3)-C(2)-N(1)	119.7(6)	C(2)-C(3)-C(4)	121.3(8)
C(3)-C(4)-C(5)	119.0(7)	C(4)-C(5)-C(6)	118.0(7)
C(5)-C(6)-N(1)	123.5(8)	Fe(1)-N(1)-C(2)	92.3(4)
Fe(1)-N(1)-C(6)	148.7(6)	C(2)-N(1)-C(6)	118.5(6)
Fe(1)-C(13)-Si(3)	111.3(4)	Fe(1)-C(13)-Si(4)	113.4(3)
Si(3)-C(13)-Si(4)	119.2(4)	Fe(1)-C(13)-C(14)	87.2(5)
Si(3)-C(13)-C(14)	109.1(5)	Si(4)-C(13)-C(14)	112.2(6)
C(13)-C(14)-C(15)	130.7(9)	C(13)-C(14)-N(2)	113.6(9)
C(15)-C(14)-N(2)	115.7(9)	C(14)-C(15)-C(16)	117.2(11)
C(15)-C(16)-C(17)	120.4(18)	C(16)-C(17)-C(18)	120.4(18)
C(17)-C(18)-N(2)	122.7(13)	Fe(1)-N(2)-C(14)	91.7(6)
Fe(1)-N(2)-C(18)	144.5(9)	C(14)-N(2)-C(18)	123.6(10)
C(25)-Fe(2)-N(3)	67.3(2)	C(25)-Fe(2)-C(37)	161.7(2)
N(3)-Fe(2)-C(37)	123.4(2)	C(25)-Fe(2)-N(4)	123.1(2)
N(3)-Fe(2)-N(4)	117.2(2)	C(37)-Fe(2)-N(4)	67.7(2)
C(25)-Si(5)-C(31)	110.9(3)	C(25)-Si(5)-C(32)	112.8(4)
C(31)-Si(5)-C(32)	105.8(4)	C(25)-Si(5)-C(33)	113.4(4)
C(31)-Si(5)-C(33)	107.2(4)	C(32)-Si(5)-C(33)	106.3(4)
C(25)-Si(6)-C(34)	113.1(4)	C(25)-Si(6)-C(35)	112.8(4)
C(34)-Si(6)-C(35)	106.8(4)	C(25)-Si(6)-C(36)	114.0(3)
C(34)-Si(6)-C(36)	105.6(4)	C(35)-Si(6)-C(36)	103.7(4)
C(37)-Si(7)-C(43)	112.6(4)	C(37)-Si(7)-C(44)	109.9(3)
C(43)-Si(7)-C(44)	106.9(5)	C(37)-Si(7)-C(45)	114.7(4)
C(43)-Si(7)-C(45)	108.3(4)	C(44)-Si(7)-C(45)	103.8(5)
C(37)-Si(8)-C(46)	109.4(3)	C(37)-Si(8)-C(47)	111.6(4)
C(46)-Si(8)-C(47)	107.7(4)	C(37)-Si(8)-C(48)	115.4(3)
C(46)-Si(8)-C(48)	105.3(5)	C(47)-Si(8)-C(48)	107.0(4)
Fe(2)-C(25)-Si(5)	114.5(4)	Fe(2)-C(25)-Si(6)	110.1(3)
Si(5)-C(25)-Si(6)	118.7(4)	Fe(2)-C(25)-C(26)	86.9(4)
Si(5)-C(25)-C(26)	113.5(4)	Si(6)-C(25)-C(26)	108.7(5)
C(25)-C(26)-C(27)	127.1(7)	C(25)-C(26)-N(3)	113.5(5)
C(27)-C(26)-N(3)	119.4(6)	C(26)-C(27)-C(28)	119.7(8)
C(27)-C(28)-C(29)	120.2(7)	C(28)-C(29)-C(30)	118.9(8)
C(29)-C(30)-N(3)	121.7(8)	Fe(2)-N(3)-C(26)	91.7(4)
Fe(2)-N(3)-C(30)	148.1(6)	C(26)-N(3)-C(30)	120.1(6)
Fe(2)-C(37)-Si(7)	111.4(3)	Fe(2)-C(37)-Si(8)	113.6(3)
Si(7)-C(37)-Si(8)	117.7(3)	Fe(2)-C(37)-C(38)	87.4(4)
Si(7)-C(37)-C(38)	111.1(4)	Si(8)-C(37)-C(38)	111.5(5)
C(37)-C(38)-C(39)	128.1(6)	C(37)-C(38)-N(4)	113.6(6)
C(39)-C(38)-N(4)	118.3(6)	C(38)-C(39)-C(40)	119.3(7)
C(39)-C(40)-C(41)	121.6(9)	C(40)-C(41)-C(42)	117.1(8)
C(41)-C(42)-N(4)	123.5(7)	Fe(2)-N(4)-C(38)	90.5(4)
Fe(2)-N(4)-C(42)	148.4(5)	C(38)-N(4)-C(42)	120.2(6)

©1996 American Chemical Society Organometallics V15 Page 1785 Leung Supplemental Page 6

L1792-6

Table 4. Anisotropic thermal parameters* ($Å^2 \times 10^4$ for Cr; $\times 10^3$ for others).

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	469(6)	567(6)	551(7)	-55(5)	23(1)	-12(6)
Si(1)	53(1)	83(2)	49(1)	-9(1)	22(1)	-6(1)
Si(2)	76(2)	60(2)	120(2)	16(1)	26(2)	-7(2)
Si(3)	45(1)	89(2)	72(2)	-10(1)	24(1)	-23(1)
Si(4)	58(1)	100(2)	122(2)	-29(1)	53(2)	-58(2)
C(1)	46(4)	52(5)	60(5)	4(3)	20(4)	-4(4)
C(2)	46(4)	52(5)	57(5)	3(4)	16(4)	5(4)
C(3)	46(5)	110(7)	71(6)	5(5)	9(4)	-27(6)
C(4)	56(5)	111(8)	76(7)	7(5)	16(5)	-5(6)
C(5)	76(6)	90(7)	53(5)	-22(5)	3(5)	-5(5)
C(6)	73(6)	87(6)	63(6)	-11(5)	34(5)	-5(5)
N(1)	51(4)	62(4)	45(4)	-7(3)	13(3)	-13(3)
C(7)	118(8)	132(8)	61(6)	-35(7)	20(5)	-19(6)
C(8)	93(7)	143(9)	96(7)	-33(7)	59(6)	-15(7)
C(9)	90(6)	90(7)	82(7)	2(5)	22(5)	20(5)
C(10)	211(14)	89(8)	190(13)	47(9)	46(11)	40(9)
C(11)	112(8)	104(9)	265(15)	28(7)	83(10)	-59(9)
C(12)	117(8)	65(7)	214(12)	-11(6)	51(8)	-44(8)
C(13)	52(4)	62(5)	58(5)	-20(4)	32(4)	-15(4)
C(14)	72(6)	98(7)	63(6)	-40(6)	31(5)	-34(5)
C(15)	108(8)	155(11)	114(9)	-61(8)	70(7)	-30(8)
C(16)	276(23)	196(19)	92(11)	-181(17)	98(15)	-15(11)
C(17)	236(23)	152(15)	103(12)	-47(17)	-9(15)	19(10)
C(18)	141(11)	131(12)	105(10)	-61(9)	26(8)	17(8)
N(2)	108(6)	66(5)	65(5)	-33(5)	18(5)	25(4)
C(19)	67(6)	243(14)	151(10)	-34(8)	40(7)	-97(10)
C(20)	99(7)	87(6)	67(6)	-18(5)	25(5)	-17(5)
C(21)	114(8)	97(7)	101(8)	13(6)	14(6)	17(6)
C(22)	143(10)	189(12)	123(10)	-64(9)	78(8)	-81(9)
C(23)	89(7)	148(10)	288(16)	-39(7)	104(9)	-120(11)
C(24)	109(8)	73(7)	190(11)	-30(6)	74(8)	-43(7)
Fe(2)	343(5)	435(6)	552(7)	17(5)	184(5)	-27(5)
Si(5)	56(1)	51(1)	100(2)	9(1)	31(1)	-10(1)
Si(6)	45(1)	81(2)	62(1)	-8(1)	24(1)	-13(1)
Si(7)	43(1)	95(2)	57(1)	-8(1)	16(1)	2(1)
Si(8)	61(1)	48(1)	95(2)	14(1)	43(1)	7(1)
C(25)	35(4)	54(4)	53(5)	0(3)	13(3)	-14(4)
C(26)	36(4)	54(5)	50(5)	6(3)	14(4)	8(4)
C(27)	42(5)	73(6)	81(6)	-18(4)	8(4)	-14(5)
C(28)	47(5)	105(8)	82(7)	-14(5)	5(5)	8(6)
C(29)	82(6)	92(7)	84(7)	-46(6)	9(5)	-30(6)
C(30)	87(6)	73(6)	87(6)	-18(5)	36(5)	-34(6)
N(3)	52(4)	48(4)	52(4)	-9(3)	16(3)	-7(3)
C(31)	99(7)	60(6)	162(10)	-2(5)	52(7)	-31(6)
C(32)	97(7)	84(7)	128(9)	14(6)	22(6)	4(6)
C(33)	95(7)	84(7)	206(12)	36(6)	81(8)	-10(7)
C(34)	119(8)	138(9)	78(7)	-30(7)	37(6)	-41(7)
C(35)	101(7)	114(8)	95(7)	19(6)	42(6)	36(6)
C(36)	63(6)	158(10)	97(7)	-11(6)	39(5)	9(7)
C(37)	35(4)	47(4)	53(5)	3(3)	20(3)	9(4)
C(38)	44(4)	47(4)	52(5)	-2(3)	17(4)	-7(4)

L1792-7

C(39)	61(5)	73(6)	100(7)	10(4)	53(5)	18(5)
C(40)	108(8)	86(7)	86(7)	-19(6)	60(6)	21(6)
C(41)	76(6)	74(6)	74(6)	-6(5)	16(5)	20(5)
C(42)	58(5)	53(5)	70(6)	-3(4)	6(4)	22(5)
N(4)	39(3)	47(4)	53(4)	4(3)	11(3)	5(3)
C(43)	147(10)	189(12)	63(7)	-38(9)	-5(6)	44(7)
C(44)	122(9)	149(10)	122(9)	-22(8)	29(7)	-70(8)
C(45)	53(5)	243(14)	104(8)	-36(7)	29(5)	-30(8)
C(46)	143(9)	102(8)	94(7)	-10(7)	54(7)	-38(6)
C(47)	90(6)	58(5)	140(8)	2(5)	63(6)	14(5)
C(48)	93(7)	84(7)	198(11)	39(6)	90(7)	24(7)

*The exponent takes the form: $-2\pi^2\sum\sum U_{ij}h_ih_j\mathbf{a}_i^*.\mathbf{a}_j^*$.

L1792-8

Table 5. Hydrogen atom coordinates (x 10^4) and assigned isotropic temperature factors* (Å^2 x 10^3).

Atom	x	y	z	U
H(3)	3311	5774	8156	100
H(4)	3736	6531	9352	100
H(5)	3132	7163	10049	100
H(6)	2120	6943	9548	100
H(7A)	1778	5070	5375	160
H(7B)	1605	5898	4935	160
H(7C)	1222	5518	5461	160
H(8A)	3005	5801	6217	160
H(8B)	3049	6585	6750	160
H(8C)	2766	6602	5756	160
H(9A)	1371	6995	6560	160
H(9B)	1717	7363	5976	160
H(9C)	2000	7345	6970	160
H(10A)	2319	4146	8735	160
H(10B)	2960	4359	8744	160
H(10C)	2702	3515	8440	160
H(11A)	2844	4418	6341	160
H(11B)	3033	3683	6949	160
H(11C)	3291	4527	7252	160
H(12A)	1561	3998	6196	160
H(12B)	1406	3837	7045	160
H(12C)	1837	3268	6768	160
H(15)	-318	5213	8524	100
H(16)	-82	3978	9329	100
H(17)	756	3366	9438	100
H(18)	1428	3915	8883	100
H(19A)	-884	5357	6930	160
H(19B)	-1036	5616	5971	160
H(19C)	-952	6261	6687	160
H(20A)	545	4823	6250	160
H(20B)	-98	4777	5634	160
H(20C)	52	4410	6552	160
H(21A)	432	6639	5902	160
H(21B)	-115	7076	6032	160
H(21C)	-199	6431	5316	160
H(22A)	617	6342	9680	160
H(22B)	755	7254	9761	160
H(22C)	1197	6665	9538	160
H(23A)	-562	6836	8418	160
H(23B)	-560	7389	7650	160
H(23C)	-331	7711	8587	160
H(24A)	1148	7597	7952	160
H(24B)	766	8195	8291	160
H(24C)	537	7872	7353	160
H(27)	5786	4474	3249	100
H(28)	6137	5494	4235	100
H(29)	5485	6252	4722	100
H(30)	4489	5980	4219	100
H(31A)	4087	2346	1730	160
H(31B)	3940	2383	2600	160
H(31C)	4385	1749	2465	160

L1792-9

H(32A)	5450	3182	4196	160
H(32B)	5262	2288	4050	160
H(32C)	4817	2922	4185	160
H(33A)	5360	2772	1726	160
H(33B)	5565	2141	2458	160
H(33C)	5818	3008	2595	160
H(34A)	4392	3245	647	160
H(34B)	4244	3972	21	160
H(34C)	3808	3720	525	160
H(35A)	3835	5366	1250	160
H(35B)	4200	5563	625	160
H(35C)	4443	5793	1593	160
H(36A)	5568	4136	1403	160
H(36B)	5540	5022	1687	160
H(36C)	5298	4791	719	160
H(39)	2144	4237	3592	100
H(40)	2300	3251	4635	100
H(41)	3150	2464	4975	100
H(42)	3838	2709	4265	100
H(43A)	2305	5613	855	160
H(43B)	2167	4924	182	160
H(43C)	2819	5146	663	160
H(44A)	3083	3428	1258	160
H(44B)	2440	3244	700	160
H(44C)	2653	2982	1660	160
H(45A)	1488	4654	1711	160
H(45B)	1642	3761	1947	160
H(45C)	1429	4024	987	160
H(46A)	3623	5616	4318	160
H(46B)	3032	5427	4509	160
H(46C)	3203	6310	4393	160
H(47A)	3565	6332	2513	160
H(47B)	3159	6985	2719	160
H(47C)	2946	6500	1867	160
H(48A)	1827	5999	2291	160
H(48B)	2048	6556	3089	160
H(48C)	1877	5673	3205	160

*The exponent takes the form: $-8\pi^2 U \sin^2\theta/\lambda^2$.

©1996 American Chemical Society Organometallics V15 Page 1785 Leung Supplemental Page 10

L1792-10

STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{24}H_{44}FeN_2Si_4$
Color; Habit	dark brown , inside capillary
Crystal size (mm)	0.36 x 0.40 x 0.60
Crystal System	Monoclinic
Space Group	$P2_1/c$
Unit Cell Dimensions	$\underline{a}$ = 23.882(5) Å
	$\underline{b}$ = 16.820(4) Å
	$\underline{c}$ = 16.406(4) Å
	β = 107.320(10)°
Volume	6291(3) $Å^3$
Z	8
Formula weight	528.8
Density(calc.)	1.117 Mg/m^3
Absorption Coefficient	0.645 mm^{-1}
F(000)	2272

L1792-11

Data Collection

Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	293
Monochromator	Highly oriented graphite crystal
2θ Range	3.0 to 50.0°
Scan Type	Wyckoff
Scan Speed	Variable; 3.08 to 29.30°/min. in ω
Scan Range (ω)	0.80°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 0.5% of total scan time
Standard Reflections	2 measured every 123 reflections
Index Ranges	$-28 \leq h \leq 27$, $-20 \leq k \leq 0$ $0 \leq l \leq 19$
Reflections Collected	11349
Independent Reflections	10957 (R_{int} = 2.40%)
Observed Reflections	4418 ($F > 6.0\sigma(F)$)
Absorption Correction	Semi-empirical
Min./Max. Transmission	0.691 / 0.819

L1792-12

Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o-F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0008F^2$
Number of Parameters Refined	559
Final R Indices (obs. data)	R = 4.11 %, wR = 6.21 %
R Indices (all data)	R = 9.34 %, wR = 6.94 %
Goodness-of-Fit	1.44
Largest and Mean Δ/σ	0.003, 0.000
Data-to-Parameter Ratio	7.9:1
Largest Difference Peak	0.30 $eÅ^{-3}$
Largest Difference Hole	-0.26 $eÅ^{-3}$

COMPOUND 3

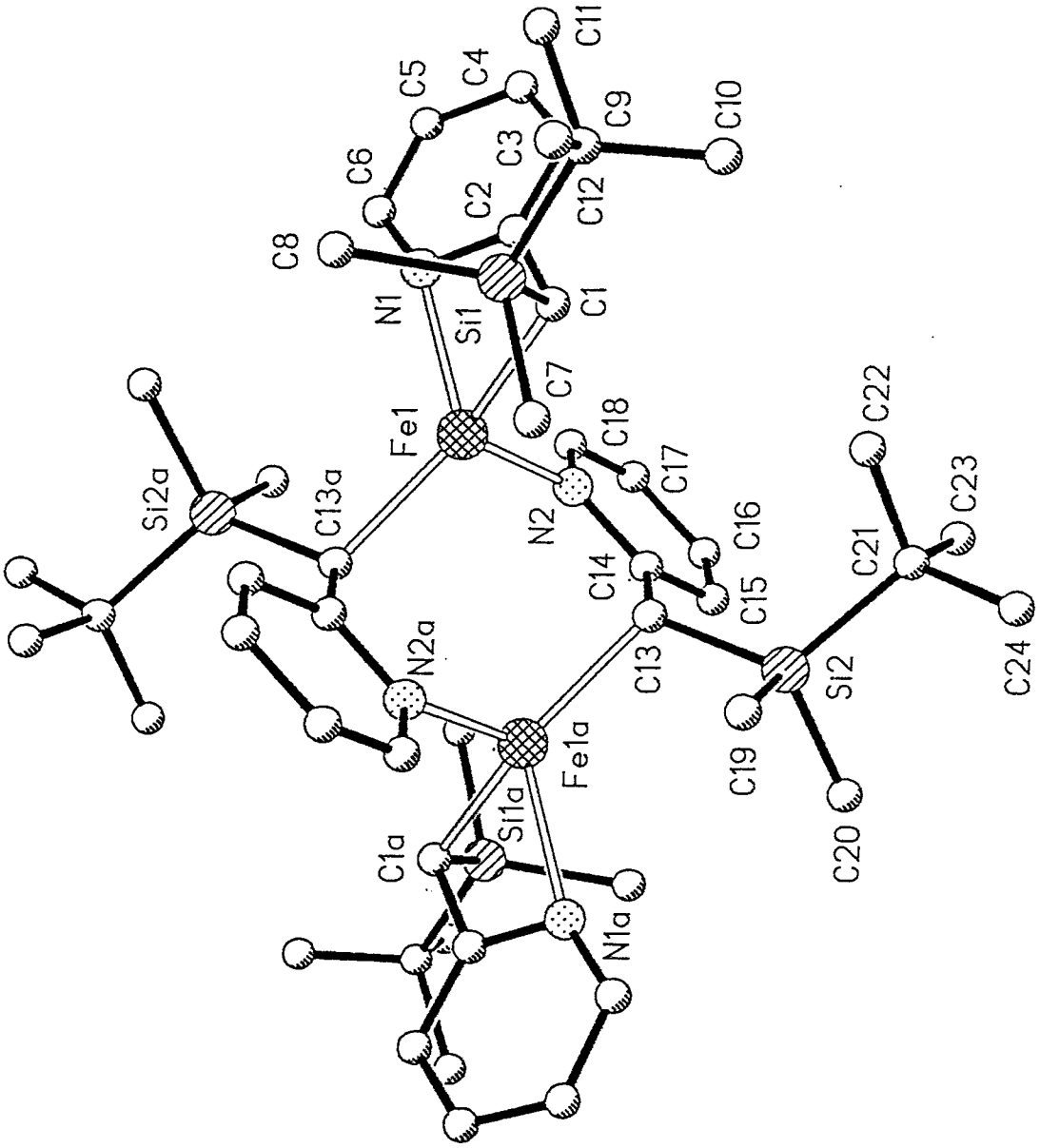
Cpd(3)

L1792-13

Table 1. Data collection and processing parameters.

Molecular formula	$[C(CH_3)_3Si(CH_3)_2C(C_5H_4N)]_2$ Fe
Molecular weight	468.6
Color and habit	greenish-brown prism
Crystal size	0.40 x 0.48 x 0.44 mm^3
Crystal system	triclinic
Space group	$P\bar{1}$ (No. 2)
Unit cell parameters	a = 10.850(2) Å α = 75.74(2) °
	b = 11.254(2) β = 84.32(2)
	c = 11.580(2) γ = 80.92(2)
	V = 1350.6(4) $Å^3$ Z = 2 $F(000)$ = 504
Density (measd)	g cm^{-3} (flotation in)
Density (calcd)	1.152 g cm^{-3}
Radiation	graphite-monochromatized Mo$K\alpha$, λ = 0.71073 Å
Standard reflections	(1,5,-1); (-1,3,-4)
Intensity variation	±1.2%
R_{int} (from merging of eqiv. reflections)	0.012
Absorption coefficient	0.66 mm^{-1}
Mean μr	0.14
Transmission factors	0.7841 to 0.885
Scan type and rate	ω-scan; 3.0-14.6 deg min^{-1}
Scan range	0.60° below $K\alpha_1$ to 0.60° above $K\alpha_2$
Background counting	stationary counts for one-fifth of scan time at each end of scan range
Collection range	$0 \le h \le 12$, $-13 \le k \le 13$, $-13 \le \ell \le 13$; $2\theta_{max}$ = 50°
Unique data measured	4762
Obs. data with $\|F_o\| \ge 3\sigma(\|F_o\|)$, n	4049
No. of variables, p	262
Weighting scheme	$w = [\sigma^2\|F_o\| + 0.0002\|F_o\|^2]^{-1}$
$R_F = \sum\|\|F_o\| - \|F_c\|\| / \sum\|F_o\|$	0.035
$wR = [\sum w^2(\|F_o\| - \|F_c\|)^2 / \sum w^2\|F_o\|^2]^{1/2}$	0.046
$S = [\sum w(\|F_o\| - \|F_c\|)^2/(n-p)]^{1/2}$	2.0
Largest and mean Δ/σ	0.000, 0.000
Residual extrema in final difference map	+0.61 to -0.38 $eÅ^{-3}$

L1792-14


C11
C5
C4
C9
C10
C6
C3
C12
C2
C8
N1
Si1
C1
C7
Fe1
C18
C22
Si2a
C13a
C17
C23
N2
C16
C21
C14
C15
N2a
C13
Si2
C24
Fe1a
C19
C20
Si1a
C1a
N1a

L1792-15

Table 2. Atomic coordinates (x 10^5 for Fe; x 10^4 for others) and equivalent isotropic temperature factors* (Å^2 x 10^4 for Fe; x 10^3 for others)

Atom	x	y	z	U_{eq}
Fe(1)	46425(3)	10196(3)	34522(3)	368(1)
Si(1)	6806(1)	2754(1)	2110(1)	47(1)
N(1)	3837(2)	1962(2)	1750(2)	50(1)
C(1)	6000(2)	1460(2)	2007(2)	42(1)
C(2)	4969(2)	1677(2)	1209(2)	44(1)
C(3)	5041(3)	1557(3)	33(3)	68(1)
C(4)	3979(3)	1792(4)	-579(3)	86(2)
C(5)	2849(3)	2133(3)	-40(3)	80(1)
C(6)	2811(3)	2212(3)	1118(3)	66(1)
C(7)	7696(3)	2250(3)	3497(3)	71(1)
C(8)	5661(3)	4146(3)	2232(3)	80(1)
C(9)	7971(3)	3216(3)	794(3)	76(1)
C(10)	8820(4)	2085(4)	545(5)	139(3)
C(11)	7285(5)	3869(4)	-340(3)	126(2)
C(12)	8787(4)	4098(5)	1064(4)	136(3)
Si(2)	7838(1)	-2225(1)	5162(1)	42(1)
N(2)	4513(2)	-848(2)	3574(2)	36(1)
C(13)	6236(2)	-1364(2)	4879(2)	37(1)
C(14)	5303(2)	-1745(2)	4274(2)	36(1)
C(15)	5169(3)	-2991(2)	4384(3)	53(1)
C(16)	4272(3)	-3298(3)	3796(3)	62(1)
C(17)	3484(3)	-2383(3)	3096(3)	60(1)
C(18)	3640(2)	-1187(3)	3007(2)	49(1)
C(19)	8657(2)	-1190(3)	5772(3)	56(1)
C(20)	7859(3)	-3749(3)	6287(3)	61(1)
C(21)	8798(2)	-2527(3)	3767(2)	52(1)
C(22)	8759(4)	-1336(3)	2784(3)	92(2)
C(23)	8306(3)	-3501(3)	3275(3)	82(2)
C(24)	10150(3)	-3015(3)	4064(3)	79(1)

*U_{eq} defined as one third of the trace of the orthogonalized U tensor.

L1792-16

Table 3. Bond lengths (Å) and bond angles (°).

Fe(1)-N(1)	2.189 (2)	Fe(1)-C(1)	2.133 (2)
Fe(1)-N(2)	2.097 (2)	Fe(1)-C(13)	2.163 (2)
Si(1)-C(1)	1.847 (3)	Si(1)-C(7)	1.876 (3)
Si(1)-C(8)	1.865 (3)	Si(1)-C(9)	1.904 (3)
N(1)-C(2)	1.352 (3)	N(1)-C(6)	1.347 (4)
C(1)-C(2)	1.473 (4)	C(2)-C(3)	1.395 (4)
C(3)-C(4)	1.368 (5)	C(4)-C(5)	1.363 (5)
C(5)-C(6)	1.362 (5)	C(9)-C(10)	1.520 (6)
C(9)-C(11)	1.538 (5)	C(9)-C(12)	1.534 (7)
Si(2)-C(13)	1.868 (2)	Si(2)-C(19)	1.872 (3)
Si(2)-C(20)	1.880 (3)	Si(2)-C(21)	1.907 (3)
N(2)-C(14)	1.369 (3)	N(2)-C(18)	1.355 (4)
C(13)-C(14)	1.458 (4)	C(13)-Fe(1A)	2.163 (2)
C(14)-C(15)	1.405 (4)	C(15)-C(16)	1.372 (5)
C(16)-C(17)	1.377 (4)	C(17)-C(18)	1.361 (4)
C(21)-C(22)	1.527 (4)	C(21)-C(23)	1.537 (5)
C(21)-C(24)	1.525 (4)		

N(1)-Fe(1)-C(1)	66.1(1)	N(1)-Fe(1)-N(2)	103.2(1)
C(1)-Fe(1)-N(2)	103.6(1)	N(1)-Fe(1)-C(13)	121.0(1)
C(1)-Fe(1)-C(13)	148.0(1)	N(2)-Fe(1)-C(13)	104.4(1)
C(1)-Si(1)-C(7)	107.9(1)	C(1)-Si(1)-C(8)	111.0(1)
C(7)-Si(1)-C(8)	108.3(2)	C(1)-Si(1)-C(9)	113.4(1)
C(7)-Si(1)-C(9)	107.7(1)	C(8)-Si(1)-C(9)	108.5(1)
Fe(1)-N(1)-C(2)	87.6(1)	Fe(1)-N(1)-C(6)	145.9(2)
C(2)-N(1)-C(6)	119.4(2)	Fe(1)-C(1)-Si(1)	112.4(1)
Fe(1)-C(1)-C(2)	86.9(1)	Si(1)-C(1)-C(2)	120.3(2)
N(1)-C(2)-C(1)	113.0(2)	N(1)-C(2)-C(3)	119.2(2)
C(1)-C(2)-C(3)	127.7(2)	C(2)-C(3)-C(4)	119.9(3)
C(3)-C(4)-C(5)	120.3(3)	C(4)-C(5)-C(6)	118.2(3)
N(1)-C(6)-C(5)	122.9(3)		
Si(1)-C(9)-C(10)	110.8(3)	Si(1)-C(9)-C(11)	110.7(3)
C(10)-C(9)-C(11)	108.1(4)	Si(1)-C(9)-C(12)	110.0(3)
C(10)-C(9)-C(12)	108.4(3)	C(11)-C(9)-C(12)	108.7(3)
C(13)-Si(2)-C(19)	105.0(1)	C(13)-Si(2)-C(20)	114.0(1)
C(19)-Si(2)-C(20)	108.2(1)	C(13)-Si(2)-C(21)	114.4(1)
C(19)-Si(2)-C(21)	107.3(1)	C(20)-Si(2)-C(21)	107.5(1)
Fe(1)-N(2)-C(14)	119.2(2)	Fe(1)-N(2)-C(18)	121.6(1)
C(14)-N(2)-C(18)	119.2(2)	Si(2)-C(13)-C(14)	124.8(2)
Si(2)-C(13)-Fe(1a)	108.4(1)	C(14)-C(13)-Fe(1a)	107.6(1)
N(2)-C(14)-C(13)	118.5(2)	N(2)-C(14)-C(15)	118.4(2)
C(13)-C(14)-C(15)	123.1(2)	C(14)-C(15)-C(16)	120.7(2)
C(15)-C(16)-C(17)	120.2(3)	C(16)-C(17)-C(18)	117.7(3)
N(2)-C(18)-C(17)	123.8(2)	Si(2)-C(21)-C(22)	110.3(2)
Si(2)-C(21)-C(23)	111.9(2)	C(22)-C(21)-C(23)	107.9(3)
Si(2)-C(21)-C(24)	109.7(2)	C(22)-C(21)-C(24)	109.4(3)
C(23)-C(21)-C(24)	107.4(3)		

L1792-17

Symmetry transformation: a (-x, -y, -z)

4792-18

Table 4. Anisotropic thermal parameters* ($Å^2 \times 10^4$ for Fe; $\times 10^3$ for others).

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	346(2)	392(2)	351(2)	-39(1)	-27(1)	-63(1)
Si(1)	41(1)	49(1)	50(1)	-11(1)	-1(1)	-8(1)
N(1)	42(1)	63(1)	41(1)	-1(1)	-7(1)	-6(1)
C(1)	39(1)	42(1)	42(1)	-6(1)	-2(1)	-5(1)
C(2)	44(1)	46(1)	40(1)	-9(1)	-1(1)	-5(1)
C(3)	52(2)	108(3)	47(2)	-11(2)	3(1)	-28(2)
C(4)	73(2)	146(3)	48(2)	-18(2)	-10(2)	-34(2)
C(5)	61(2)	124(3)	53(2)	-12(2)	-22(2)	-9(2)
C(6)	42(2)	96(2)	53(2)	2(1)	-11(1)	-7(2)
C(7)	61(2)	88(2)	69(2)	-21(2)	-14(2)	-18(2)
C(8)	74(2)	56(2)	109(3)	-5(2)	-6(2)	-20(2)
C(9)	74(2)	81(2)	73(2)	-39(2)	18(2)	-8(2)
C(10)	107(3)	138(4)	152(5)	-24(3)	80(3)	-29(3)
C(11)	172(5)	136(4)	64(2)	-69(4)	4(3)	14(2)
C(12)	131(4)	157(5)	134(4)	-106(4)	28(3)	-20(3)
Si(2)	36(1)	43(1)	42(1)	3(1)	-4(1)	-8(1)
N(2)	31(1)	43(1)	36(1)	-5(1)	-2(1)	-14(1)
C(13)	35(1)	37(1)	38(1)	0(1)	-2(1)	-12(1)
C(14)	35(1)	39(1)	36(1)	-6(1)	6(1)	-12(1)
C(15)	56(2)	40(1)	62(2)	-9(1)	2(1)	-13(1)
C(16)	65(2)	53(2)	78(2)	-25(1)	10(2)	-30(2)
C(17)	51(2)	79(2)	67(2)	-26(2)	5(1)	-40(2)
C(18)	39(1)	67(2)	48(1)	-9(1)	-3(1)	-24(1)
C(19)	43(1)	70(2)	57(2)	-5(1)	-9(1)	-16(1)
C(20)	59(2)	54(2)	58(2)	8(1)	-5(1)	-1(1)
C(21)	44(1)	58(2)	49(1)	8(1)	-1(1)	-13(1)
C(22)	111(3)	83(2)	60(2)	13(2)	28(2)	-4(2)
C(23)	73(2)	104(3)	74(2)	0(2)	2(2)	-43(2)
C(24)	50(2)	103(3)	81(2)	12(2)	6(2)	-34(2)

*The exponent takes the form: $-2\pi^2 \sum\sum U_{ij} h_i h_j a_i^* . a_j^*$.

Table 5. Hydrogen atom coordinates (x 10^4) and assigned isotropic temperature factors* (Å^2 x 10^3).

21792-19

Atom	x	y	z	U
H(1A)	6583	745	1925	80
H(3B)	5834	1305	-345	80
H(4B)	4031	1722	-1392	80
H(5B)	2101	2312	-466	80
H(6A)	2018	2453	1502	80
H(7D)	7131	2009	4178	80
H(7E)	8323	1560	3433	80
H(7F)	8090	2924	3591	80
H(8D)	5066	3927	2891	80
H(8E)	6096	4778	2359	80
H(8F)	5232	4449	1508	80
H(10D)	9398	2342	-119	120
H(10E)	9274	1671	1236	120
H(10F)	8324	1531	358	120
H(11D)	7888	4096	-992	180
H(11E)	6786	3317	-527	180
H(11F)	6755	4599	-213	180
H(12D)	9366	4320	392	150
H(12E)	8272	4831	1206	150
H(12F)	9240	3692	1758	150
H(13A)	6005	-621	5161	80
H(15A)	5712	-3634	4873	80
H(16A)	4192	-4152	3875	80
H(17A)	2849	-2582	2682	80
H(18A)	3094	-545	2519	80
H(19A)	8197	-1018	6478	80
H(19B)	9484	-1593	5967	80
H(19C)	8712	-429	5184	80
H(20A)	7381	-3626	7002	80
H(20B)	7500	-4314	5964	80
H(20C)	8706	-4085	6471	80
H(22B)	9247	-1504	2089	120
H(22C)	7910	-1035	2587	120
H(22D)	9099	-723	3057	120
H(23B)	8813	-3627	2576	80
H(23C)	8343	-4267	3871	80
H(23D)	7456	-3216	3072	80
H(24B)	10632	-3166	3360	80
H(24C)	10496	-2415	4351	80
H(24D)	10174	-3773	4669	80

*The exponent takes the form: $-8\pi^2 U \sin^2\theta/\lambda^2$.

©1996 American Chemical Society Organometallics V15 Page 1785 Leung Supplemental Page 20

L1792-20

STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{24}H_{40}FeN_2Si_2$
Color; Habit	black prism
Crystal size (mm)	0.40 x 0.48 x 0.44
Crystal System	Triclinic
Space Group	$P\bar{1}$
Unit Cell Dimensions	$\underline{a}$ = 10.850(2) Å
	$\underline{b}$ = 11.254(2) Å
	$\underline{c}$ = 11.580(2) Å
	α = 75.74(2)°
	β = 84.32(2)°
	γ = 80.92(2)°
Volume	1350.6(4) $Å^3$
Z	2
Formula weight	468.6
Density(calc.)	1.152 g/cm^3
Absorption Coefficient	0.659 mm^{-1}
F(000)	504

L1792-21

Data Collection

Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	294
Monochromator	Highly oriented graphite crystal
2θ Range	3.0 to 50.0°
Scan Type	ω
Scan Speed	Variable; 3.00 to 14.60°/min. in ω
Scan Range (ω)	1.80°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	2 measured every 125 reflections
Index Ranges	$0 \leq h \leq 12$, $-13 \leq k \leq 13$ $-13 \leq l \leq 13$
Reflections Collected	4762
Independent Reflections	4762 (R_{int} = 0.00%)
Observed Reflections	4049 ($F > 4.0\sigma(F)$)
Absorption Correction	Semi-empirical
Min./Max. Transmission	0.4648 / 0.5155

L1792-22

Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0002F^2$
Number of Parameters Refined	262
Final R Indices (obs. data)	R = 3.54 %, wR = 4.63 %
R Indices (all data)	R = 4.22 %, wR = 4.70 %
Goodness-of-Fit	2.00
Largest and Mean Δ/σ	0.000, 0.000
Data-to-Parameter Ratio	15.5:1
Largest Difference Peak	0.61 eÅ^{-3}
Largest Difference Hole	-0.38 eÅ^{-3}

COMPOUND 5 Fd(5)

Table 1. Data collection and processing parameters.

L1792-23

Molecular formula	$C_{21}H_{34}N_3ClSiFe$
Molecular weight	447.9
Color and habit	dark red prism
Crystal size	.50 x 0.40 x 0.16 mm^3
Crystal system	monoclinic
Space group	$P2_1/n$ (No. 14)
Unit cell parameters	a = 10.598(2)Å β = 96.290(0)°
	b = 14.205(6) V = 2444(1)Å^3
	c = 16.334(4) Z = 4 $F(000)$ = 952
Density (calcd)	1.217 g cm^{-3}
Radiation	graphite-monochromatized Mo$K\alpha$, λ = 0.71073 Å
Standard reflections	(1,2,2); (3,2,1); (3,2,-1)
Intensity variation	±1.1%
R_{int} (from merging of eqiv. reflections)	0.039
Absorption coefficient	0.79 mm^{-1}
Mean μr	0.1
Scan type and rate	ω-scan; 3 - 45 deg min^{-1}
Scan range	0.60° below $K\alpha_1$ to 0.60° above $K\alpha_2$
Background counting	stationary counts for one-fifth of scan time at each end of scan range
Collection range	$0 \le h \le 12$, $0 \le k \le 16$, $-19 \le \ell \le 19$; $2\theta_{max}$ = 45°
Unique data measured	4281
Obs. data with $\|F_o\| \ge 4\sigma(\|F_o\|)$, n	2137
No. of variables, p	244
Weighting scheme	$w = [\sigma^2\|F_o\| + 0.0005\|F_o\|^2]^{-1}$
$R_F = \sum\|\|F_o\| - \|F_c\|\| / \sum\|F_o\|$	0.0596
$wR = [\sum w^2(\|F_o\| - \|F_c\|)^2 / \sum w^2\|F_o\|^2]^{1/2}$	0.0596
$S = [\sum w(\|F_o\| - \|F_c\|)^2/(n-p)]^{1/2}$	1.212
Largest and mean Δ/σ	.000, .000
Residual extrema in final difference map	+0.48 to -0.36 eÅ^{-3}

L1792-24

Table 2. Atomic coordinates (x 10^5 for Fe; x 10^4 for others) and equivalent isotropic temperature factors* ($Å^2$ x 10^4 for Fe; x 10^3 for others)

Atom	x	y	z	U_{eq}
Fe(1)	25392(9)	19954(7)	12152(5)	425(3)
Si(1)	2501(2)	3945(2)	173(1)	59(1)
Cl(1)	2662(2)	2688(1)	2501(1)	67(1)
N(1)	515(5)	2306(4)	815(3)	48(2)
N(2)	4565(5)	1426(4)	1416(4)	57(2)
N(3)	2151(6)	491(4)	1408(4)	63(3)
C(1)	-682(8)	2297(5)	996(4)	59(3)
C(2)	-1701(8)	2494(6)	434(5)	75(3)
C(3)	-1466(8)	2685(5)	-358(5)	72(3)
C(4)	-241(7)	2711(5)	-549(4)	54(3)
C(5)	759(7)	2545(5)	52(4)	45(2)
C(6)	2125(6)	2659(4)	-10(4)	45(2)
C(7)	2591(7)	2234(5)	-756(4)	55(3)
C(8)	1949(8)	1513(6)	-1220(4)	67(3)
C(9)	2384(10)	1134(6)	-1911(5)	91(4)
C(10)	3480(12)	1426(8)	-2176(6)	102(5)
C(11)	4177(9)	2112(8)	-1739(6)	92(4)
C(12)	3731(8)	2506(6)	-1037(5)	74(3)
C(13)	1375(7)	4471(5)	847(4)	73(3)
C(14)	2305(8)	4613(6)	-827(5)	86(4)
C(15)	4126(8)	4173(6)	704(5)	91(4)
C(16)	3365(10)	-13(6)	1548(6)	94(4)
C(17)	4404(9)	598(7)	1915(6)	106(5)
C(18)	5073(7)	1233(6)	638(5)	85(4)
C(19)	5521(7)	2023(7)	1905(5)	92(4)
C(20)	1456(8)	404(6)	2138(5)	93(4)
C(21)	1339(9)	84(5)	714(6)	99(4)

*U_{eq} defined as one third of the trace of the orthogonalized U tensor.

L1792-25

Table 3. Bond lengths (Å) and bond angles (°).

Fe(1)-Cl(1)	2.310(2)	Fe(1)-N(1)	2.218(6)
Fe(1)-N(2)	2.284(6)	Fe(1)-N(3)	2.206(6)
Fe(1)-C(6)	2.212(6)	Si(1)-C(6)	1.887(7)
Si(1)-C(13)	1.867(8)	Si(1)-C(14)	1.880(8)
Si(1)-C(15)	1.871(8)	N(1)-C(1)	1.333(10)
N(1)-C(5)	1.345(8)	N(2)-C(17)	1.451(12)
N(2)-C(18)	1.460(10)	N(2)-C(19)	1.485(10)
N(3)-C(16)	1.468(12)	N(3)-C(20)	1.474(11)
N(3)-C(21)	1.464(10)	C(1)-C(2)	1.367(11)
C(2)-C(3)	1.371(12)	C(3)-C(4)	1.369(11)
C(4)-C(5)	1.384(9)	C(5)-C(6)	1.471(10)
C(6)-C(7)	1.492(10)	C(7)-C(8)	1.404(10)
C(7)-C(12)	1.394(11)	C(8)-C(9)	1.376(12)
C(9)-C(10)	1.348(17)	C(10)-C(11)	1.375(15)
C(11)-C(12)	1.404(13)	C(16)-C(17)	1.477(13)

Cl(1)-Fe(1)-N(1)	98.0(2)	Cl(1)-Fe(1)-N(2)	93.5(2)
N(1)-Fe(1)-N(2)	167.6(2)	Cl(1)-Fe(1)-N(3)	106.0(2)
N(1)-Fe(1)-N(3)	92.6(2)	N(2)-Fe(1)-N(3)	79.8(2)
Cl(1)-Fe(1)-C(6)	128.8(2)	N(1)-Fe(1)-C(6)	63.8(2)
N(2)-Fe(1)-C(6)	111.8(2)	N(3)-Fe(1)-C(6)	121.3(2)
C(6)-Si(1)-C(13)	110.1(3)	C(6)-Si(1)-C(14)	110.5(3)
C(13)-Si(1)-C(14)	107.1(4)	C(6)-Si(1)-C(15)	114.1(3)
C(13)-Si(1)-C(15)	105.8(4)	C(14)-Si(1)-C(15)	108.9(4)
Fe(1)-N(1)-C(1)	147.8(5)	Fe(1)-N(1)-C(5)	92.6(4)
C(1)-N(1)-C(5)	119.5(6)	Fe(1)-N(2)-C(17)	101.6(5)
Fe(1)-N(2)-C(18)	111.8(4)	C(17)-N(2)-C(18)	114.4(7)
Fe(1)-N(2)-C(19)	116.8(5)	C(17)-N(2)-C(19)	106.0(6)
C(18)-N(2)-C(19)	106.3(6)	Fe(1)-N(3)-C(16)	108.7(5)
Fe(1)-N(3)-C(20)	108.3(5)	C(16)-N(3)-C(20)	109.9(6)
Fe(1)-N(3)-C(21)	112.1(5)	C(16)-N(3)-C(21)	111.0(6)
C(20)-N(3)-C(21)	106.9(6)	N(1)-C(1)-C(2)	123.4(7)
C(1)-C(2)-C(3)	117.5(8)	C(2)-C(3)-C(4)	119.7(7)
C(3)-C(4)-C(5)	120.4(7)	N(1)-C(5)-C(4)	119.4(6)
N(1)-C(5)-C(6)	112.4(5)	C(4)-C(5)-C(6)	128.0(6)
Fe(1)-C(6)-Si(1)	104.6(3)	Fe(1)-C(6)-C(5)	89.5(4)
Si(1)-C(6)-C(5)	106.7(5)	Fe(1)-C(6)-C(7)	121.1(4)
Si(1)-C(6)-C(7)	116.0(5)	C(5)-C(6)-C(7)	115.3(5)
C(6)-C(7)-C(8)	123.5(7)	C(6)-C(7)-C(12)	122.2(6)
C(8)-C(7)-C(12)	114.2(7)	C(7)-C(8)-C(9)	122.9(8)
C(8)-C(9)-C(10)	121.4(9)	C(9)-C(10)-C(11)	119.0(10)
C(10)-C(11)-C(12)	119.8(9)	C(7)-C(12)-C(11)	122.7(8)
N(3)-C(16)-C(17)	112.3(7)	N(2)-C(17)-C(16)	112.1(8)

L1792-26

Table 4. Anisotropic thermal parameters* ($Å^2 \times 10^4$ for Fe; $\times 10^3$ for others).

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	525(6)	429(5)	319(5)	14(5)	33(4)	4(6)
Si(1)	65(1)	56(1)	55(1)	-5(1)	1(1)	15(1)
Cl(1)	86(1)	74(1)	40(1)	11(1)	-2(1)	-13(1)
N(1)	47(4)	55(4)	42(3)	-2(3)	9(3)	1(3)
N(2)	58(4)	54(4)	59(4)	8(3)	7(3)	12(3)
N(3)	77(5)	42(4)	68(4)	-10(4)	6(4)	9(3)
C(1)	63(5)	70(6)	45(4)	-7(4)	12(4)	-3(4)
C(2)	50(5)	99(6)	79(6)	-6(5)	17(5)	-11(5)
C(3)	73(6)	75(6)	63(5)	5(5)	-16(5)	-10(4)
C(4)	48(5)	73(6)	42(4)	3(4)	3(4)	-2(4)
C(5)	62(5)	43(4)	30(3)	1(4)	8(3)	0(3)
C(6)	48(4)	43(4)	45(4)	5(3)	14(3)	2(3)
C(7)	58(5)	62(6)	45(4)	18(4)	16(4)	19(4)
C(8)	86(6)	65(5)	50(5)	16(5)	15(5)	-1(4)
C(9)	144(10)	73(6)	60(6)	45(6)	22(6)	-9(5)
C(10)	147(11)	105(9)	63(6)	61(8)	52(7)	24(6)
C(11)	93(7)	118(9)	75(6)	41(7)	50(6)	46(6)
C(12)	74(6)	85(6)	67(5)	18(5)	24(5)	17(5)
C(13)	95(6)	54(5)	68(5)	7(5)	-2(5)	-1(4)
C(14)	95(7)	78(6)	85(6)	1(5)	13(5)	39(5)
C(15)	90(7)	86(7)	94(7)	-28(5)	-2(5)	14(5)
C(16)	109(8)	53(6)	118(8)	2(6)	3(7)	9(5)
C(17)	98(8)	96(8)	121(9)	37(7)	4(7)	49(7)
C(18)	75(6)	115(8)	66(6)	21(5)	15(5)	-15(5)
C(19)	61(5)	123(8)	86(6)	2(6)	-9(5)	-16(6)
C(20)	109(7)	72(6)	101(7)	-11(5)	28(6)	29(5)
C(21)	129(9)	49(5)	114(8)	-35(6)	-7(7)	-15(5)

*The exponent takes the form: $-2\pi^2 \sum\sum U_{ij} h_i h_j a_i^* . a_j^*$.

L1792-27

Table 5. Hydrogen atom coordinates (x 10^4) and assigned isotropic temperature factors* (Å^2 x 10^3).

Atom	x	y	z	U
H(1A)	-835	2142	1549	80
H(2A)	-2552	2492	584	80
H(3A)	-2159	2808	-773	80
H(4A)	-69	2841	-1103	80
H(8A)	1165	1288	-1050	80
H(9A)	1897	656	-2217	110
H(10A)	3778	1154	-2657	110
H(11A)	4972	2308	-1914	110
H(12A)	4218	2992	-742	80
H(13A)	1449	4143	1364	80
H(13B)	1566	5125	942	80
H(13C)	524	4409	583	80
H(14A)	2882	4361	-1186	110
H(14B)	1450	4549	-1084	110
H(14C)	2492	5266	-725	110
H(15A)	4231	3837	1218	110
H(15B)	4753	3963	363	110
H(15C)	4229	4835	807	110
H(16A)	3580	-259	1034	110
H(16B)	3263	-534	1909	110
H(17A)	4223	793	2453	110
H(17B)	5181	245	1979	110
H(18A)	5926	998	733	110
H(18B)	4542	771	342	110
H(18C)	5064	1802	321	110
H(19A)	6329	1709	1949	110
H(19B)	5586	2616	1632	110
H(19C)	5274	2127	2446	110
H(20A)	1277	-246	2238	110
H(20B)	1963	661	2609	110
H(20C)	674	748	2043	110
H(21A)	1183	-570	814	110
H(21B)	548	418	647	110
H(21C)	1754	146	223	110

*The exponent takes the form: $-8\pi^2 U \sin^2\theta/\lambda^2$.

©1996 American Chemical Society Organometallics V15 Page 1785 Leung Supplemental Page 28

L1792-28

STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{21}\ H_{34}\ Cl\ Fe\ N_3\ Si$
Color; Habit	DARK RED PRISM
Crystal size (mm)	.5 x .4 x .16
Crystal System	Monoclinic
Space Group	$P2_1/n$
Unit Cell Dimensions	$\underline{a}$ = 10.598(2) Å
	$\underline{b}$ = 14.205(6) Å
	$\underline{c}$ = 16.334(4) Å
	β = 96.290(0)°
Volume	2444.1(14) $Å^3$
Z	4
Formula weight	447.9
Density(calc.)	1.217 Mg/m^3
Absorption Coefficient	0.785 mm^{-1}
F(000)	952

L1792-29

Data Collection

Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	293
Monochromator	Highly oriented graphite crystal
2θ Range	7.0 to 45.0°
Scan Type	ω
Scan Speed	Variable; 3.00 to 45.00°/min. in ω
Scan Range (ω)	0.60°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 0.5% of total scan time
Standard Reflections	3 measured every 100 reflections
Index Ranges	$0 \leq h \leq 12$, $0 \leq k \leq 16$ $-19 \leq l \leq 19$
Reflections Collected	4527
Independent Reflections	4281 (R_{int} = 3.88%)
Observed Reflections	2137 ($F > 4.0\sigma(F)$)
Absorption Correction	N/A

4792-30

Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Patterson Interpretation
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0005F^2$
Number of Parameters Refined	244
Final R Indices (obs. data)	R = 5.96 %, wR = 5.96 %
R Indices (all data)	R = 12.65 %, wR = 7.37 %
Goodness-of-Fit	1.21
Largest and Mean Δ/σ	0.000, 0.000
Data-to-Parameter Ratio	8.8:1
Largest Difference Peak	0.48 $e\text{Å}^{-3}$
Largest Difference Hole	-0.36 $e\text{Å}^{-3}$

COMPOUND 7 (C50H74)

L1792-31

Table 1. Data collection and processing parameters.

Molecular formula	$C_{48}H_{81}N_1Si_2S_2Fe$
Molecular weight	848.29
Color and habit	yellow prism
Crystal size	0.30 x 0.30 x 1.00 mm^3
Crystal system	monoclinic
Space group	$P2_1/c$ (No. 14)
Unit cell parameters	a = 14.585(5)Å β = 111.16(1)°
	b = 19.894(6) V = 5213(3)Å^3
	c = 19.266(5) Z = 4 $F(000)$ = 1848
Density (calcd)	1.081 g cm^{-3}
Radiation	graphite-monochromatized Mo$K\alpha$, λ = 0.71073 Å
Standard reflections	(2,3,1); (0,3,-1)
Intensity variation	±1.0%
R_{int} (from merging of eqiv. reflections)	0.024
Absorption coefficient	0.44 mm^{-1}
Mean μr	0.10
Transmission factors	0.921 to 0.965
Scan type and rate	ω–2G qscan; 4.19–29.3 deg min^{-1}
Scan range	1.00° below $K\alpha_1$ to 1.00° above $K\alpha_2$
Background counting	stationary counts for one-fifth of scan time at each end of scan range
Collection range	$0 \le h \le 15$, $0 \le k \le 22$, $-21 \le \ell \le 20$; $2\theta_{max}$ = 45°
Unique data measured	6826
Obs. data with $\|F_o\| \ge 4\sigma(\|F_o\|)$, n	3656
No. of variables, p	487
Weighting scheme	$w = [\sigma^2\|F_o\| + 0.0035\|F_o\|^2]^{-1}$
$R_F = \sum\|\|F_o\| - \|F_c\|\| / \sum\|F_o\|$	0.0845
$wR = [\sum w^2(\|F_o\| - \|F_c\|)^2 / \sum w^2\|F_o\|^2]^{1/2}$	0.1251
$S = [\sum w(\|F_o\| - \|F_c\|)^2/(n-p)]^{1/2}$	1.60
Largest and mean Δ/σ	.004, .000
Residual extrema in final difference map	+0.85 to −0.45 e Å^{-3}

L1792-32

Table 2. Atomic coordinates (x 10^5 for Fe; x 10^4 for others) and equivalent isotropic temperature factors* (Å^2 x 10^4 for Fe; x 10^3 for others)

Atom	x	y	z	U_{eq}
Fe(1)	1519(1)	8381(9)	28031(9)	446(7)
Si(1)	3216(3)	-1082(2)	3511(2)	55(2)
Si(2)	2018(3)	-725(2)	4610(2)	62(2)
N(1)	891(6)	-117(4)	2588(5)	38(4)
C(1)	47(10)	-174(7)	1996(7)	58(6)
C(2)	-477(9)	-745(7)	1806(7)	64(6)
C(3)	-168(9)	-1303(7)	2244(7)	53(6)
C(4)	708(9)	-1258(7)	2839(7)	58(6)
C(5)	1221(8)	-662(6)	3026(6)	39(5)
C(6)	2182(8)	-619(5)	3675(5)	36(4)
C(7)	437(1)	-669(7)	4070(9)	96(8)
C(8)	302(1)	-1012(8)	2512(8)	92(9)
C(9)	329(1)	-2007(7)	3742(9)	90(8)
C(10)	310(1)	-31(1)	5338(8)	13(1)
C(11)	90(2)	-33(2)	457(1)	21(2)
C(12)	203(2)	-1605(9)	490(1)	16(2)
S(1)	554(2)	1742(2)	2338(2)	55(1)
C(13)	-632(8)	1524(6)	1671(6)	44(5)
C(14)	-76(1)	1491(6)	892(7)	56(6)
C(15)	-1688(9)	1313(7)	408(7)	55(6)
C(16)	-251(1)	1204(6)	611(7)	51(5)
C(17)	-235(1)	1251(6)	1361(6)	50(6)
C(18)	-1438(7)	1429(5)	1896(6)	35(4)
C(19)	16(10)	1604(8)	556(7)	69(7)
C(20)	81(1)	1017(9)	789(8)	98(9)
C(21)	52(1)	2302(9)	786(10)	12(1)
C(22)	-40(1)	160(1)	-293(8)	11(1)
C(23)	-347(1)	1009(9)	12(8)	77(7)
C(24)	-428(1)	98(1)	334(9)	12(1)
C(25)	-342(1)	36(1)	-33(1)	16(1)
C(26)	-379(1)	159(1)	-56(1)	15(1)
C(27)	-1386(9)	1479(6)	2715(6)	44(5)
C(28)	-73(1)	912(7)	3212(7)	64(6)
C(29)	-243(1)	1392(7)	2770(7)	71(7)
C(30)	-1025(9)	2164(6)	3060(7)	60(6)
S(2)	3099(2)	1025(2)	3546(2)	48(1)
C(31)	3264(8)	1878(5)	3298(6)	33(4)
C(32)	3015(7)	2420(6)	3670(6)	36(5)
C(33)	2985(9)	3051(6)	3363(7)	53(6)
C(34)	3227(8)	3186(6)	2751(7)	46(5)
C(35)	3591(9)	2653(6)	2461(7)	51(6)
C(36)	3665(8)	2001(6)	2744(6)	43(5)
C(37)	2844(8)	2367(6)	4416(6)	46(5)
C(38)	3743(9)	2031(7)	4989(7)	70(6)
C(39)	276(1)	3072(7)	4746(7)	75(7)
C(40)	190(1)	1988(8)	4370(7)	82(8)
C(41)	312(1)	3891(7)	2392(8)	65(7)
C(42)	313(2)	4439(9)	295(1)	18(2)
C(43)	398(2)	4049(9)	218(1)	15(2)
C(44)	214(2)	393(1)	176(1)	20(2)

C(45)	421(1)	1479(7)	2431(7)	55(6)
C(46)	352(1)	947(8)	1944(9)	95(9)
C(47)	478(1)	1807(8)	1972(9)	91(9)
C(48)	506(1)	1158(8)	3107(8)	79(7)

L1792-33

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 3. Bond lengths (Å) and bond angles (°).

Fe(1)-N(1)	2.086	(9)	Fe(1)-S(1)	2.259	(4)
Fe(1)-S(2)	2.261	(3)	Si(1)-C(6)	1.89	(1)
Si(1)-C(7)	1.83	(1)	Si(1)-C(8)	1.85	(2)
Si(1)-C(9)	1.89	(2)	Si(2)-C(6)	1.91	(1)
Si(2)-C(10)	1.88	(2)	Si(2)-C(11)	1.79	(3)
Si(2)-C(12)	1.84	(2)	N(1)-C(1)	1.35	(1)
N(1)-C(5)	1.35	(1)	C(1)-C(2)	1.35	(2)
C(2)-C(3)	1.37	(2)	C(3)-C(4)	1.38	(2)
C(4)-C(5)	1.38	(2)	C(5)-C(6)	1.51	(1)
S(1)-C(13)	1.80	(1)	C(13)-C(14)	1.44	(2)
C(13)-C(18)	1.41	(2)	C(14)-C(15)	1.38	(2)
C(14)-C(19)	1.52	(2)	C(15)-C(16)	1.40	(2)
C(16)-C(17)	1.38	(2)	C(16)-C(23)	1.52	(2)
C(17)-C(18)	1.40	(1)	C(18)-C(27)	1.56	(2)
C(19)-C(20)	1.59	(2)	C(19)-C(21)	1.56	(2)
C(19)-C(22)	1.53	(2)	C(23)-C(24)	1.52	(3)
C(23)-C(25)	1.46	(3)	C(23)-C(26)	1.55	(3)
C(27)-C(28)	1.56	(2)	C(27)-C(29)	1.57	(2)
C(27)-C(30)	1.52	(2)	S(2)-C(31)	1.80	(1)
C(31)-C(32)	1.41	(2)	C(31)-C(36)	1.41	(2)
C(32)-C(33)	1.38	(2)	C(32)-C(37)	1.55	(2)
C(33)-C(34)	1.37	(2)	C(34)-C(35)	1.39	(2)
C(34)-C(41)	1.55	(2)	C(35)-C(36)	1.40	(2)
C(36)-C(45)	1.55	(2)	C(37)-C(38)	1.53	(2)
C(37)-C(39)	1.56	(2)	C(37)-C(40)	1.54	(2)
C(41)-C(42)	1.53	(3)	C(41)-C(43)	1.48	(3)
C(41)-C(44)	1.51	(2)	C(45)-C(46)	1.53	(2)
C(45)-C(47)	1.56	(2)	C(45)-C(48)	1.57	(2)

N(1)-Fe(1)-S(1)	118.7(2)	N(1)-Fe(1)-S(2)	123.4(2)
S(1)-Fe(1)-S(2)	117.8(1)	C(6)-Si(1)-C(7)	107.6(6)
C(6)-Si(1)-C(8)	107.7(6)	C(6)-Si(1)-C(9)	114.4(7)
C(7)-Si(1)-C(8)	110.2(8)	C(7)-Si(1)-C(9)	109.8(6)
C(8)-Si(1)-C(9)	107.1(8)	C(6)-Si(2)-C(10)	107.2(7)
C(6)-Si(2)-C(11)	109.4(8)	C(6)-Si(2)-C(12)	113.8(8)
C(10)-Si(2)-C(11)	110(1)	C(10)-Si(2)-C(12)	106(1)
C(11)-Si(2)-C(12)	110(1)	Fe(1)-N(1)-C(1)	116.5(8)
Fe(1)-N(1)-C(5)	125.1(6)	C(1)-N(1)-C(5)	118(1)
N(1)-C(1)-C(2)	124(1)	C(1)-C(2)-C(3)	119(1)

L1792-34

C(2)-C(3)-C(4)	117(1)	C(3)-C(4)-C(5)	122(1)
N(1)-C(5)-C(4)	119.3(9)	N(1)-C(5)-C(6)	119.2(9)
C(4)-C(5)-C(6)	121(1)	Si(1)-C(6)-Si(2)	118.9(5)
Si(1)-C(6)-C(5)	113.2(8)	Si(2)-C(6)-C(5)	112.3(9)
Fe(1)-S(1)-C(13)	113.1(4)	S(1)-C(13)-C(14)	119(1)
S(1)-C(13)-C(18)	120.6(8)	C(14)-C(13)-C(18)	120.2(9)
C(13)-C(14)-C(15)	116(1)	C(13)-C(14)-C(19)	127(1)
C(15)-C(14)-C(19)	117(1)	C(14)-C(15)-C(16)	125(1)
C(15)-C(16)-C(17)	116(1)	C(15)-C(16)-C(23)	119(1)
C(17)-C(16)-C(23)	125(1)	C(16)-C(17)-C(18)	123(1)
C(13)-C(18)-C(17)	119(1)	C(13)-C(18)-C(27)	124.4(9)
C(17)-C(18)-C(27)	117(1)	C(14)-C(19)-C(20)	111(1)
C(14)-C(19)-C(21)	111(1)	C(14)-C(19)-C(22)	113(1)
C(20)-C(19)-C(21)	111(1)	C(20)-C(19)-C(22)	105(1)
C(21)-C(19)-C(22)	106(1)	C(16)-C(23)-C(24)	110(1)
C(16)-C(23)-C(25)	113(1)	C(16)-C(23)-C(26)	108(1)
C(24)-C(23)-C(25)	109(2)	C(24)-C(23)-C(26)	104(1)
C(25)-C(23)-C(26)	113(2)	C(18)-C(27)-C(28)	112(1)
C(18)-C(27)-C(29)	111.5(9)	C(18)-C(27)-C(30)	113(1)
C(28)-C(27)-C(29)	106(1)	C(28)-C(27)-C(30)	109.9(8)
C(29)-C(27)-C(30)	105(1)	Fe(1)-S(2)-C(31)	101.0(3)
S(2)-C(31)-C(32)	119.9(9)	S(2)-C(31)-C(36)	119.7(9)
C(32)-C(31)-C(36)	120(1)	C(31)-C(32)-C(33)	117(1)
C(31)-C(32)-C(37)	125(1)	C(33)-C(32)-C(37)	118(1)
C(32)-C(33)-C(34)	125(1)	C(33)-C(34)-C(35)	117(1)
C(33)-C(34)-C(41)	123(1)	C(35)-C(34)-C(41)	120(1)
C(34)-C(35)-C(36)	123(1)	C(31)-C(36)-C(35)	117(1)
C(31)-C(36)-C(45)	126(1)	C(35)-C(36)-C(45)	117(1)
C(32)-C(37)-C(38)	108(1)	C(32)-C(37)-C(39)	112(1)
C(32)-C(37)-C(40)	115(1)	C(38)-C(37)-C(39)	105.7(9)
C(38)-C(37)-C(40)	110.0(9)	C(39)-C(37)-C(40)	106(1)
C(34)-C(41)-C(42)	111(1)	C(34)-C(41)-C(43)	111(1)
C(34)-C(41)-C(44)	108(1)	C(42)-C(41)-C(43)	104(2)
C(42)-C(41)-C(44)	108(2)	C(43)-C(41)-C(44)	115(2)
C(36)-C(45)-C(46)	113(1)	C(36)-C(45)-C(47)	113(1)
C(36)-C(45)-C(48)	108(1)	C(46)-C(45)-C(47)	108(1)
C(46)-C(45)-C(48)	112(1)	C(47)-C(45)-C(48)	103(1)

©1996 American Chemical Society Organometallics V15 Page 1785 Leung Supplemental Page 35

L1792-35

STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{48}\ H_{81}\ Fe\ N\ S_2\ Si_2$
Color; Habit	yellow prism
Crystal size (mm)	0.30 x 0.30 x1.00
Crystal System	Monoclinic
Space Group	$P2_1/c$
Unit Cell Dimensions	$\underline{a}$ = 14.585(5) Å
	$\underline{b}$ = 19.894(6) Å
	$\underline{c}$ = 19.266(5) Å
	β = 111.16(1)°
Volume	5213(3) $Å^3$
Z	4
Formula weight	848.3
Density(calc.)	1.081 Mg/m^3
Absorption Coefficient	0.445 mm^{-1}
F(000)	1848

L1792-36

Data Collection

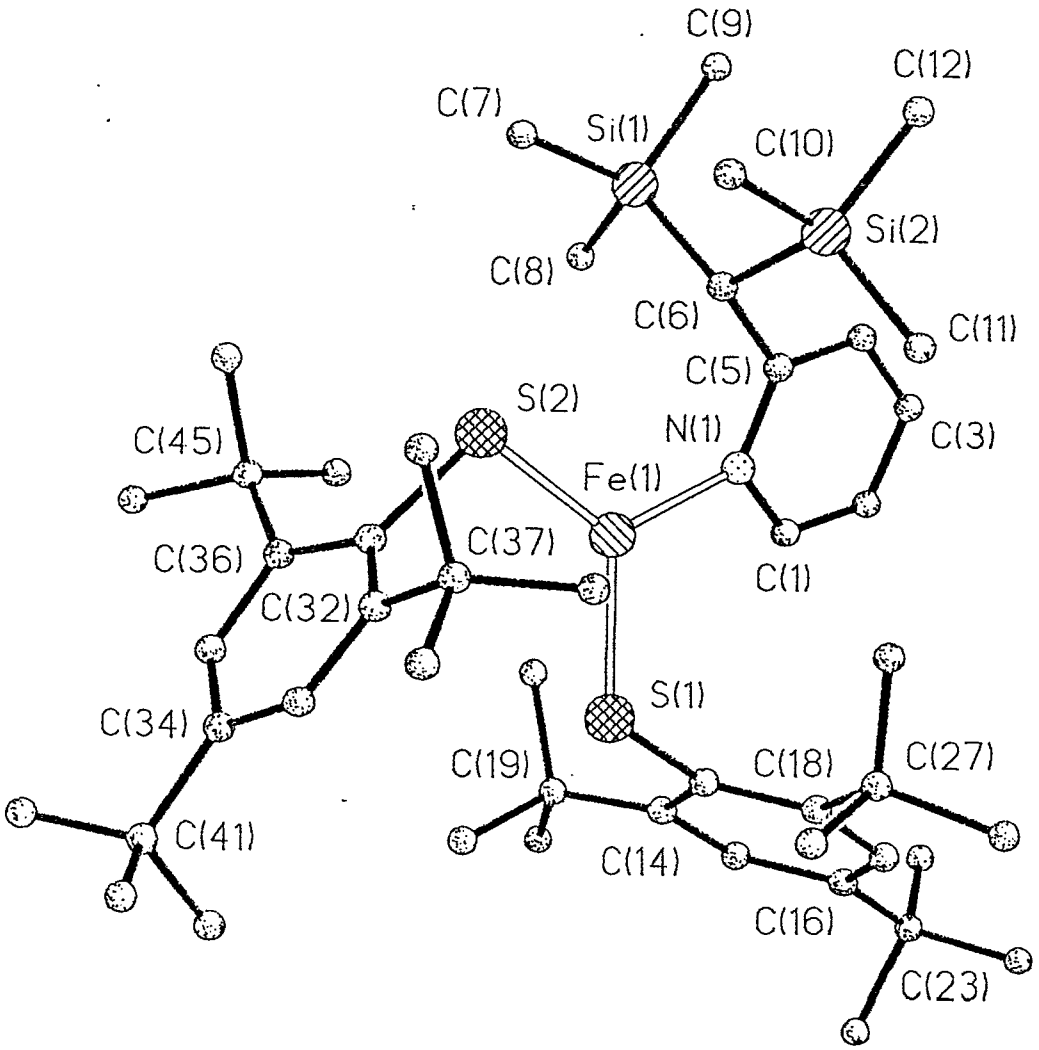
Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	293
Monochromator	Highly oriented graphite crystal
2θ Range	3.0 to 45.0°
Scan Type	$\omega/2\theta$
Scan Speed	Variable; 4.19 to 29.30°/min. in ω
Scan Range (ω)	1.00°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 0.5% o f total scan time
Standard Reflections	2 measured every 123 reflections
Index Ranges	$0 \leq h \leq 15$, $0 \leq k \leq 22$ $-21 \leq l \leq 20$
Reflections Collected	7185
Independent Reflections	6826 (R_{int} = 2.41%)
Observed Reflections	3656 ($F > 4.0\sigma(F)$)
Absorption Correction	Semi-empirical
Min./Max. Transmission	0.921 / 0.965

L1792-37

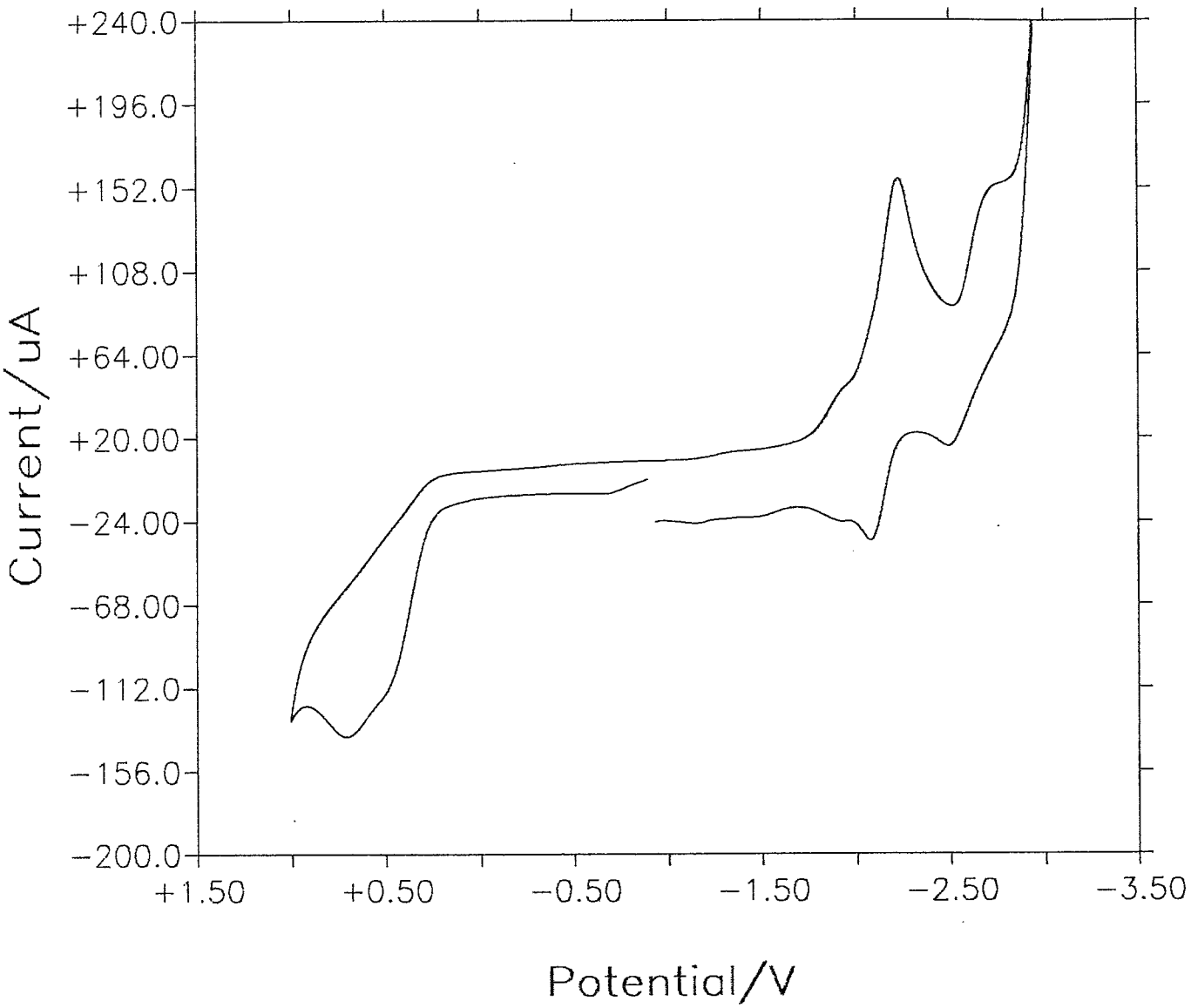
Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0035F^2$
Number of Parameters Refined	487
Final R Indices (obs. data)	R = 8.45 %, wR = 12.51 %
R Indices (all data)	R = 14.71 %, wR = 17.21 %
Goodness-of-Fit	1.60
Largest and Mean Δ/σ	0.004, 0.000
Data-to-Parameter Ratio	7.5:1
Largest Difference Peak	0.85 eÅ^{-3}
Largest Difference Hole	-0.45 eÅ^{-3}

L1792-38


C(9)
C(12)
C(7)
Si(1)
C(10)
Si(2)
C(8)
C(6)
C(11)
C(5)
S(2)
C(45)
N(1)
C(3)
Fe(1)
C(36)
C(37)
C(1)
C(32)
S(1)
C(34)
C(19)
C(18)
C(27)
C(41)
C(14)
C(16)
C(23)

L1792-39



14−Aug−95
17:01:18
Mode: CV
Fe(Pic")2

Init E (mV) = 0
High E (mV) = 1900
Low E (mV) = −2100
Init P/N = P
V (mV/s) = 100
Sweep Segments = 3
Smpl Int (mV) = 2
Quiet T (s) = 2
Sens (A/V) = 1E−4

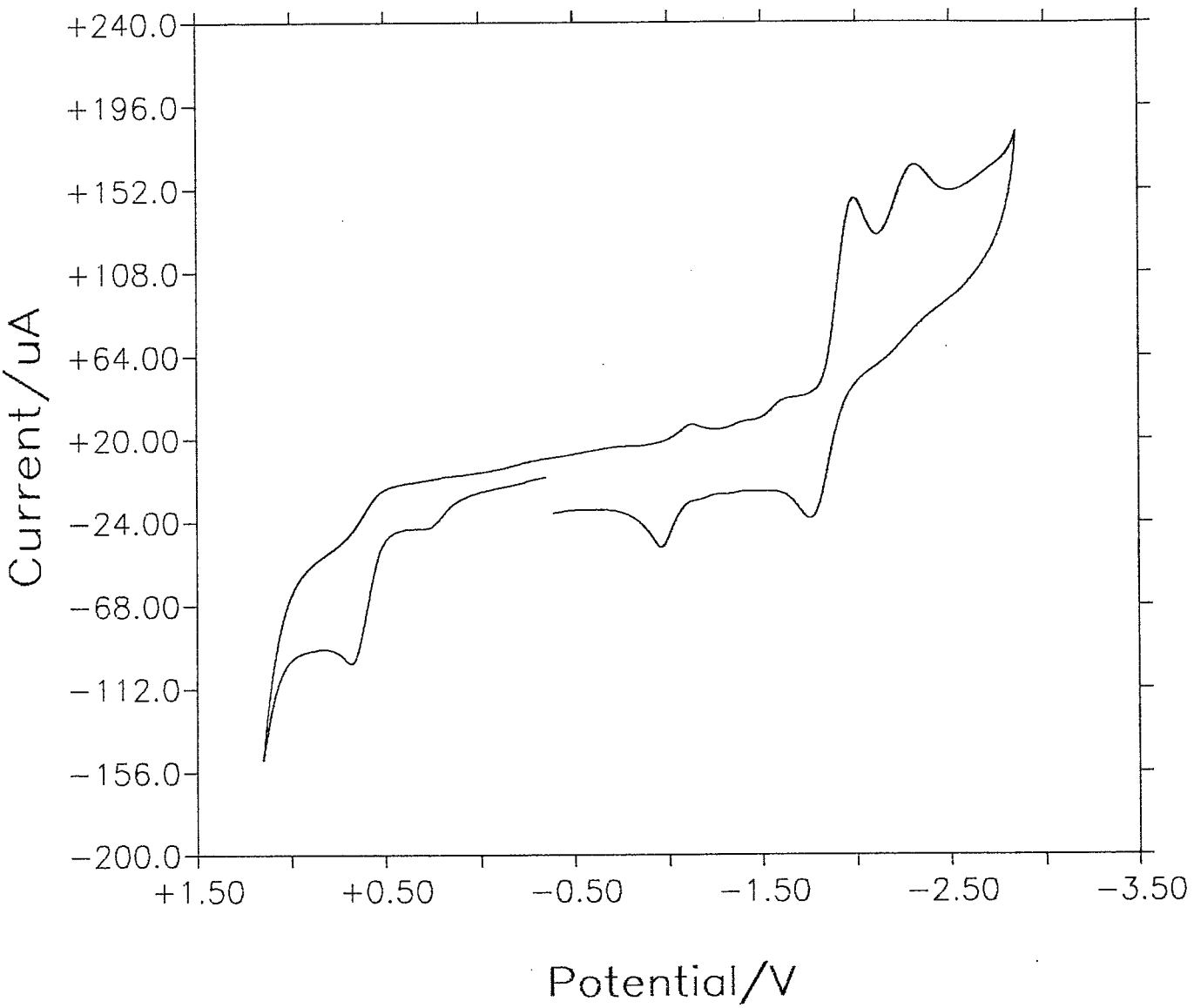
Segment 2:
Ep (mV) = −2219
ip (A) = +8.1396E−5

Segment 3:
Ep (mV) = −2075
ip (A) = −5.6470E−5

Ep (mV) = −1143
ip (A) = −2.8142E−6

Cpd 1

L1792.40



12−Jul−95
18:37:55
Mode: CV
Fe(PicPh)2

Init E (mV) = 0
High E (mV) = 1500
Low E (mV) = −2500
Init P/N = P
V (mV/s) = 100
Sweep Segments = 3
Smpl Int (mV) = 2
Quiet T (s) = 2
Sens (A/V) = 1E−4

Segment 1:
Ep (mV) = +682
ip (A) = −7.0241E−5

Segment 2:
Ep (mV) = −1125
ip (A) = +1.0165E−5

Ep (mV) = −1987
ip (A) = +1.0076E−4

Segment 3:
Ep (mV) = −1769
ip (A) = −5.6149E−5

Cpd 2