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Supporting Information: Preparation and Data of the New Compounds

1) Preparation of 4 and 5.

To a stirred solution of **3** (470 mg = 0.602 mmol) in toluene (20 mL) were added equimolar amounts of the lactones **1** or **2**. After stirring for 30 min. the solution was concentrated to ca. 3 mL, layered with 20 mL of pentane and stored at -30°C for 20 h to give **4** or **5** as yellow, microcrystalline solids in yields of 58% and 41% respectively.

Data for **4** are as follows. Anal. calcd. for $C_{51}H_{50}F_3FeN_3O_4Si_3Zr$: C, 57.99; H, 4.74; N, 3.98. Found: C, 57.69; H, 4.78; N, 3.52. ^{1}H-NMR (C_6D_6, 295 K): δ -0.18 (s, HC(Si...)$_3$), 0.42, 0.55 (s, (Si(CH_3)$_2$), 1.74 (6'-CH_3), 2.09 (4'-CH_3), 3.85 (s, C_5H_5), 5.62-7.57 (m, 2-FC_6H_4 and lactone **2**). ^{13}C-NMR (C_6D_6, 295 K): δ 3.9, 4.8 (Si(CH_3)$_2$), 7.7 (HC(Si...)$_3$), 20.9 (ArCH_3), 21.1 (ArCH_3), 87.2 (C_5H_5), 115.2 (d, $^2J_{FC}$ = 22.1 Hz, C^3 of 2-FC_6H_4), 120.3 (C^4 of 2-FC_6H_4), 124.2 (C^5 of 2-FC_6H_4), 126.7 (C^6 of 2-FC_6H_4), 141.8 (d, $^2J_{FC}$ = 13.1 Hz, C^1 of 2-FC_6H_4), 157.9 (d, $^1J_{FC}$ = 235.4 Hz, C^2 of 2-FC_6H_4), 211.2, 212.2 (CO), 296.2 (ZrO(...)COFe), 115.9, 117.0, 119.4, 121.8, 122.7, 126.1, 126.7, 127.5, 128.5, 132.7, 132.9, 155.2, 161.8 (lactone **2**). ^{19}F-NMR (C_6D_6, 295 K): δ -122.0. ^{29}Si-NMR (C_6D_6, 295 K): δ 2.0. IR (benzene): ν(CO) = 2028, 1985 cm^{-1}.

Data for **5** are as follows. Anal. calcd. for $C_{51}H_{50}F_3FeN_3O_6Si_3Zr$: C, 56.28; H, 4.60; N, 3.86. Found: C, 56.36; H, 4.77; N, 3.58. ^{1}H-NMR (C_6D_6, 295 K): δ -0.17 (s, HC(Si...)$_3$), 0.43, 0.54 (s, (Si(CH_3)$_2$), 2.96 (6'-CH_3), 3.41 (4'-OCH_3), 3.93 (s, C_5H_5), 5.60-7.50 (m, 2-FC_6H_4 and lactone **3**). ^{13}C-NMR (C_6D_6, 295 K): δ 4.0, 4.3 (Si(CH_3)$_2$), 7.8 (HC(Si...)$_3$), 54.6 (OCH_3), 55.4 (OCH_3), 87.1 (C_5H_5), 115.2 (d, $^2J_{FC}$ = 22.1 Hz, C^3 of 2-FC_6H_4), 120.3 (C^4 of 2-FC_6H_4), 124.2 (C^5 of 2-FC_6H_4), 126.7 (C^6 of 2-FC_6H_4), 141.7 (d, $^2J_{FC}$ = 13.1 Hz, C^1 of 2-FC_6H_4), 157.9 (d, $^1J_{FC}$ = 235.4 Hz, C^2 of 2-FC_6H_4), 210.6, 211.5 (CO), 297.6 (ZrO(...)COFe), 115.9, 117.8, 121.8, 123.1, 126.0, 129.5, 132.9, 133.5, 155.7, 158.7, 161.9, 163.7 (lactone **3**). ^{19}F-NMR (C_6D_6, 295 K): δ = -121.9. ^{29}Si-NMR (C_6D_6, 295 K): δ 2.1. IR (benzene): ν(CO) 2030, 1991 cm^{-1}.

2) Preparation of 6 and 7.

A solution of **4** or **5** (0.2 mmol) was stirred at ambient temperature in pentane (15 mL) for, respectively, 15h and 72h. During this period the decarbonylation was monitored by infrared spectroscopy. After completion of the conversion, the solvent was removed in vacuo. The residues contained the pure reaction products as bright yellow powders. It proved extremely difficult to obtain single crystals of wither of the products and the crystal employed in the X-ray crystallographic study grew during the course of the decarbonylation.

Data for **6** are as follows. Anal. calcd. for $C_{50}H_{50}F_3FeN_3O_3Si_3Zr$: C, 58.35; H, 4.90; N, 4.08. Found: C, 57.98; H, 4.73; N, 3.94. ^{1}H-NMR (C_6D_6, 295 K): δ -0.35 (s, HC(Si...)$_3$), 0.22, 0.31 (s, (Si(CH_3)$_2$), 1.70 (6'-CH_3), 2.10 (4'-CH_3), 4.23 (s, C_5H_5), 6.33-7.64 (m, 2-FC_6H_4 and lactone **2**). ^{13}C-NMR (C_6D_6, 295 K): δ 3.1, 4.9 (Si(CH_3)$_2$), 8.8 (HC(Si...)$_3$), 20.9 (ArCH_3), 21.5 (ArCH_3), 86.4 (C_5H_5), 115.0 (d, $^2J_{FC}$ = 23.1 Hz, C^3 of 2-FC_6H_4), 120.1 (C^4 of 2-FC_6H_4), 122.2 (C^5 of 2-FC_6H_4), 125.3 (C^6 of 2-FC_6H_4), 139.9 (d, $^2J_{FC}$ = 12.1 Hz, C^1 of 2-FC_6H_4), 158.1 (d, $^1J_{FC}$ = 227.4 Hz, C^2 of 2-FC_6H_4), 214.2, 217.2 (CO), 117.1, 119.0, 124.1, 124.6, 124.9, 125.6, 129.3, 132.1, 132.7, 144.8, 146.9, 148.4, 160.5 (lactone **2**). ^{19}F-NMR (C_6D_6, 295 K): δ -123.0. ^{29}Si-NMR (C_6D_6, 295 K): δ 3.3. IR (benzene): ν(CO) = 2000, 1956 cm^{-1}.

Data for **7** are as follows. Anal. calcd. for $C_{50}H_{50}F_3FeN_3O_5Si_3Zr$: C, 56.59; H, 4.75; N, 3.96. Found: C, 56.39; H, 4.49; N, 3.90. ^{1}H-NMR (C_6D_6, 295 K): δ -0.37 (s, HC(Si...)$_3$), 0.24, 0.30 (s, (Si(CH_3)$_2$), 3.01 (6'-OCH_3), 3.48 (4'-OCH_3), 4.15 (s, C_5H_5), 6.30-7.68 (m, 2-FC_6H_4 and lactone 3). ^{13}C-NMR (C_6D_6, 295 K): δ 3.0, 5.1 (Si(CH_3)$_2$), 8.7 (HC(Si...)$_3$), 54.2 (ArOCH_3), 55.1 (ArOCH_3), 86.8 (C_5H_5), 114.4 (d, $^2J_{FC}$ = 22.8 Hz, C^3 of 2-FC_6H_4), 120.0 (C^4 of 2-FC_6H_4), 122.6 (C^5 of 2-FC_6H_4), 125.4 (C^6 of 2-FC_6H_4), 140.3 (d, $^2J_{FC}$ = 12.0 Hz, C^1 of 2-FC_6H_4), 158.5 (d, $^1J_{FC}$ = 228.6 Hz, C^2 of 2-FC_6H_4), 214.1, 217.8 (CO), 117.2, 119.3, 124.1, 124.7, 124.7, 125.5, 129.9, 133.0, 132.8, 145.2, 146.7, 148.9, 161.3 (lactone **3**). ^{19}F-NMR (C_6D_6, 295 K): δ -124.1. ^{29}Si-NMR (C_6D_6, 295 K): δ 3.4. IR (benzene): 1997, 1954 cm^{-1}.

Table 1. Crystal data and structure refinement for 7.

formula	$C_{53.50}\ H_{54}\ F_3\ Fe\ N_3\ O_5\ Si_3\ Zr$
fw	1107.34
crystal size, mm^3	0.34 x 0.36 x 0.44
crystal system	Monoclinic
space group	C2/c
cell dimensions determn	
a, Å	40.373(7)
b, Å	13.056(4)
c, Å	20.130(4)
α, °	90
β, °	96.068(0)
γ, °	90
V, $Å^3$	10551(4)
Z	8
ρ_{calc}, gcm^{-3}	1.394
diffractometer	CAD4 (Enraf-Nonius)
radiation	Mo-K_α (0.70930 Å), graphite monochromator, Zr filter (factor ?)
temp, K	297(2)
μ, mm^{-1}	0.600
2Θ (max), °	42.00
tot. no. of reflcns scanned	6662
no. of unique rflcns	5668 [R(int) = 0.0867]
no. of data	5101
no. of obsd rflcns [$I>2\sigma(I)$]	2689
param	581 (full-matrix least-squares on F^2 (SHELXL-93))
final R indices [$I>2\sigma(I)$]	$R_1 = 0.0852$, $wR_2 = 0.1623$
R indices (all data)	$R_1 = 0.2011$, $wR_2 = 0.2310$
resid electron density, $eÅ^{-3}$	0.432 / -0.450

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 7. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zr(1)	6458(1)	7866(1)	5200(1)	42(1)
Fe(2)	5635(1)	4276(2)	4130(1)	53(1)
Si(1)	7090(1)	9407(4)	5374(2)	68(1)
Si(2)	6363(1)	10284(3)	5441(2)	62(1)
Si(3)	6595(1)	9569(3)	4061(2)	59(1)
N(1)	6895(3)	8335(8)	5734(5)	48(3)
N(2)	6148(3)	9089(9)	5363(5)	50(3)
N(3)	6556(3)	8254(8)	4228(5)	46(3)
F(1)	6486(2)	7415(9)	6458(4)	113(4)
F(2A)	5786(4)	8090(13)	4395(8)	68(5)
F(2B)	5791(5)	9907(19)	6336(11)	115(9)
F(3)	6783(2)	6461(6)	4677(4)	64(2)
O(51)	5289(3)	3557(10)	5208(6)	99(4)
O(61)	5587(3)	2229(10)	3567(6)	112(5)
O(72)	6191(2)	6617(7)	5258(4)	42(2)
O(74)	5428(2)	6283(7)	6917(5)	67(3)
O(76)	5951(2)	3346(7)	6102(5)	57(3)
C(1)	6719(3)	10079(10)	4925(6)	46(4)
C(2)	7311(4)	10286(12)	6005(8)	100(7)
C(3)	7406(4)	8965(12)	4859(7)	79(5)
C(4)	6078(4)	11322(10)	5110(8)	81(6)
C(5)	6503(4)	10585(12)	6344(7)	93(6)
C(6)	6918(4)	9829(12)	3485(7)	87(6)
C(7)	6195(4)	10111(12)	3660(7)	84(6)
C(11)	7028(3)	7892(8)	6364(4)	54(4)
C(12)	7361(3)	7890(9)	6620(6)	83(5)
C(13)	7458(3)	7438(10)	7235(7)	122(9)
C(14)	7221(4)	6988(9)	7595(5)	122(9)
C(15)	6887(4)	6990(9)	7339(6)	103(7)
C(16)	6791(2)	7442(9)	6724(7)	85(6)
C(21)	5807(3)	9067(10)	5345(8)	63(5)
C(22)	5638(4)	9499(8)	5843(6)	87(7)
C(23)	5294(4)	9400(9)	5817(7)	119(9)
C(24)	5119(3)	8868(11)	5294(9)	108(9)
C(25)	5288(4)	8435(9)	4797(6)	94(6)
C(26)	5632(4)	8534(9)	4822(6)	73(5)
C(31)	6590(2)	7455(7)	3750(5)	53(4)
C(32)	6515(3)	7571(8)	3064(5)	83(6)
C(33)	6561(3)	6757(11)	2638(4)	97(7)
C(34)	6682(3)	5827(9)	2899(6)	113(8)
C(35)	6756(3)	5711(6)	3585(7)	82(6)

C(36)	6710(2)	6525(8)	4010(4)	61(5)
C(41)	5371(4)	4898(12)	3257(8)	69(5)
C(42)	5729(4)	5162(12)	3270(8)	63(5)
C(43)	5809(4)	5737(12)	3881(9)	68(5)
C(44)	5516(5)	5847(12)	4219(8)	71(5)
C(45)	5243(4)	5308(12)	3842(8)	65(5)
C(51)	5449(4)	3852(13)	4807(8)	60(5)
C(61)	5617(5)	3036(14)	3800(9)	82(6)
C(81)	6255(3)	4387(10)	5159(7)	34(3)
C(82)	6101(3)	4041(11)	4536(8)	49(4)
C(83)	6321(4)	3495(12)	4136(8)	62(5)
C(84)	6631(4)	3236(10)	4360(7)	51(4)
C(85)	6790(4)	3535(10)	4985(8)	41(4)
C(86)	6582(3)	4146(11)	5381(7)	38(4)
C(87)	6741(4)	4482(10)	5995(7)	46(4)
C(88)	7056(4)	4218(14)	6235(9)	77(5)
C(89)	7249(4)	3569(14)	5858(10)	78(6)
C(810)	7107(4)	3264(11)	5256(10)	64(5)
C(71)	6049(3)	4919(11)	5629(6)	32(3)
C(72)	6018(3)	6015(11)	5647(6)	38(4)
C(73)	5812(3)	6482(11)	6068(7)	44(4)
C(74)	5642(3)	5910(12)	6492(7)	48(4)
C(75)	5684(3)	4842(11)	6504(6)	46(4)
C(76)	5884(3)	4391(11)	6095(6)	39(4)
C(77A)	5455(8)	7432(22)	6953(14)	54(10)
C(77B)	5285(7)	7265(24)	6775(14)	49(9)
C(78)	5768(4)	2741(11)	6532(7)	85(6)
C(7S)	5000	9771(55)	7500	141(24)
C(6S)	5000	12620(34)	7500	61(13)
C(5S)	4862(6)	10746(26)	7356(14)	54(9)
C(4S)	4742(9)	12373(32)	7192(19)	93(14)
C(3S)	4822(11)	11696(44)	7272(24)	121(17)
C(2S)	4596(9)	11264(30)	7120(17)	84(12)
C(1S)	4662(12)	10083(41)	7166(24)	156(19)

Table 3. Bond lengths [Å] for 7.

Zr(1)-O(72)	1.965(9)
Zr(1)-N(1)	2.062(1)
Zr(1)-N(2)	2.076(1)
Zr(1)-N(3)	2.100(0)
Zr(1)-F(3)	2.548(8)
Zr(1)-F(1)	2.591(9)
Zr(1)-Si(2)	3.223(5)
Zr(1)-Si(1)	3.240(5)
Fe(2)-C(51)	1.72(2)
Fe(2)-C(61)	1.75(2)
Fe(2)-C(82)	1.994(4)
Fe(2)-C(43)	2.11(2)
Fe(2)-C(45)	2.116(4)
Fe(2)-C(44)	2.12(2)
Fe(2)-C(41)	2.12(2)
Fe(2)-C(42)	2.15(2)
Si(1)-N(1)	1.797(1)
Si(1)-C(3)	1.82(2)
Si(1)-C(2)	1.869(4)
Si(1)-C(1)	1.884(3)
Si(2)-N(2)	1.785(2)
Si(2)-C(4)	1.856(4)
Si(2)-C(1)	1.880(3)
Si(2)-C(5)	1.89(2)
Si(3)-N(3)	1.761(1)
Si(3)-C(6)	1.865(4)
Si(3)-C(7)	1.866(4)
Si(3)-C(1)	1.881(3)
N(1)-C(11)	1.445(2)
N(2)-C(21)	1.374(3)
N(3)-C(31)	1.435(2)
F(1)-C(16)	1.291(1)
F(2A)-C(26)	1.25(2)
F(2B)-C(22)	1.23(2)
F(3)-C(36)	1.346(1)
O(51)-C(51)	1.15(2)
O(61)-C(61)	1.15(2)
O(72)-C(72)	1.355(4)
O(74)-C(74)	1.369(4)
O(74)-C(77B)	1.42(3)
O(74)-C(77A)	1.51(3)
O(76)-C(76)	1.39(2)
O(76)-C(78)	1.43(2)
C(11)-C(12)	1.39
C(11)-C(16)	1.39
C(12)-C(13)	1.39
C(13)-C(14)	1.39

C(14)-C(15)	1.39
C(15)-C(16)	1.39
C(21)-C(22)	1.39
C(21)-C(26)	1.39
C(22)-C(23)	1.39
C(23)-C(24)	1.39
C(24)-C(25)	1.39
C(25)-C(26)	1.39
C(31)-C(32)	1.39
C(31)-C(36)	1.39
C(32)-C(33)	1.39
C(33)-C(34)	1.39
C(34)-C(35)	1.39
C(35)-C(36)	1.39
C(41)-C(45)	1.44(2)
C(41)-C(42)	1.48(2)
C(42)-C(43)	1.45(2)
C(43)-C(44)	1.43(2)
C(44)-C(45)	1.45(2)
C(81)-C(86)	1.38(2)
C(81)-C(82)	1.41(2)
C(81)-C(71)	1.50(2)
C(82)-C(83)	1.45(2)
C(83)-C(84)	1.33(2)
C(84)-C(85)	1.41(2)
C(85)-C(810)	1.38(2)
C(85)-C(86)	1.46(2)
C(86)-C(87)	1.40(2)
C(87)-C(88)	1.36(2)
C(88)-C(89)	1.42(2)
C(89)-C(810)	1.34(2)
C(71)-C(76)	1.39(2)
C(71)-C(72)	1.44(2)
C(72)-C(73)	1.39(2)
C(73)-C(74)	1.37(2)
C(74)-C(75)	1.41(2)
C(75)-C(76)	1.35(2)
C(7S)-C(5S)#1	1.41(6)
C(7S)-C(5S)	1.41(6)
C(7S)-C(1S)#1	1.51(5)
C(7S)-C(1S)	1.51(5)
C(6S)-C(4S)#1	1.20(4)
C(6S)-C(4S)	1.20(4)
C(6S)-C(3S)#1	1.45(6)
C(6S)-C(3S)	1.45(6)
C(5S)-C(5S)#1	1.20(5)
C(5S)-C(1S)	1.22(5)
C(5S)-C(3S)	1.26(5)
C(5S)-C(2S)	1.31(4)
C(5S)-C(3S)#1	1.88(5)

C(4S)-C(3S)	0.95(6)
C(4S)-C(2S)	1.56(5)
C(3S)-C(2S)	1.09(5)
C(3S)-C(3S)#1	1.62(9)
C(3S)-C(5S)#1	1.88(4)
C(2S)-C(1S)	1.57(6)

Table 4. Bond angles [°] for 7.

O(72)-Zr(1)-N(1)	131.3(4)
O(72)-Zr(1)-N(2)	106.6(4)
N(1)-Zr(1)-N(2)	100.8(4)
O(72)-Zr(1)-N(3)	114.5(4)
N(1)-Zr(1)-N(3)	100.3(4)
N(2)-Zr(1)-N(3)	98.0(4)
O(72)-Zr(1)-F(3)	74.7(3)
N(1)-Zr(1)-F(3)	88.8(3)
N(2)-Zr(1)-F(3)	164.8(3)
N(3)-Zr(1)-F(3)	68.4(3)
O(72)-Zr(1)-F(1)	73.8(3)
N(1)-Zr(1)-F(1)	67.1(4)
N(2)-Zr(1)-F(1)	89.2(4)
N(3)-Zr(1)-F(1)	166.6(4)
F(3)-Zr(1)-F(1)	105.6(3)
O(72)-Zr(1)-Si(2)	136.8(3)
N(1)-Zr(1)-Si(2)	74.9(3)
N(2)-Zr(1)-Si(2)	30.6(3)
N(3)-Zr(1)-Si(2)	86.7(3)
F(3)-Zr(1)-Si(2)	147.4(2)
F(1)-Zr(1)-Si(2)	94.0(3)
O(72)-Zr(1)-Si(1)	160.0(3)
N(1)-Zr(1)-Si(1)	30.4(3)
N(2)-Zr(1)-Si(1)	89.2(3)
N(3)-Zr(1)-Si(1)	74.1(3)
F(3)-Zr(1)-Si(1)	93.3(2)
F(1)-Zr(1)-Si(1)	94.8(2)
Si(2)-Zr(1)-Si(1)	58.70(3)
C(51)-Fe(2)-C(61)	89.9(8)
C(51)-Fe(2)-C(82)	95.6(6)
C(61)-Fe(2)-C(82)	90.8(7)
C(51)-Fe(2)-C(43)	131.6(8)
C(61)-Fe(2)-C(43)	138.4(8)
C(82)-Fe(2)-C(43)	85.0(5)
C(51)-Fe(2)-C(45)	92.5(7)
C(61)-Fe(2)-C(45)	119.1(7)
C(82)-Fe(2)-C(45)	149.1(6)
C(43)-Fe(2)-C(45)	67.5(6)
C(51)-Fe(2)-C(44)	97.0(7)
C(61)-Fe(2)-C(44)	158.1(7)
C(82)-Fe(2)-C(44)	109.1(6)
C(43)-Fe(2)-C(44)	39.6(5)
C(45)-Fe(2)-C(44)	40.1(5)
C(51)-Fe(2)-C(41)	123.8(7)
C(61)-Fe(2)-C(41)	92.4(7)
C(82)-Fe(2)-C(41)	140.4(6)
C(43)-Fe(2)-C(41)	67.0(6)

C(45)-Fe(2)-C(41)	39.7(5)
C(44)-Fe(2)-C(41)	66.4(6)
C(51)-Fe(2)-C(42)	160.5(7)
C(61)-Fe(2)-C(42)	101.3(7)
C(82)-Fe(2)-C(42)	100.1(6)
C(43)-Fe(2)-C(42)	39.8(5)
C(45)-Fe(2)-C(42)	68.1(6)
C(44)-Fe(2)-C(42)	66.9(6)
C(41)-Fe(2)-C(42)	40.7(5)
N(1)-Si(1)-C(3)	110.2(6)
N(1)-Si(1)-C(2)	113.8(6)
C(3)-Si(1)-C(2)	105.6(7)
N(1)-Si(1)-C(1)	101.3(6)
C(3)-Si(1)-C(1)	116.4(7)
C(2)-Si(1)-C(1)	109.9(7)
N(1)-Si(1)-Zr(1)	35.5(4)
C(3)-Si(1)-Zr(1)	109.4(5)
C(2)-Si(1)-Zr(1)	140.3(6)
C(1)-Si(1)-Zr(1)	70.1(4)
N(2)-Si(2)-C(4)	109.3(6)
N(2)-Si(2)-C(1)	102.7(6)
C(4)-Si(2)-C(1)	112.8(6)
N(2)-Si(2)-C(5)	111.1(6)
C(4)-Si(2)-C(5)	107.7(7)
C(1)-Si(2)-C(5)	113.2(7)
N(2)-Si(2)-Zr(1)	36.3(4)
C(4)-Si(2)-Zr(1)	137.8(5)
C(1)-Si(2)-Zr(1)	70.5(4)
C(5)-Si(2)-Zr(1)	108.7(5)
N(3)-Si(3)-C(6)	112.2(6)
N(3)-Si(3)-C(7)	111.2(6)
C(6)-Si(3)-C(7)	107.0(7)
N(3)-Si(3)-C(1)	100.9(5)
C(6)-Si(3)-C(1)	112.1(7)
C(7)-Si(3)-C(1)	113.5(6)
C(11)-N(1)-Si(1)	121.9(8)
C(11)-N(1)-Zr(1)	123.9(8)
Si(1)-N(1)-Zr(1)	114.1(6)
C(21)-N(2)-Si(2)	119.9(0)
C(21)-N(2)-Zr(1)	126.9(0)
Si(2)-N(2)-Zr(1)	113.0(6)
C(31)-N(3)-Si(3)	124.3(8)
C(31)-N(3)-Zr(1)	119.4(7)
Si(3)-N(3)-Zr(1)	116.3(5)
C(16)-F(1)-Zr(1)	109.9(8)
C(36)-F(3)-Zr(1)	107.4(6)
C(72)-O(72)-Zr(1)	146.7(8)
C(74)-O(74)-C(77B)	118(2)
C(74)-O(74)-C(77A)	110(2)
C(76)-O(76)-C(78)	116.0(0)

Si(2)-C(1)-Si(3)	114.7(7)
Si(2)-C(1)-Si(1)	114.7(7)
Si(3)-C(1)-Si(1)	113.6(7)
C(12)-C(11)-C(16)	120.0
C(12)-C(11)-N(1)	125.6(0)
C(16)-C(11)-N(1)	114.6(0)
C(11)-C(12)-C(13)	120.0
C(14)-C(13)-C(12)	120.0
C(15)-C(14)-C(13)	120.0
C(14)-C(15)-C(16)	120.0
F(1)-C(16)-C(15)	121.6(1)
F(1)-C(16)-C(11)	118.5(1)
C(15)-C(16)-C(11)	120.0
N(2)-C(21)-C(22)	122.8(4)
N(2)-C(21)-C(26)	117.3(4)
C(22)-C(21)-C(26)	120.0
F(2B)-C(22)-C(21)	121(2)
F(2B)-C(22)-C(23)	119(2)
C(21)-C(22)-C(23)	120.0
C(24)-C(23)-C(22)	120.0
C(23)-C(24)-C(25)	120.0
C(26)-C(25)-C(24)	120.0
F(2A)-C(26)-C(25)	120(2)
F(2A)-C(26)-C(21)	120(2)
C(25)-C(26)-C(21)	120.0
C(32)-C(31)-C(36)	120.0
C(32)-C(31)-N(3)	124.1(9)
C(36)-C(31)-N(3)	115.9(9)
C(31)-C(32)-C(33)	120.0
C(34)-C(33)-C(32)	120.0
C(33)-C(34)-C(35)	120.0
C(36)-C(35)-C(34)	120.0
F(3)-C(36)-C(35)	122.5(9)
F(3)-C(36)-C(31)	117.5(9)
C(35)-C(36)-C(31)	120.0
C(45)-C(41)-C(42)	109.5(4)
C(45)-C(41)-Fe(2)	70.0(9)
C(42)-C(41)-Fe(2)	70.7(8)
C(43)-C(42)-C(41)	105.5(4)
C(43)-C(42)-Fe(2)	68.7(9)
C(41)-C(42)-Fe(2)	68.6(9)
C(44)-C(43)-C(42)	109.5(4)
C(44)-C(43)-Fe(2)	70.6(0)
C(42)-C(43)-Fe(2)	71.5(9)
C(43)-C(44)-C(45)	109.0(4)
C(43)-C(44)-Fe(2)	69.9(9)
C(45)-C(44)-Fe(2)	69.8(9)
C(41)-C(45)-C(44)	106.9(4)
C(41)-C(45)-Fe(2)	70.3(8)
C(44)-C(45)-Fe(2)	70.1(8)

O(51)-C(51)-Fe(2)	171.7(4)
O(61)-C(61)-Fe(2)	176(2)
C(86)-C(81)-C(82)	122.1(3)
C(86)-C(81)-C(71)	118.6(2)
C(82)-C(81)-C(71)	119.2(2)
C(81)-C(82)-C(83)	114.4(3)
C(81)-C(82)-Fe(2)	128.7(1)
C(83)-C(82)-Fe(2)	117.1(2)
C(84)-C(83)-C(82)	123.3(4)
C(83)-C(84)-C(85)	124.0(4)
C(810)-C(85)-C(84)	127(2)
C(810)-C(85)-C(86)	119.2(4)
C(84)-C(85)-C(86)	114.1(3)
C(81)-C(86)-C(87)	123.2(4)
C(81)-C(86)-C(85)	122.3(3)
C(87)-C(86)-C(85)	114.8(3)
C(88)-C(87)-C(86)	124(2)
C(87)-C(88)-C(89)	120(2)
C(810)-C(89)-C(88)	117(2)
C(89)-C(810)-C(85)	125(2)
C(76)-C(71)-C(72)	115.4(3)
C(76)-C(71)-C(81)	122.5(2)
C(72)-C(71)-C(81)	122.4(3)
O(72)-C(72)-C(73)	118.5(3)
O(72)-C(72)-C(71)	120.9(3)
C(73)-C(72)-C(71)	120.9(3)
C(74)-C(73)-C(72)	120.8(4)
O(74)-C(74)-C(73)	126.0(4)
O(74)-C(74)-C(75)	115.3(4)
C(73)-C(74)-C(75)	119.0(4)
C(76)-C(75)-C(74)	120.2(3)
C(75)-C(76)-C(71)	123.9(4)
C(75)-C(76)-O(76)	123.4(3)
C(71)-C(76)-O(76)	112.9(2)
C(5S)#1-C(7S)-C(5S)	50(3)
C(5S)#1-C(7S)-C(1S)#1	49(3)
C(5S)-C(7S)-C(1S)#1	100(5)
C(5S)#1-C(7S)-C(1S)	100(5)
C(5S)-C(7S)-C(1S)	49(3)
C(1S)#1-C(7S)-C(1S)	149(7)
C(4S)#1-C(6S)-C(4S)	149(6)
C(4S)#1-C(6S)-C(3S)#1	41(3)
C(4S)-C(6S)-C(3S)#1	108(5)
C(4S)#1-C(6S)-C(3S)	108(5)
C(4S)-C(6S)-C(3S)	41(3)
C(3S)#1-C(6S)-C(3S)	68(4)
C(5S)#1-C(5S)-C(1S)	135(3)
C(5S)#1-C(5S)-C(3S)	100(3)
C(1S)-C(5S)-C(3S)	126(4)
C(5S)#1-C(5S)-C(2S)	149(2)

C(1S)-C(5S)-C(2S)	76(3)
C(3S)-C(5S)-C(2S)	50(3)
C(5S)#1-C(5S)-C(7S)	65(2)
C(1S)-C(5S)-C(7S)	70(3)
C(3S)-C(5S)-C(7S)	164(4)
C(2S)-C(5S)-C(7S)	146(3)
C(5S)#1-C(5S)-C(3S)#1	42(2)
C(1S)-C(5S)-C(3S)#1	174(4)
C(3S)-C(5S)-C(3S)#1	58(4)
C(2S)-C(5S)-C(3S)#1	107(3)
C(7S)-C(5S)-C(3S)#1	106(3)
C(3S)-C(4S)-C(6S)	84(5)
C(3S)-C(4S)-C(2S)	43(4)
C(6S)-C(4S)-C(2S)	127(4)
C(4S)-C(3S)-C(2S)	100(5)
C(4S)-C(3S)-C(5S)	167(6)
C(2S)-C(3S)-C(5S)	68(4)
C(4S)-C(3S)-C(6S)	55(4)
C(2S)-C(3S)-C(6S)	153(6)
C(5S)-C(3S)-C(6S)	136(4)
C(4S)-C(3S)-C(3S)#1	111(4)
C(2S)-C(3S)-C(3S)#1	146(4)
C(5S)-C(3S)-C(3S)#1	80(3)
C(6S)-C(3S)-C(3S)#1	56(2)
C(4S)-C(3S)-C(5S)#1	153(5)
C(2S)-C(3S)-C(5S)#1	106(5)
C(5S)-C(3S)-C(5S)#1	39(2)
C(6S)-C(3S)-C(5S)#1	98(3)
C(3S)#1-C(3S)-C(5S)#1	41(2)
C(3S)-C(2S)-C(5S)	62(3)
C(3S)-C(2S)-C(4S)	37(3)
C(5S)-C(2S)-C(4S)	99(3)
C(3S)-C(2S)-C(1S)	111(5)
C(5S)-C(2S)-C(1S)	49(2)
C(4S)-C(2S)-C(1S)	148(4)
C(5S)-C(1S)-C(7S)	61(4)
C(5S)-C(1S)-C(2S)	55(3)
C(7S)-C(1S)-C(2S)	116(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+3/2

Table 5. Anisotropic displacement parameters ($Å^2$ x 10^3) for 7.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U]$

	U11	U22	U33	U23	U13	U12
Zr(1)	62(1)	26(1)	37(1)	2(1)	4(1)	-1(1)
Fe(2)	64(2)	49(2)	45(1)	-11(1)	-3(1)	0(1)
Si(1)	85(3)	45(3)	69(3)	2(3)	-6(3)	-13(3)
Si(2)	95(4)	36(3)	54(3)	-5(2)	6(3)	4(3)
Si(3)	91(3)	35(3)	50(3)	7(2)	4(3)	-2(3)
N(1)	64(8)	38(7)	44(8)	-2(6)	11(6)	5(7)
N(2)	52(8)	51(8)	46(8)	3(7)	0(6)	11(7)
N(3)	75(8)	33(7)	32(7)	-1(6)	22(6)	0(6)
F(1)	110(8)	144(10)	75(7)	49(7)	-36(6)	-60(7)
F(3)	84(6)	40(5)	67(6)	17(5)	6(5)	7(5)
O(51)	78(9)	139(12)	83(10)	-15(9)	22(7)	-33(8)
O(61)	163(13)	65(9)	96(10)	-30(9)	-35(8)	8(10)
O(72)	47(6)	44(6)	35(6)	-3(5)	11(5)	-7(5)
O(74)	93(8)	50(7)	65(7)	6(6)	44(7)	16(6)
O(76)	82(7)	42(7)	52(7)	8(5)	29(6)	5(6)
C(1)	75(10)	18(8)	44(9)	9(7)	-5(8)	-9(8)
C(2)	120(15)	71(14)	98(15)	1(12)	-41(12)	-32(12)
C(3)	86(13)	75(13)	74(13)	2(11)	-2(10)	-19(11)
C(4)	121(15)	32(10)	94(14)	5(10)	29(11)	19(10)
C(5)	138(16)	57(12)	83(13)	-28(11)	2(12)	-4(12)
C(6)	122(14)	71(13)	71(13)	11(11)	23(11)	-21(12)
C(7)	134(15)	52(11)	63(12)	18(10)	-6(11)	15(11)
C(11)	64(11)	26(9)	68(12)	2(9)	-18(10)	11(9)
C(12)	74(13)	96(15)	71(13)	2(12)	-27(10)	21(12)
C(13)	154(21)	98(19)	99(18)	4(14)	-54(16)	52(16)
C(14)	179(24)	94(18)	79(16)	13(14)	-55(17)	11(19)
C(15)	144(19)	78(15)	80(15)	26(13)	-19(13)	-41(15)
C(16)	105(16)	62(13)	80(15)	32(11)	-31(13)	-35(12)
C(21)	77(14)	50(12)	62(13)	24(10)	10(12)	35(11)
C(22)	63(13)	81(16)	124(20)	52(15)	40(14)	30(13)
C(23)	191(30)	72(17)	98(19)	30(14)	41(18)	38(18)
C(24)	113(17)	86(17)	139(21)	58(16)	79(18)	60(15)
C(25)	119(19)	83(15)	74(15)	32(13)	-16(14)	3(15)
C(26)	68(14)	70(14)	86(16)	29(12)	22(12)	13(12)
C(31)	62(10)	69(13)	28(9)	-1(9)	6(8)	10(9)
C(32)	147(16)	68(13)	31(10)	-15(10)	-5(10)	9(12)
C(33)	154(18)	91(16)	44(12)	7(12)	-1(12)	-24(15)
C(34)	183(21)	98(19)	65(15)	-12(14)	44(15)	-5(16)
C(35)	101(13)	19(10)	134(18)	-17(12)	47(13)	14(10)
C(36)	90(13)	37(11)	53(12)	-5(10)	-5(10)	21(10)
C(41)	76(13)	68(12)	61(12)	-10(10)	0(10)	48(11)
C(42)	83(13)	47(11)	52(11)	13(9)	-24(10)	8(10)
C(43)	77(12)	47(11)	76(13)	24(11)	-14(11)	31(10)
C(44)	79(13)	50(11)	81(13)	-15(10)	-9(11)	23(11)
C(45)	67(11)	57(12)	68(12)	-4(10)	-12(10)	16(10)
C(51)	44(10)	84(14)	56(12)	-27(10)	19(9)	-20(9)
C(61)	112(15)	70(14)	61(13)	-11(11)	-6(11)	3(13)
C(81)	39(10)	33(9)	29(9)	14(8)	4(8)	6(8)
C(82)	64(11)	28(9)	59(12)	30(8)	23(10)	0(9)

C(83)	49(11)	69(13)	64(12)	-14(10)	-10(10)	-1(10)
C(84)	82(13)	34(10)	38(10)	-18(8)	10(9)	-2(9)
C(85)	44(10)	19(9)	62(11)	11(8)	10(9)	8(8)
C(86)	38(9)	34(9)	42(10)	12(8)	1(8)	-7(8)
C(87)	52(10)	38(10)	48(10)	4(8)	1(9)	2(9)
C(88)	52(12)	94(16)	81(14)	23(12)	-13(10)	6(12)
C(89)	61(13)	73(14)	94(16)	33(13)	-23(12)	31(11)
C(810)	45(11)	44(11)	104(15)	18(11)	12(10)	25(9)
C(71)	41(9)	40(10)	15(8)	-11(7)	-2(7)	-3(8)
C(72)	45(9)	43(11)	28(9)	-6(8)	13(7)	-8(8)
C(73)	46(9)	32(9)	53(10)	3(9)	8(8)	-3(8)
C(74)	53(10)	48(11)	49(10)	-1(9)	27(8)	6(9)
C(75)	68(11)	40(11)	30(9)	15(8)	11(8)	-13(9)
C(76)	56(10)	37(10)	27(9)	2(8)	20(8)	14(8)
C(78)	138(15)	41(11)	88(13)	-6(11)	71(12)	8(11)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 7.

	x	y	z	U(eq)
H(1)	6800(3)	10772(10)	4849(6)	56
H(2A)	7156(4)	10547(12)	6293(8)	150
H(2B)	7406(4)	10846(12)	5780(8)	150
H(2C)	7485(4)	9918(12)	6266(8)	150
H(3A)	7306(4)	8506(12)	4523(7)	119
H(3B)	7579(4)	8614(12)	5134(7)	119
H(3C)	7499(4)	9541(12)	4649(7)	119
H(4A)	5901(4)	11396(10)	5391(8)	122
H(4B)	5986(4)	11154(10)	4665(8)	122
H(4C)	6200(4)	11953(10)	5105(8)	122
H(5A)	6651(4)	10058(12)	6528(7)	140
H(5B)	6312(4)	10619(12)	6591(7)	140
H(5C)	6616(4)	11232(12)	6372(7)	140
H(6A)	7128(4)	9560(12)	3675(7)	131
H(6B)	6937(4)	10554(12)	3421(7)	131
H(6C)	6855(4)	9506(12)	3062(7)	131
H(7A)	6022(4)	9992(12)	3943(7)	126
H(7B)	6138(4)	9785(12)	3236(7)	126
H(7C)	6220(4)	10834(12)	3595(7)	126
H(12)	7520(4)	8191(13)	6379(9)	99
H(13)	7681(3)	7437(15)	7406(10)	146
H(14)	7285(6)	6686(13)	8006(6)	147
H(15)	6728(5)	6689(13)	7579(9)	123
H(23)	5181(7)	9690(13)	6149(9)	143
H(24)	4889(3)	8801(16)	5276(14)	129
H(25)	5172(6)	8079(12)	4447(8)	113
H(32)	6435(4)	8193(9)	2890(8)	99
H(33)	6512(4)	6834(15)	2180(4)	117
H(34)	6713(4)	5282(11)	2614(9)	136
H(35)	6837(4)	5089(7)	3759(10)	99
H(83)	6241(4)	3316(12)	3701(8)	74
H(84)	6750(4)	2833(10)	4087(7)	61
H(87)	6623(4)	4912(10)	6254(7)	56
H(88)	7146(4)	4463(14)	6649(9)	93
H(89)	7463(4)	3366(14)	6021(10)	94
H(810)	7231(4)	2841(11)	5005(10)	77
H(73)	5790(3)	7191(11)	6062(7)	52
H(75)	5574(3)	4445(11)	6794(6)	55
H(77A)	5305(8)	7691(22)	7251(14)	80
H(77B)	5400(8)	7718(22)	6516(14)	80
H(77C)	5679(8)	7621(22)	7116(14)	80
H(77D)	5140(7)	7435(24)	7108(14)	73

H(77E)	5159(7)	7254(24)	6343(14)	73
H(77F)	5458(7)	7768(24)	6779(14)	73
H(78A)	5832(4)	2035(11)	6502(7)	127
H(78B)	5534(4)	2809(11)	6397(7)	127
H(78C)	5817(4)	2973(11)	6984(7)	127