© 2003 American Chemical Society, J. Am. Chem. Soc., Slep ja030377f Supporting Info Page 1

SUPPORTING INFORMATION

SUPPORTING INFORMATION

The Mixed-valent $\{Fe^{IV}(\mu\text{-}O)(\mu\text{-carboxylato})_2Fe^{III}\}^{3+}$ Core.

Leonardo D. Slep, Ana Mijovilovich, Wolfram Meyer-Klaucke, Thomas Weyhermüller, Eckhard Bill, Eberhard Bothe, Frank Neese, Karl Wieghardt

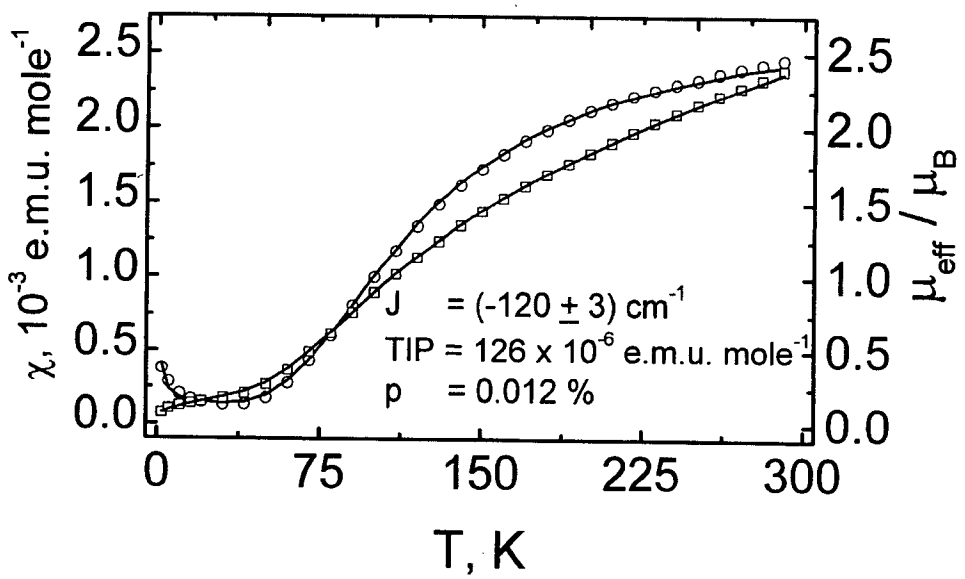

Figure S1. Plot of χ *vs.* T (circles) and μ_{eff} *vs.* T (squares) for a powder sample of $[(tpb)Fe^{III}(\mu\text{-}O)(\mu\text{-}CH_3CO_2)_2Fe^{III}(Me_3[9]aneN_3)]PF_6 \cdot 0.5\ MeCN \cdot 0.25\ Et_2O$. The solid lines represent de best fit to the isotropic Heisemberg model for electron exchange (see text).

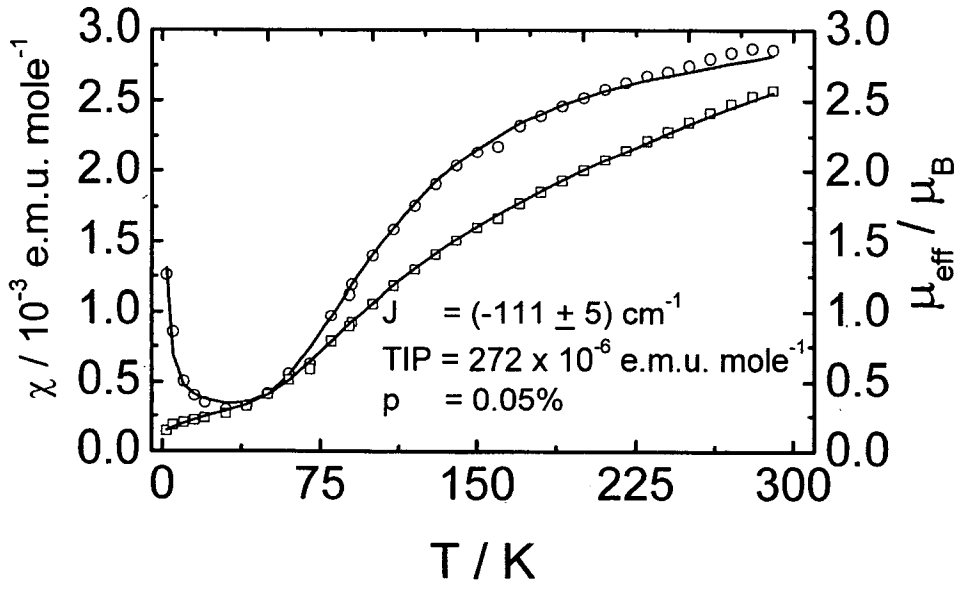

Figure S2. Plot of χ *vs.* T (circles) and μ_{eff} *vs.* T (squares) for a powder sample of $[([9]aneN_3)Fe^{III}(\mu\text{-}O)(\mu\text{-}CH_3CO_2)_2Fe^{III}([9]aneN_3)](PF_6)_2$. The solid lines represent de best fit to the isotropic Heisemberg model for electron exchange (see text).

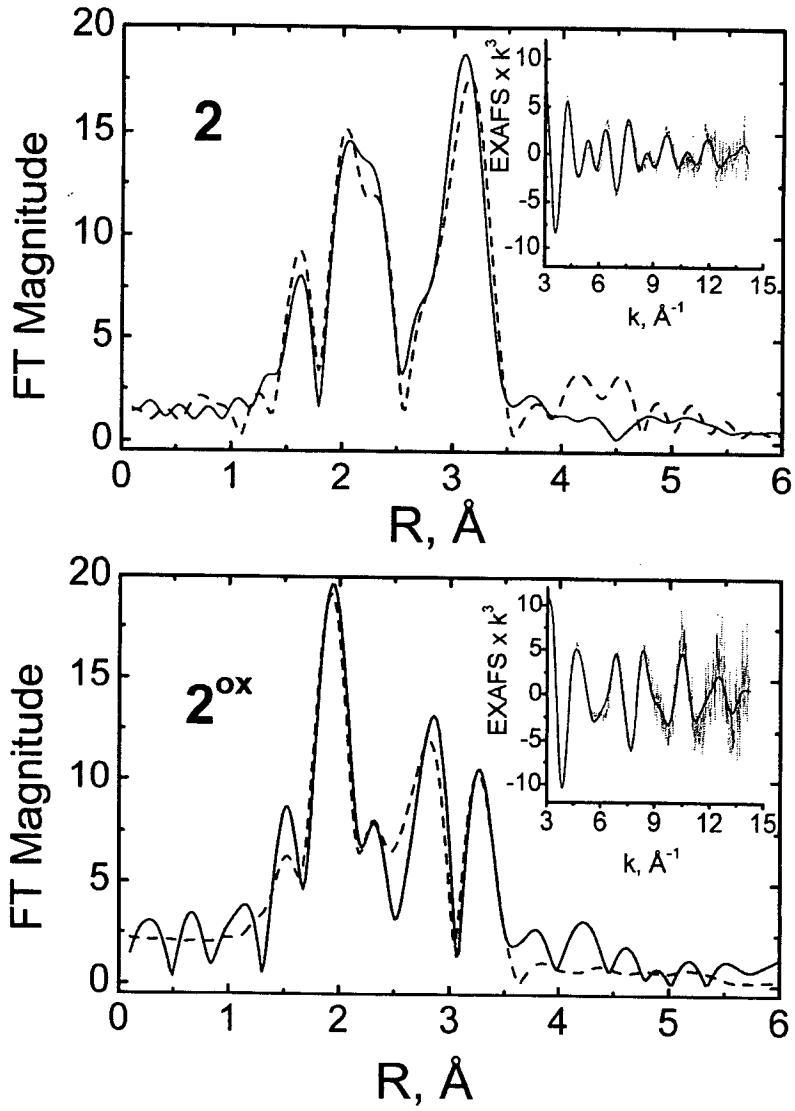

Figure S3. Fourier transform of the EXAFS data for **2** and **2**^{ox} in frozen acetonitrile solution. The dashed line represents the best fit based on the structural parameters described in the text. Inset: raw EXAFS data for the same compounds.

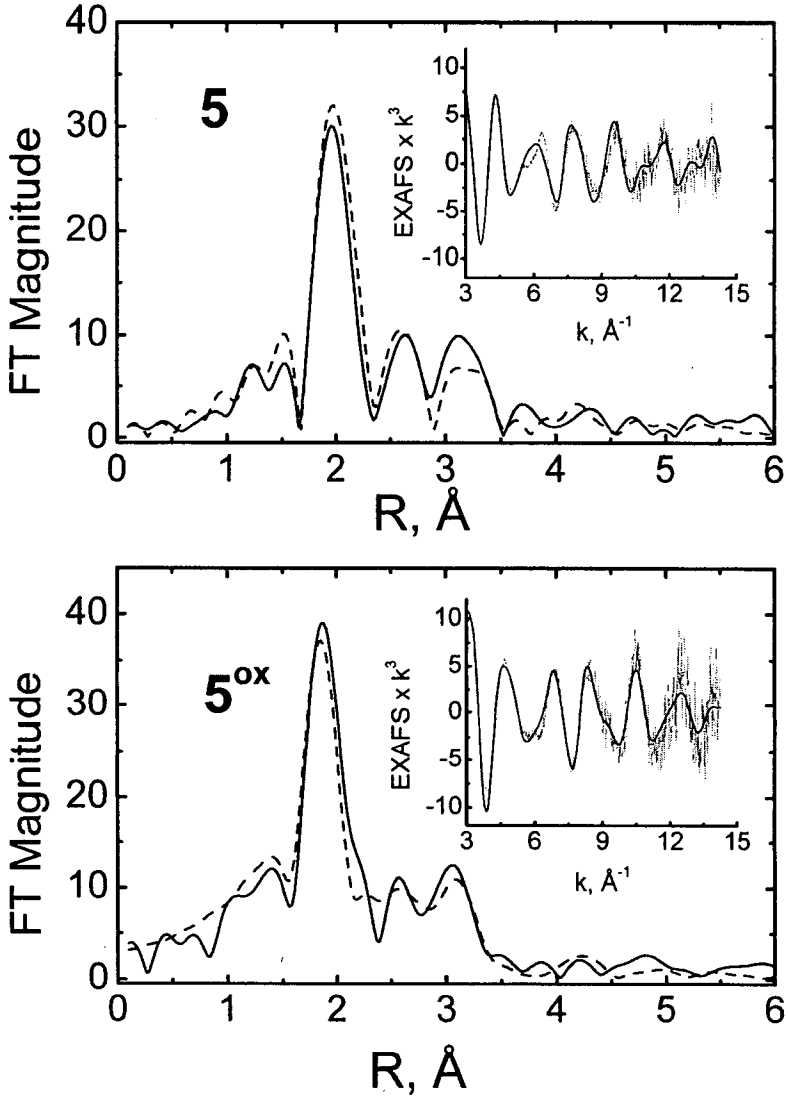

Figure S4. Fourier transform of the EXAFS data for **5** and **5**^{ox} in frozen acetonitrile solution. The dashed line represents the best fit based on the structural parameters described in the text. Inset: raw EXAFS data for the same compounds.

Table 1. Crystal data and structure refinement for 4

Identification code	ST3629
Empirical formula	C_{22} H_{37} B F_6 Fe_2 N_9 O_5 P 0.5 MeCN, 0.25 Et_2O
Formula weight	814.14
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Fdd2 No. 43
Unit cell dimensions	a = 32.721(4) Å alpha = 90 deg. b = 49.518(5) Å beta = 90 deg. c = 8.6090(8) Å gamma = 90 deg.
Volume	13949(3) Å^3
Z	16
Density (calculated)	1.551 Mg/m^3
Absorption coefficient	0.959 mm^-1
F(000)	6712
Crystal size	0.46 x 0.21 x 0.14 mm
Theta range for data collection	1.49 to 34.11 deg.
Index ranges	-51<=h<=47, -76<=k<=58, -13<=l<=11
Reflections collected	38686
Independent reflections	12034 [R(int) = 0.0492]
Absorption correction	SADABS, G.M. Sheldrick 1994
Max. and min. transmission	0.862 and 0.611
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12012 / 1 / 506
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0541, wR2 = 0.1063
R indices (all data)	R1 = 0.0859, wR2 = 0.1165
Absolute structure parameter	0.033(13)
Largest diff. peak and hole	1.086 and -1.121 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	3971(1)	753(1)	9034(1)	20(1)
Fe(2)	3079(1)	667(1)	7817(1)	15(1)
B(1)	2341(1)	466(1)	5512(4)	20(1)
O(1)	3623(1)	656(1)	7527(2)	19(1)
O(2)	3736(1)	532(1)	10786(3)	30(1)
O(3)	3079(1)	502(1)	10023(2)	20(1)
O(4)	3693(1)	1100(1)	9684(3)	24(1)
O(5)	3055(1)	1050(1)	8761(3)	21(1)
N(1)	4467(1)	864(1)	10755(4)	28(1)
N(2)	4392(1)	984(1)	7559(4)	30(1)
N(3)	4428(1)	437(1)	8561(3)	26(1)
C(1)	4721(1)	1075(1)	10064(5)	45(1)
C(2)	4616(2)	1174(1)	8636(8)	108(3)
C(3)	4671(2)	798(1)	6837(8)	91(3)
C(4)	4616(2)	517(1)	7090(6)	54(1)
C(5)	4731(2)	432(1)	9848(6)	62(2)
C(6)	4696(2)	617(1)	11031(8)	94(3)
C(7)	4295(1)	960(1)	12237(5)	48(1)
C(8)	4165(1)	1149(1)	6436(4)	29(1)
C(9)	4235(1)	171(1)	8373(7)	54(1)
N(11)	2597(1)	691(1)	4754(3)	22(1)
N(12)	2915(1)	810(1)	5534(3)	20(1)
C(13)	3072(1)	995(1)	4579(4)	26(1)
C(14)	2859(1)	995(1)	3177(4)	36(1)
C(15)	2565(1)	802(1)	3339(4)	31(1)
N(16)	2161(1)	580(1)	7015(3)	20(1)
N(17)	2413(1)	682(1)	8117(3)	19(1)
C(18)	2174(1)	782(1)	9239(4)	22(1)
C(19)	1762(1)	743(1)	8874(4)	27(1)
C(20)	1767(1)	615(1)	7450(4)	25(1)
N(21)	2633(1)	231(1)	5928(3)	20(1)
N(22)	2951(1)	275(1)	6915(3)	19(1)
C(23)	3153(1)	41(1)	7030(4)	22(1)
C(24)	2968(1)	-155(1)	6127(4)	26(1)
C(25)	2639(1)	-26(1)	5427(4)	24(1)
C(26)	3369(1)	453(1)	10948(4)	20(1)
C(27)	3279(1)	288(1)	12369(4)	32(1)
C(28)	3334(1)	1183(1)	9422(3)	19(1)
C(29)	3239(1)	1466(1)	9955(4)	25(1)
P(1)	5975(1)	664(1)	7858(1)	37(1)
F(11)	5706(2)	482(1)	8849(8)	56(2)
F(12)	5629(2)	706(2)	6578(7)	64(2)
F(13)	6226(2)	908(1)	6898(7)	53(1)
F(14)	6313(2)	700(2)	9142(7)	55(2)
F(11X)	6011(3)	453(1)	9320(8)	88(3)
F(12X)	5554(1)	503(1)	7393(8)	54(2)
F(13X)	5946(3)	823(1)	6340(8)	78(2)
F(14X)	6405(2)	767(2)	8117(17)	117(4)
F(15)	5743(1)	902(1)	8761(3)	59(1)
F(16)	6193(1)	428(1)	6928(4)	66(1)
O(30)	5000	0	13130(10)	46(2)
C(30)	5331(5)	91(4)	13932(18)	91(5)
C(31)	5659(4)	216(3)	13106(18)	66(4)

C(41)	5747(7)	310(3)	13552(21)	94(7)
C(40)	5605(5)	36(3)	13672(13)	64(3)
N(40)	4506(6)	181(3)	13735(13)	131(6)

Table 3. Bond lengths [Å] and angles [deg] for 4.

Fe(1)-O(1)	1.790(2)
Fe(1)-O(2)	2.015(2)
Fe(1)-O(4)	2.022(2)
Fe(1)-N(2)	2.196(3)
Fe(1)-N(3)	2.203(3)
Fe(1)-N(1)	2.266(3)
Fe(2)-O(1)	1.799(2)
Fe(2)-O(5)	2.065(2)
Fe(2)-O(3)	2.068(2)
Fe(2)-N(22)	2.130(2)
Fe(2)-N(12)	2.157(3)
Fe(2)-N(17)	2.195(2)
B(1)-N(16)	1.529(4)
B(1)-N(11)	1.539(4)
B(1)-N(21)	1.547(4)
O(2)-C(26)	1.271(4)
O(3)-C(26)	1.261(4)
O(4)-C(28)	1.265(4)
O(5)-C(28)	1.264(3)
N(1)-C(6)	1.456(5)
N(1)-C(1)	1.462(5)
N(1)-C(7)	1.473(5)
N(2)-C(3)	1.437(5)
N(2)-C(8)	1.466(4)
N(2)-C(2)	1.510(6)
N(3)-C(4)	1.463(5)
N(3)-C(9)	1.470(5)
N(3)-C(5)	1.487(5)
C(1)-C(2)	1.366(7)
C(3)-C(4)	1.420(7)
C(5)-C(6)	1.375(7)
N(11)-C(15)	1.340(4)
N(11)-N(12)	1.371(4)
N(12)-C(13)	1.334(4)
C(13)-C(14)	1.393(5)
C(14)-C(15)	1.364(5)
N(16)-C(20)	1.353(4)
N(16)-N(17)	1.356(3)
N(17)-C(18)	1.336(4)
C(18)-C(19)	1.399(4)
C(19)-C(20)	1.379(5)
N(21)-C(25)	1.344(4)
N(21)-N(22)	1.361(3)
N(22)-C(23)	1.340(4)
C(23)-C(24)	1.382(4)
C(24)-C(25)	1.391(5)
C(26)-C(27)	1.500(4)
C(28)-C(29)	1.505(4)
P(1)-F(14X)	1.516(7)
P(1)-F(11)	1.520(5)
P(1)-F(13X)	1.528(6)
P(1)-F(14)	1.575(6)
P(1)-F(16)	1.588(3)
P(1)-F(12)	1.592(6)
P(1)-F(15)	1.603(3)
P(1)-F(11X)	1.639(6)
P(1)-F(12X)	1.639(5)
P(1)-F(13)	1.680(6)
O(30)-C(30)#1	1.360(14)

O(30)-C(30)	1.360(14)
C(30)-C(31)	1.43(2)
C(41)-C(40)	1.44(2)
C(40)-N(40)#1	1.14(2)
N(40)-C(40)#1	1.14(2)
O(1)-Fe(1)-O(2)	98.93(9)
O(1)-Fe(1)-O(4)	98.21(9)
O(2)-Fe(1)-O(4)	94.81(10)
O(1)-Fe(1)-N(2)	96.83(10)
O(2)-Fe(1)-N(2)	162.69(10)
O(4)-Fe(1)-N(2)	89.94(10)
O(1)-Fe(1)-N(3)	96.18(10)
O(2)-Fe(1)-N(3)	90.64(10)
O(4)-Fe(1)-N(3)	163.62(9)
N(2)-Fe(1)-N(3)	80.59(10)
O(1)-Fe(1)-N(1)	173.67(10)
O(2)-Fe(1)-N(1)	85.16(10)
O(4)-Fe(1)-N(1)	86.20(10)
N(2)-Fe(1)-N(1)	78.55(11)
N(3)-Fe(1)-N(1)	78.88(10)
O(1)-Fe(2)-O(5)	96.75(8)
O(1)-Fe(2)-O(3)	96.63(9)
O(5)-Fe(2)-O(3)	90.13(8)
O(1)-Fe(2)-N(22)	96.81(9)
O(5)-Fe(2)-N(22)	166.44(9)
O(3)-Fe(2)-N(22)	88.57(9)
O(1)-Fe(2)-N(12)	97.39(10)
O(5)-Fe(2)-N(12)	92.69(9)
O(3)-Fe(2)-N(12)	165.27(9)
N(22)-Fe(2)-N(12)	85.31(10)
O(1)-Fe(2)-N(17)	178.70(10)
O(5)-Fe(2)-N(17)	83.33(8)
O(3)-Fe(2)-N(17)	84.67(8)
N(22)-Fe(2)-N(17)	83.11(9)
N(12)-Fe(2)-N(17)	81.30(9)
N(16)-B(1)-N(11)	107.6(2)
N(16)-B(1)-N(21)	108.6(2)
N(11)-B(1)-N(21)	107.7(2)
Fe(1)-O(1)-Fe(2)	121.39(12)
C(26)-O(2)-Fe(1)	127.5(2)
C(26)-O(3)-Fe(2)	131.0(2)
C(28)-O(4)-Fe(1)	130.1(2)
C(28)-O(5)-Fe(2)	129.1(2)
C(6)-N(1)-C(1)	112.0(4)
C(6)-N(1)-C(7)	109.0(4)
C(1)-N(1)-C(7)	109.9(3)
C(6)-N(1)-Fe(1)	105.7(2)
C(1)-N(1)-Fe(1)	108.4(2)
C(7)-N(1)-Fe(1)	111.7(2)
C(3)-N(2)-C(8)	113.1(4)
C(3)-N(2)-C(2)	110.8(5)
C(8)-N(2)-C(2)	107.8(3)
C(3)-N(2)-Fe(1)	108.4(3)
C(8)-N(2)-Fe(1)	110.6(2)
C(2)-N(2)-Fe(1)	105.8(3)
C(4)-N(3)-C(9)	109.2(3)
C(4)-N(3)-C(5)	111.6(4)
C(9)-N(3)-C(5)	110.6(4)
C(4)-N(3)-Fe(1)	104.7(3)
C(9)-N(3)-Fe(1)	111.5(2)
C(5)-N(3)-Fe(1)	109.1(2)
C(2)-C(1)-N(1)	118.5(4)

C(1)-C(2)-N(2)	117.0(4)
C(4)-C(3)-N(2)	118.8(4)
C(3)-C(4)-N(3)	116.8(4)
C(6)-C(5)-N(3)	119.0(3)
C(5)-C(6)-N(1)	118.9(4)
C(15)-N(11)-N(12)	109.2(3)
C(15)-N(11)-B(1)	129.7(3)
N(12)-N(11)-B(1)	121.1(2)
C(13)-N(12)-N(11)	106.6(3)
C(13)-N(12)-Fe(2)	133.8(2)
N(11)-N(12)-Fe(2)	119.6(2)
N(12)-C(13)-C(14)	109.9(3)
C(15)-C(14)-C(13)	105.4(3)
N(11)-C(15)-C(14)	108.9(3)
C(20)-N(16)-N(17)	109.8(3)
C(20)-N(16)-B(1)	130.4(3)
N(17)-N(16)-B(1)	119.7(2)
C(18)-N(17)-N(16)	106.7(2)
C(18)-N(17)-Fe(2)	132.7(2)
N(16)-N(17)-Fe(2)	120.6(2)
N(17)-C(18)-C(19)	110.5(3)
C(20)-C(19)-C(18)	104.6(3)
N(16)-C(20)-C(19)	108.4(3)
C(25)-N(21)-N(22)	109.8(2)
C(25)-N(21)-B(1)	130.3(3)
N(22)-N(21)-B(1)	119.8(2)
C(23)-N(22)-N(21)	106.6(2)
C(23)-N(22)-Fe(2)	131.7(2)
N(21)-N(22)-Fe(2)	121.5(2)
N(22)-C(23)-C(24)	110.6(3)
C(23)-C(24)-C(25)	104.9(3)
N(21)-C(25)-C(24)	108.1(3)
O(3)-C(26)-O(2)	125.6(3)
O(3)-C(26)-C(27)	118.2(3)
O(2)-C(26)-C(27)	116.2(3)
O(5)-C(28)-O(4)	125.6(3)
O(5)-C(28)-C(29)	118.3(3)
O(4)-C(28)-C(29)	116.2(3)
F(14X)-P(1)-F(13X)	90.5(6)
F(11)-P(1)-F(14)	94.7(4)
F(14X)-P(1)-F(16)	84.5(4)
F(11)-P(1)-F(16)	96.2(2)
F(13X)-P(1)-F(16)	88.6(3)
F(14)-P(1)-F(16)	96.9(3)
F(11)-P(1)-F(12)	93.1(4)
F(14)-P(1)-F(12)	165.9(4)
F(16)-P(1)-F(12)	93.9(2)
F(14X)-P(1)-F(15)	96.8(4)
F(11)-P(1)-F(15)	83.7(2)
F(13X)-P(1)-F(15)	90.4(2)
F(14)-P(1)-F(15)	84.7(3)
F(16)-P(1)-F(15)	178.3(2)
F(12)-P(1)-F(15)	84.5(2)
F(14X)-P(1)-F(11X)	92.0(6)
F(13X)-P(1)-F(11X)	171.3(4)
F(16)-P(1)-F(11X)	83.4(3)
F(15)-P(1)-F(11X)	97.5(3)
F(14X)-P(1)-F(12X)	168.7(4)
F(13X)-P(1)-F(12X)	89.3(5)
F(16)-P(1)-F(12X)	84.2(2)
F(15)-P(1)-F(12X)	94.5(2)
F(11X)-P(1)-F(12X)	86.6(4)
F(11)-P(1)-F(13)	170.2(3)

© 2003 American Chemical Society, J. Am. Chem. Soc., Slep ja030377f Supporting Info Page 12

F(14)-P(1)-F(13)	85.3(4)
F(16)-P(1)-F(13)	93.5(2)
F(12)-P(1)-F(13)	85.0(4)
F(15)-P(1)-F(13)	86.6(2)
C(30)#1-O(30)-C(30)	119(2)
O(30)-C(30)-C(31)	119.3(13)
N(40)#1-C(40)-C(41)	178.6(14)

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

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 4.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1)	14(1)	20(1)	25(1)	2(1)	-2(1)	-2(1)
Fe(2)	13(1)	16(1)	17(1)	-1(1)	-1(1)	-1(1)
B(1)	18(1)	23(2)	18(2)	-3(1)	-2(1)	-1(1)
O(1)	13(1)	21(1)	23(1)	-2(1)	-1(1)	-3(1)
O(2)	19(1)	40(1)	31(1)	10(1)	-5(1)	-6(1)
O(3)	18(1)	25(1)	17(1)	3(1)	0(1)	-1(1)
O(4)	17(1)	27(1)	29(1)	-5(1)	-4(1)	1(1)
O(5)	17(1)	19(1)	27(1)	-3(1)	-3(1)	-3(1)
N(1)	20(1)	31(1)	34(2)	0(1)	-8(1)	-1(1)
N(2)	19(1)	33(1)	38(2)	12(1)	-1(1)	1(1)
N(3)	16(1)	23(1)	39(2)	-2(1)	-5(1)	0(1)
C(1)	48(2)	45(2)	42(2)	-25(2)	18(2)	-28(2)
C(2)	112(5)	111(5)	102(5)	71(4)	-80(4)	-100(4)
C(3)	98(4)	80(4)	94(5)	46(3)	75(4)	53(3)
C(4)	87(3)	31(2)	45(3)	-18(2)	28(2)	-16(2)
C(5)	66(3)	72(3)	48(3)	-18(2)	-28(2)	52(3)
C(6)	115(5)	41(3)	127(6)	-30(3)	-100(5)	40(3)
C(7)	35(2)	87(3)	22(2)	3(2)	-7(2)	-24(2)
C(8)	28(2)	33(2)	26(2)	7(1)	0(1)	-4(1)
C(9)	25(2)	19(2)	119(5)	1(2)	6(2)	2(1)
N(11)	26(1)	22(1)	17(1)	-3(1)	-2(1)	3(1)
N(12)	20(1)	21(1)	19(1)	0(1)	0(1)	1(1)
C(13)	26(2)	26(2)	25(2)	4(1)	8(1)	-1(1)
C(14)	47(2)	38(2)	23(2)	11(1)	5(2)	-2(2)
C(15)	42(2)	35(2)	16(2)	1(1)	-6(1)	2(2)
N(16)	15(1)	21(1)	24(1)	1(1)	-3(1)	0(1)
N(17)	17(1)	20(1)	18(1)	1(1)	-2(1)	1(1)
C(18)	24(1)	23(1)	17(2)	6(1)	5(1)	3(1)
C(19)	20(1)	31(2)	30(2)	10(1)	9(1)	6(1)
C(20)	14(1)	28(2)	33(2)	7(1)	0(1)	0(1)
N(21)	20(1)	20(1)	21(1)	-2(1)	-2(1)	-4(1)
N(22)	15(1)	20(1)	23(1)	-1(1)	-1(1)	-3(1)
C(23)	19(1)	19(1)	29(2)	-2(1)	0(1)	0(1)
C(24)	24(2)	16(1)	39(2)	-5(1)	4(1)	-2(1)
C(25)	24(1)	23(1)	25(2)	-6(1)	1(1)	-7(1)
C(26)	22(1)	18(1)	20(1)	2(1)	-2(1)	-1(1)
C(27)	29(2)	43(2)	24(2)	12(1)	0(1)	-3(2)
C(28)	19(1)	21(1)	18(1)	1(1)	0(1)	-2(1)
C(29)	27(2)	19(1)	30(2)	-5(1)	-4(1)	0(1)
P(1)	22(1)	49(1)	39(1)	2(1)	3(1)	1(1)
F(11)	62(3)	33(3)	72(5)	2(3)	33(3)	-7(2)
F(12)	41(3)	107(5)	43(3)	-27(4)	-9(3)	13(3)
F(13)	57(3)	58(3)	45(3)	-5(3)	21(3)	-4(3)
F(14)	35(3)	85(5)	45(3)	-12(3)	-15(2)	19(3)
F(11X)	162(8)	49(3)	52(4)	12(3)	-45(5)	10(4)
F(12X)	24(2)	53(3)	86(5)	-23(3)	1(2)	7(2)
F(13X)	116(6)	62(4)	55(4)	30(3)	53(4)	46(4)
F(14X)	52(4)	44(4)	254(15)	-12(7)	-40(7)	-16(3)
F(15)	69(2)	68(2)	38(2)	-6(1)	13(1)	15(1)
F(16)	43(1)	53(2)	100(3)	-10(2)	25(2)	13(1)
O(30)	34(4)	61(5)	43(5)	0	0	-1(4)
C(30)	102(11)	123(13)	47(7)	-4(8)	-9(8)	-56(10)
C(31)	44(6)	82(11)	71(10)	19(8)	-7(6)	-3(7)

C(41)	159(17)	59(8)	62(10)	-2(6)	2(9)	-64(9)
C(40)	105(11)	60(7)	26(5)	-15(5)	3(6)	-14(8)
N(40)	261(20)	94(9)	37(6)	6(6)	-23(8)	-43(11)

© 2003 American Chemical Society, J. Am. Chem. Soc., Slep ja030377f Supporting Info Page 15

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 1.

	x	y	z	U(eq)
H(1)	2119(1)	404(1)	4796(4)	23
H(1A)	4727(1)	1230(1)	10797(5)	54
H(1B)	5003(1)	1005(1)	9992(5)	54
H(2A)	4869(2)	1233(1)	8108(8)	130
H(2B)	4443(2)	1335(1)	8792(8)	130
H(3A)	4660(2)	830(1)	5703(8)	109
H(3B)	4950(2)	846(1)	7185(8)	109
H(4A)	4887(2)	429(1)	7021(6)	65
H(4B)	4447(2)	445(1)	6233(6)	65
H(5A)	4722(2)	249(1)	10319(6)	75
H(5B)	5005(2)	454(1)	9383(6)	75
H(6A)	4975(2)	669(1)	11351(8)	113
H(6B)	4568(2)	524(1)	11927(8)	113
H(7A)	4128(8)	816(2)	12701(19)	72
H(7B)	4123(8)	1119(4)	12049(7)	72
H(7C)	4517(1)	1008(6)	12947(14)	72
H(8A)	3979(5)	1270(4)	6993(4)	43
H(8B)	4007(6)	1030(1)	5748(19)	43
H(8C)	4357(1)	1256(4)	5819(20)	43
H(9A)	4108(10)	116(3)	9355(14)	82
H(9B)	4444(2)	38(2)	8081(44)	82
H(9C)	4027(8)	180(2)	7559(30)	82
H(13)	3296(1)	1110(1)	4818(4)	31
H(14)	2908(1)	1106(1)	2297(4)	43
H(15)	2369(1)	754(1)	2574(4)	37
H(18)	2271(1)	867(1)	10157(4)	26
H(19)	1530(1)	793(1)	9472(4)	33
H(20)	1534(1)	561(1)	6872(4)	30
H(23)	3390(1)	13(1)	7646(4)	27
H(24)	3048(1)	-339(1)	6009(4)	32
H(25)	2451(1)	-105(1)	4719(4)	29
H(27A)	3383(7)	382(3)	13290(5)	48
H(27B)	3413(7)	112(2)	12278(14)	48
H(27C)	2984(1)	262(5)	12466(17)	48
H(29A)	3366(6)	1596(1)	9246(17)	38
H(29B)	3346(7)	1493(2)	11006(12)	38
H(29C)	2942(1)	1493(2)	9959(28)	38
H(30A)	5446(5)	-65(4)	14508(18)	109
H(30B)	5231(5)	222(4)	14715(18)	109
H(31A)	5873(4)	271(3)	13841(18)	99
H(31B)	5557(4)	376(3)	12559(18)	99
H(31C)	5773(4)	89(3)	12352(18)	99