Electronic Supplementary Material (ESI) for Chemical Communications

Supporting information for

Stepwise syntheses of tri- and tetraphosphaporphyrinogens.

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Experimental Section

All operations were performed using canula techniques on Schlenk lines under a dry nitrogen atmosphere or in a Braun Labmaster 130 drybox under dry purified argon. Potassium fluoride was dried by protracted heating under reduced pressure at 200°C, and 18C6 was crystallised from acetonitrile prior to use; **4**[24], **6**[39] and **7**[24] were prepared according to earlier protocols. Solvents were distilled under dry nitrogen: THF and ether from sodium benzophenoneketyl, pentane from sodium benzophenoneketyl/ tetraglyme, acetonitrile from calcium hydride, methanol from sodium methoxide and dichloromethane from P_4O_{10}. $(CD_3)_2SO$ and CD_3CN were used as received from SigmaAldrich. NMR measurements were made on a Bruker Avance 300 spectrometer and are referenced to internal $(CD_3)_2SO$ and CD_3CN and external H_3PO_4 as appropriate. Mass spectra were obtained from dichloromethane solutions on a Bruker electrospray MicroTOF spectrometer; infrared spectra were taken from KBr disks prepared under argon in a glovebox and measured on a Perkin Elmer System 2000 spectroscope.

9: A THF (30mL) solution of the 2,5-*bis*(chlorocarbonyl)phosphaferrocene **6** (1g, 2.34 mmol) was added dropwise over a period of three minutes to a well- stirred -78°C solution of **7** (2.48 g, 9.37 mmol) in THF (40 mL). The mixture was allowed to return to room temperature over 15 minutes, the solvent was removed under reduced pressure and the residue was washed with pentane (3x 15mL). The purity of the phospholide **8** can be established by ^{31}P NMR at this point [δ : 151.9 (d, J_{PP} = 52.8 Hz, 2P) ; -13.6 (t, J_{PP} = 52.8 Hz, 1P)]. The dianion was redissolved in THF (80mL), treated with a further THF (20mL) solution of 2,5-di(chlorocarbonyl)phosphaferrocene **6** (810 mg, 1.90 mmol) at room temperature and, after stirring for a further 30 minutes, the solvent was removed under reduced pressure. The product was purified by flash chromatography on neutral alumina; apolar impurities were removed by washing the column with pentane and the product was collected as a red band upon elution with ether. The crude red sample of **9** (1.19 g, 48%) is sufficiently pure for use directly in the synthesis of **10**. A sample for analysis was crystallized from acetone $C_{60}H_{84}Fe_2O_4P_4Si_2$ requires: C: 62.07%, H 7.29; found: C: 62.40%, H 7.42%. νIR (KBr) 1725 cm^{-1} ^{31}P NMR (CD_2Cl_2): 70.6 (d, J_{PP} = 100.2 Hz, 2P), 46.9 (s), -48.4 (t, J_{PP} = 100.2 Hz, 1P). ^{1}H NMR (CD_2Cl_2) : 2.22 (d, J_{PH} = 3.0 Hz, 6H, Me), 2.15 (d, J_{PH} = 2.0 Hz, 6H, Me), 2.10 (d, J_{PH} = 1,7 Hz, 6H, Me), 1.81 (s, 6H, Me), 1.68 (s, 15H, Cp*), 1.51 (s, 15H, Cp*), 0.99 (s, 18H, *t*-Bu), 0.35 (s, 6H, SiMe), 0.28 (s, 6H, SiMe). ^{13}C NMR (CD_2Cl_2) : 211.8 (dd, J_{PC} = 46.2 Hz, J_{PC} = 27.8 Hz, PCO), 198.6 (dd, J_{PC} = 19.5 Hz, J_{PC} = 15.6 Hz, CO), 162.4 (d, J_{PC} = 3.3 Hz, PC<u>C</u>Me), 152.1 (d, J_{PC} = 12.1 Hz, PC<u>C</u>Me), 146.6 (d, J_{PC} = 16.7 Hz, P<u>C</u>CO), 137.4 (dd, J_{PC} = 38.9 Hz, J_{PC} = 5.8 Hz, P<u>C</u>Si), 102.9 (dd, J_{PC} = 62.6 Hz, J_{PC} = 4.8 Hz, PC), 101.9 (m, PC<u>C</u>Me), 101.4 (d, J_{PC} = 64.4 Hz, PC), 90.4 (dd, J_{PC} = 5.5 Hz, J_{PC} = 1.5 Hz, PC<u>C</u>Me), 85.6 (Cp*), 85.5 (Cp*), 28.0 (Me *t*-Bu), 20.6 (d, J_{PC} = 4.3 Hz, Me), 19.3 (Si<u>C</u>(Me)$_3$), 16.3 (d, J_{PC} = 0.9 Hz, Me), 16.0 (d, J_{PC} = 17.4 Hz, Me), 12.0 (d, J_{PC} = 6.2 Hz, Me), 10.3 (Me du Cp*), 10.2 (Me Cp*), -2.1 (d, J_{PC} = 5.6 Hz, SiMe), -3.0 (d, J_{PC} = 7.5 Hz, SiMe)ppm.

10. KF (48mg, 0.80 mmol) and 18C6 (210 mg, 0.80 mmol) were added to a toluene (10mL) solution of **9** (260 mg, 0.22 mmol) and the mixture was heated at 100°C for 4h. The solution was cooled and filtered through a frit, and the crude orange- red precipitate of **7** was collected, extracted with acetonitrile (2 x 10mL) and dried (180 mg, 53%). Monocrystals suitable for the Xray diffraction study were obtained from saturated acetonitrile solution of **10** at -30°C. νIR$_{(CO)}$ (KBr) 1620, 1637 cm^{-1}. ^{31}P NMR (CD_3CN): 213.1 (t, J_{PP} = 131.2 Hz), -55.8 (t, J_{PP} = 131.0 Hz). ^{1}H NMR (CD_3CN): 3.54 (s, 48H, 2 18C6), 2.29 (s, 12H, 4 Me), 1.98 (s, 12H, 4 Me), 1.87 (s, 30H, 2 Cp*). ^{13}C NMR (CD_3CN): 196.2 (m, CO), 153.3 (m, PC), 133.1 (PC<u>C</u>Me), 101.1 (dt, J_{CP} = 65.5 Hz, J_{CP} = 7.5 Hz), 92.8 (d, J_{CP} = 2.2 Hz, PC<u>C</u>Me), 83.2 (Cp*), 70.9 (CH_2 18C6), 15.1 (Me), 12.1 (Me), 11.1 (Me Cp*).

11: A THF (10mL) solution of 2,6-*bis*(chlorocarbonyl)pyridine (231.0 mg, 1.13 mmol) was added dropwise over a period of thirty seconds to a well- stirred room temperature solution of **8** (1 g, 1.13

mmol) in THF (10 mL). The mixture was stirred at room temperature for 15 minutes, the solvent was removed under reduced pressure and the residue was washed with pentane (3x 15mL). After filtration through an alumina plug, a red band was collected from which the solvents were removed. The product (467 mg, 44 %) was dissolved in toluene (40 mL), KF (116 mg, 1.9 mmol) and 18C6 (525 mg, 1.9 mmol) were added and the mixture was heated at 100°C for 18h. The solution was cooled and filtered through a frit, and the crude red precipitate of **11** was collected and extracted into acetonitrile (3 x 10mL). Concentration to 2mL gave the product. (342 mg, 49%). Monocrystals suitable for the Xray diffraction study were obtained from saturated acetonitrile solution of **11** at -30°C. $\nu IR_{(CO)}$ (KBr) 1645, 1634 cm^{-1} ^{31}P NMR (CD_3CN) : 217.7 (d, J_{PP} = 113.0 Hz), -25.6 (t, J_{PP} = 113.3 Hz). ^{1}H NMR (CD_3CN): 7.58 (t, J_{HH} = 7.8 Hz, 1H), 7.27 (d, J_{HH} = 7.8 Hz, 2H), 3.54 (s, 70H, 3 18C6), 2.41 (s, 6H, 2 Me), 2.28 (s, 6H, 2 Me), 2.19 (s, 6H, 2 Me), 1.76 (s, 15H, Cp*). ^{13}C NMR (CD_3CN): 198.4, 194.1, 163.9, 161.1, 141.8, 135.4, 134.1, 133.7, 122.5, 100.9, (d J_{CP} = 57.8 Hz), 96.4, (d J_{CP} = 8.3 Hz), 83.4, 71.4, (18C6) 15.8, 14.6, 12.1, 11.1 ppm.

Crystal data: Data were collected on a Nonius Kappa CCD diffractometer at 150(1) K using an Mo K_α (λ = 0.71073 Å) source and graphite monochromator. Structures were solved in SIR 97 and refined in SHELXL-97 by full-matrix least-squares using anisotropic thermal displacement parameters for all non-hydrogen atoms.

9: $C_{60}H_{84}Fe_2O_4P_4Si_2$, M = 580.52 orthorhombic, space group: $Pca2_1$, a =23.209(1), b = 25.099(1), c = 20.610(1) Å. U = 12005.8(9) $Å^3$. Z = 16, D_c = 1.285gcm^{-3}, F(000) =4928, μ = 0.674 cm^{-1}. Of 25709 unique reflections from a red plate of 0.18 x 0.16 x 0.06 mm over h = -30 to 25; k = -32 to 30; l = -26 to 19, 16505 having $I > 2\sigma(I)$ were refined. wR_2 = 0.1730, R_1 = 0.0566, GoF = 1.036.

10: $C_{48}H_{54}Fe_2O_4P_4.2(C_{16}H_{30}KN_2O_6).2(C_2H_3N)$, M = 1146.66 triclinic, space group: P-1, a =13.995(1), b = 14.050(1), c = 14.447(1)Å α=108.305, β = 106.230(1), γ = 109.092(1)°. U = 2305.8(3) $Å^3$. Z = 1, D_c = 1.285gcm^{-3}, F(000) = 944, μ = 0.538 cm^{-1}. Of 13331 unique reflections from a red block of 0.40 x 0.30 x 0.26 mm over h = -19 to 17; k = -19 to 19; l = -19 to 20, 10339 having $I > 2\sigma(I)$ were refined. wR_2 = 0.0999, R_1 = 0.0358, GoF = 1.059.

11: $C_{61}H_{84}FeK_2NO_{16}P_3,C_2H_3N$ M = 1355.31 monoclinic, space group: $P2_1/c$, a =17.606(1), b = 16.733(1), c = 27.421(1) Å, β = 125.457(2)°. U = 6580.2(6) $Å^3$. Z = 4, D_c = 1.368gcm^{-3}, F(000) = 2864, μ = 0.496 cm^{-1}. Of 11464 unique reflections from a red block of 0.22 x 0.18 x 0.02 mm over h = -20 to 19; k = -19 to 19; l = -31 to 32; 8811 were refined. wR_2 =0.165, R_1 =0.097, GoF=1.209.

Reference:

[39] D Carmichael, E Muller, XF le Goff, *Organometallics*, om-2011-00658k under submission.

Computational methods

We use a well established methodology, the GGA density functional BP86,[1,2,3] to optimise all of our geometries. These geometry optimization calculations were accelerated using the Multipole Accelerated Resolution of Identity for J (MARI-J) approximation method,[4] as implemented in Turbomole v6.1.[5] Basis sets of split valence quality, labelled def2-SVP,[6,7] and the associated auxiliary basis sets to fit Coulomb potentials,[8] were employed in the geometry optimization for all atoms.

Reed and Weinhold's NBO analysis[9,10],[11], which gives molecular charge distribution in terms of natural population analysis, as well as the NICS calculations[12] at the center of the phospholyl ring were conducted with Gaussian 09[13] at the B3LYP level using the 6-31++G(d,p) basis set all atoms.

Bibliography

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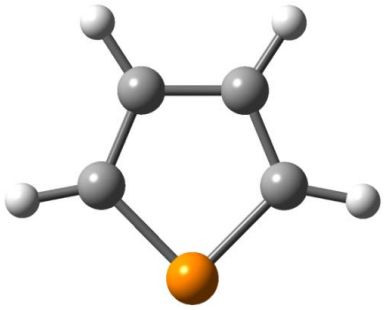
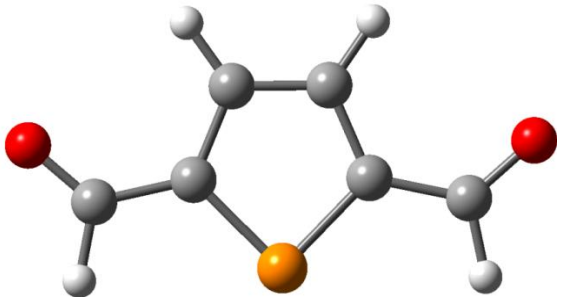
Cartesian coordinated of the located minima

- Structure and cartesian coordinates of **C**



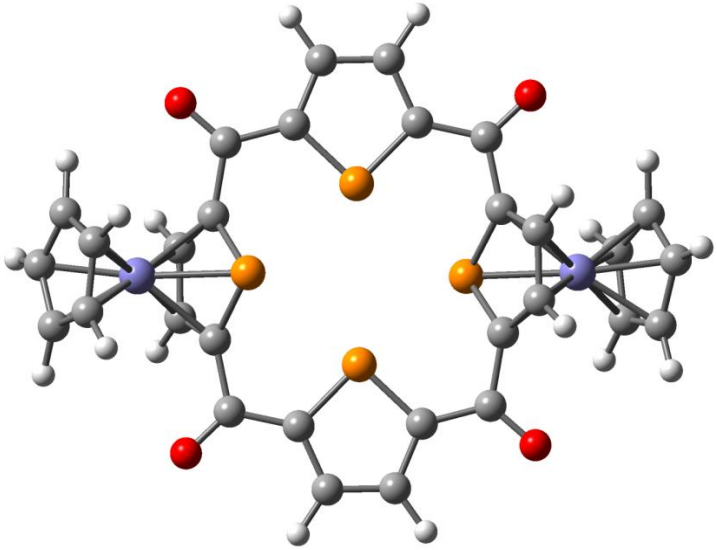
H	16.3243333	13.8216582	-1.6212699
C	15.8183743	13.6352696	-0.6574199
P	14.6132183	12.3503725	-0.3925301
C	14.4483019	12.8650509	1.3050450
H	13.7723104	12.3859610	2.0352988
C	16.0571132	14.3942236	0.5046962
C	15.2801528	13.9578712	1.6170934
H	16.7689280	15.2401882	0.5579468
H	15.3309370	14.4331992	2.6153729

- Structure and cartesian coordinates of **B**



C	16.2717153	13.8349873	-1.6183325
O	17.1073083	14.7069884	-1.8929143
C	15.6449559	13.5950662	-0.3328601
P	14.4517249	12.2980128	-0.0666195
C	14.3108430	12.7947870	1.6393089
C	13.4303628	12.1317874	2.5815932
O	13.2672473	12.4101655	3.7772565
C	15.8976818	14.3528225	0.8582563
C	15.1577750	13.9094593	1.9516599
H	15.9225285	13.1158930	-2.4309387
H	12.8471280	11.2670323	2.1213369
H	16.6089781	15.1944892	0.8723911
H	15.1948090	14.3459302	2.9628296

- Structure and cartesian coordinates of **A**



Fe	9.5585078	9.2700429	3.7074028
Fe	11.8405244	17.8773019	5.6509362
P	9.8925702	14.1466897	3.1017248
P	11.4059333	13.0201248	6.3250361
P	9.5510844	11.4736862	4.5001449
P	11.7732089	15.6554898	4.9148939
O	8.7499109	11.2175763	0.5941325
O	11.7754188	9.0398787	6.7731721
O	9.6489414	18.1290257	2.5948540
C	9.5898530	15.7361532	2.3626729
C	8.9739803	15.5876244	1.0734275
C	8.7670118	14.2541910	0.7024162
C	9.2069068	13.3085959	1.6903296
C	9.1833690	11.8453907	1.5807314
C	9.8521129	11.1234463	2.7441072
C	10.9388323	10.2070204	2.5501059
C	11.5278249	9.7683820	3.7842405
C	10.9063427	10.3492797	4.9390071
C	11.4827798	10.1702131	6.3380029
C	11.7620145	11.4301754	7.0389449
C	12.4114864	11.5803484	8.3111427
C	12.6040335	12.9146499	8.6879568
C	12.1242783	13.8600298	7.7193139
C	12.1374929	15.3241191	7.8354203
C	11.4893363	16.0495913	6.6635739
C	10.4402654	17.0113408	6.8432109
C	9.8569104	17.4412452	5.6030763
C	10.4542226	16.8175762	4.4578479
C	9.8960052	16.9954447	3.0522874
C	8.3455624	8.1196755	4.8841699

C	7.5903286	8.7176307	3.8116779
C	8.1747408	8.2957536	2.5630980
C	9.2827021	7.4238067	2.8665737
C	9.3935029	7.3190918	4.3005574
C	12.9560918	19.1374214	6.8121431
C	13.7977819	18.4202885	5.8865992
C	13.3474447	18.7186313	4.5500809
C	12.2236915	19.6167652	4.6465052
C	11.9882207	19.8814150	6.0441816
O	12.5496000	15.9503099	8.8312965
H	9.9506675	6.9551870	2.1309765
H	10.1672610	6.7797216	4.8614257
H	7.8902866	8.6610636	1.5678711
H	6.7490625	9.4127727	3.9259406
H	8.1831736	8.2777592	5.9577163
H	12.3685952	9.0613751	3.8568946
H	11.2669012	9.8767061	1.5525380
H	12.7244531	10.7112716	8.9139289
H	13.0812366	13.2339726	9.6296841
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H	8.6993315	16.4571383	0.4528882
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H	14.6082205	17.7324805	6.1584081
H	13.0115875	19.0661028	7.9055662
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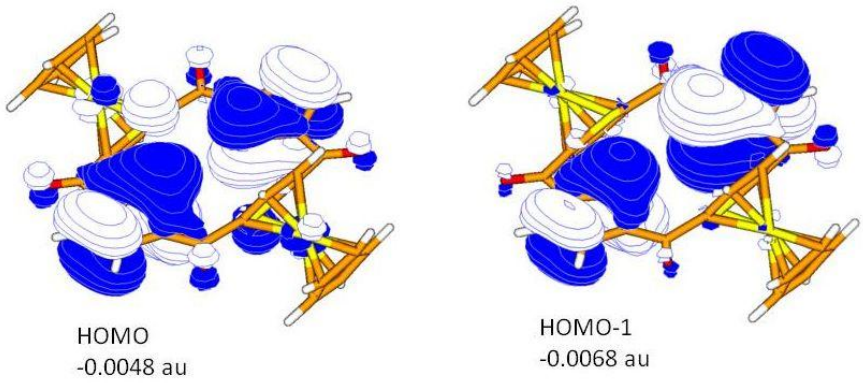

B3LYP/6-31++G(d,p)//marij-BP86/def2-SVP determined HOMO (left) and HOMO-1 (right) orbitals for macrocycle A.

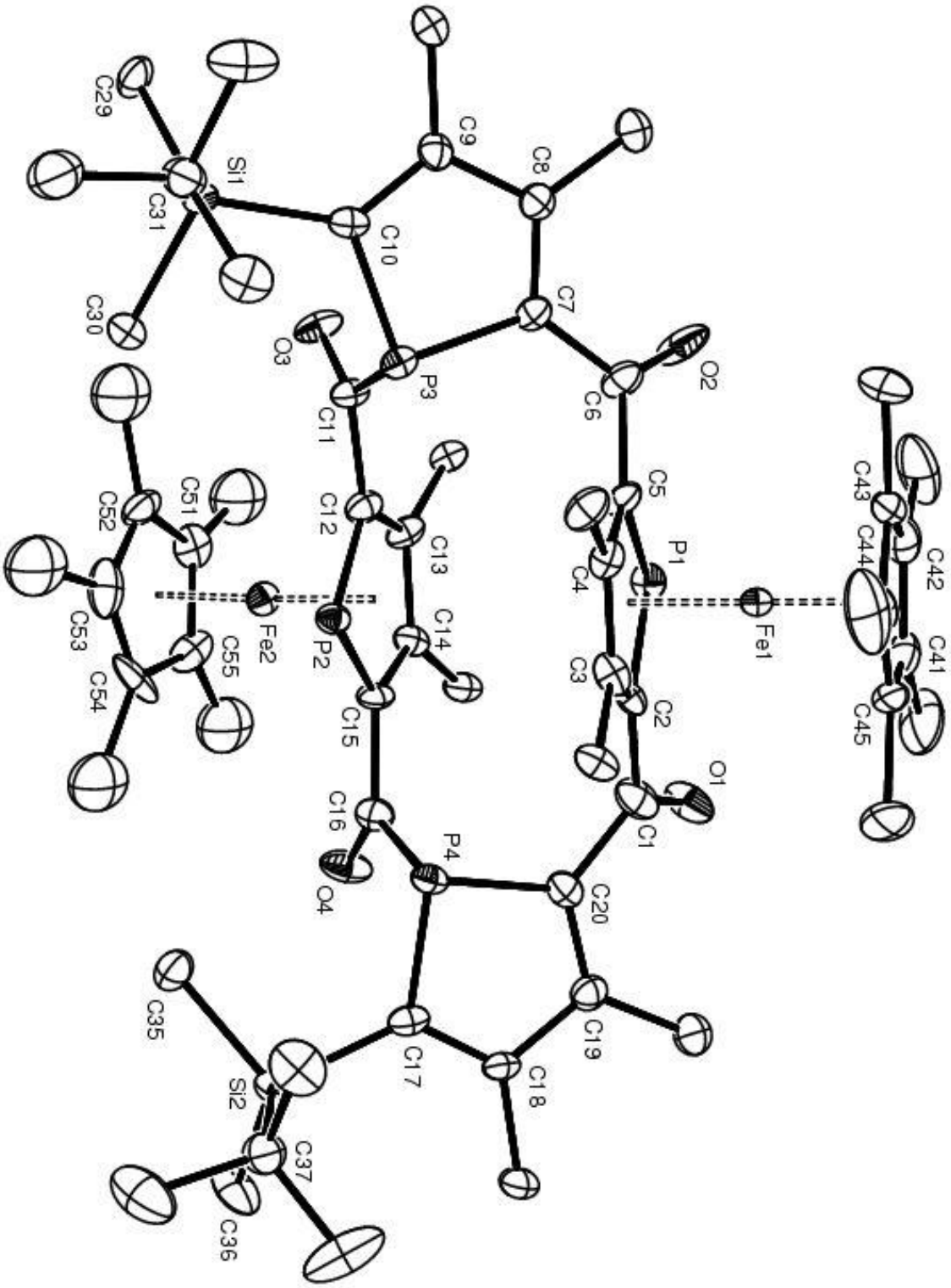

Table 1. Crystal data for **9**

Compound	em463
Molecular formula	$C_{60}H_{84}Fe_2O_4P_4Si_2$
Molecular weight	580.52
Crystal habit	Red Plate
Crystal dimensions(mm)	0.18x0.16x0.06
Crystal system	orthorhombic
Space group	$Pca2_1$
a(Å)	23.209(1)
b(Å)	25.099(1)
c(Å)	20.610(1)
α(°)	90.00
β(°)	90.00
γ(°)	90.00
V(Å^3)	12005.8(9)
Z	16
d(g-cm^{-3})	1.285
F(000)	4928
μ(cm^{-1})	0.674
Absorption corrections	multi-scan ; 0.8883 min, 0.9607 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150(1)
Scan mode	phi and omega scans
Maximum θ	27.46
HKL ranges	-30 25 ; -32 30 ; -26 19
Reflections measured	90852
Unique data	25709
Rint	0.0408
Reflections used	16505
Criterion	I > 2σ(I)
Refinement type	Fsqd
Hydrogen atoms	constr
Parameters refined	1331
Reflections / parameter	12
wR2	0.1730
R1	0.0566
Flack's parameter	0.0(4)
Weights a, b	0.0974 ; 1.0595
GoF	1.036
difference peak / hole (e Å^{-3})	0.164(0.024) / -0.115(0.024)

Table 2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **9**

atom	x	y	z	U(eq)
Fe(1)	-12260(1)	-5034(1)	1903(1)	25(1)
Fe(2)	-10221(1)	-5045(1)	-522(1)	30(1)
P(1)	-12057(1)	-5061(1)	832(1)	32(1)
P(2)	-10288(1)	-5046(1)	606(1)	28(1)
P(3)	-10598(1)	-6324(1)	1146(1)	31(1)
P(4)	-10561(1)	-3761(1)	1138(1)	31(1)
Si(1)	-9604(1)	-7192(1)	1080(1)	29(1)
Si(2)	-9603(1)	-2843(1)	1106(1)	32(1)
O(1)	-12234(2)	-3885(2)	791(2)	51(1)
O(2)	-12308(2)	-6247(2)	926(3)	64(2)
O(3)	-10566(3)	-6447(2)	-181(3)	43(1)
O(4)	-10490(3)	-3635(2)	-189(3)	50(1)
C(1)	-11806(4)	-4002(3)	1100(4)	47(2)
C(2)	-11723(3)	-4555(3)	1322(4)	29(2)
C(3)	-11415(3)	-4774(3)	1881(4)	35(2)
C(4)	-11421(3)	-5337(3)	1898(4)	32(2)
C(5)	-11746(3)	-5553(3)	1349(4)	32(2)
C(6)	-11851(3)	-6126(3)	1166(4)	39(2)
C(7)	-11364(3)	-6497(3)	1177(4)	31(2)
C(8)	-11413(3)	-7040(3)	1210(4)	32(2)
C(9)	-10869(3)	-7322(3)	1191(4)	32(2)
C(10)	-10387(4)	-7017(3)	1113(4)	32(2)
C(11)	-10584(3)	-6128(3)	261(4)	33(2)
C(12)	-10655(4)	-5533(3)	136(4)	33(2)
C(13)	-11040(3)	-5324(3)	-348(3)	32(2)
C(14)	-11028(3)	-4751(3)	-346(4)	31(2)
C(15)	-10640(3)	-4558(3)	138(4)	30(2)
C(16)	-10546(3)	-3967(3)	258(4)	36(2)
C(17)	-10383(4)	-3067(3)	1137(4)	34(2)
C(18)	-10860(4)	-2779(3)	1239(4)	31(2)
C(19)	-11402(3)	-3075(3)	1229(4)	36(2)
C(20)	-11323(3)	-3609(3)	1167(4)	36(2)
C(21)	-11112(3)	-4442(3)	2388(4)	37(2)
C(22)	-11140(4)	-5649(3)	2414(4)	41(2)
C(23)	-11964(3)	-7346(3)	1284(5)	46(2)
C(24)	-10876(3)	-7919(3)	1232(5)	45(2)
C(25)	-11459(4)	-5655(3)	-730(4)	36(2)
C(26)	-11443(4)	-4410(3)	-725(4)	39(2)
C(27)	-10890(4)	-2185(2)	1314(5)	47(2)
C(28)	-11969(4)	-2788(3)	1304(5)	50(2)
C(29)	-9448(3)	-7778(3)	541(4)	42(2)
C(30)	-9242(4)	-6577(3)	732(4)	39(2)
C(31)	-9299(4)	-7322(3)	1918(5)	42(2)
C(32)	-9560(5)	-7828(3)	2227(6)	70(3)
C(33)	-8657(4)	-7382(4)	1894(5)	67(3)
C(34)	-9456(4)	-6863(3)	2352(4)	48(2)
C(35)	-9208(4)	-3422(3)	728(5)	46(2)
C(36)	-9485(4)	-2227(3)	598(5)	61(3)
C(37)	-9298(4)	-2729(3)	1950(5)	46(2)
C(38)	-9398(4)	-3211(4)	2360(4)	61(2)
C(39)	-8654(5)	-2625(4)	1912(6)	84(4)
C(40)	-9587(6)	-2261(4)	2283(6)	94(4)
C(41)	-13057(4)	-4689(3)	2013(5)	47(2)
C(42)	-13115(4)	-5255(4)	1960(4)	46(2)
C(43)	-12808(3)	-5487(3)	2474(5)	37(2)
C(44)	-12551(5)	-5067(2)	2871(5)	39(2)
C(45)	-12726(4)	-4581(3)	2550(5)	48(2)

C(46)	-13340(4)	-4270(4)	1585(6)	107(4)
C(47)	-13462(4)	-5537(4)	1448(5)	91(3)
C(48)	-12771(4)	-6088(3)	2596(5)	74(3)
C(49)	-12219(5)	-5144(4)	3446(5)	88(3)
C(50)	-12552(5)	-4029(3)	2808(5)	117(5)
C(51)	-10087(4)	-5254(3)	-1478(4)	43(2)
C(52)	-9706(3)	-5530(2)	-1110(4)	50(2)
C(53)	-9377(4)	-5170(4)	-775(4)	60(2)
C(54)	-9544(4)	-4657(4)	-934(5)	79(4)
C(55)	-10003(5)	-4700(3)	-1396(4)	51(2)
C(56)	-10519(4)	-5439(3)	-1970(4)	102(1)
C(57)	-9657(4)	-6136(3)	-1171(4)	102(1)
C(58)	-8888(4)	-5380(4)	-323(4)	102(1)
C(59)	-9218(4)	-4178(3)	-695(4)	102(1)
C(60)	-10250(4)	-4231(3)	-1694(4)	102(1)
Fe(3)	-7726(1)	-9939(1)	5975(1)	30(1)
Fe(4)	-9761(1)	-9981(1)	3548(1)	26(1)
P(5)	-7790(1)	-9947(1)	4843(1)	29(1)
P(6)	-9560(1)	-9932(1)	4618(1)	31(1)
P(7)	-8036(1)	-11240(1)	4320(1)	28(1)
P(8)	-8127(1)	-8677(1)	4295(1)	31(1)
Si(3)	-7083(1)	-12162(1)	4351(1)	31(1)
Si(4)	-7128(1)	-7813(1)	4367(1)	32(1)
O(5)	-8107(2)	-8547(2)	5613(3)	44(1)
O(6)	-7941(2)	-11355(2)	5641(3)	42(1)
O(7)	-9707(2)	-11096(2)	4699(3)	58(2)
O(8)	-9864(2)	-8737(2)	4442(3)	57(1)
C(61)	-8129(3)	-8883(3)	5203(4)	31(2)
C(62)	-8174(3)	-9454(2)	5314(3)	24(2)
C(63)	-8557(3)	-9690(3)	5777(4)	28(2)
C(64)	-8539(3)	-10254(3)	5779(4)	27(2)
C(65)	-8128(3)	-10468(3)	5316(4)	28(2)
C(66)	-8024(3)	-11029(3)	5221(3)	28(2)
C(67)	-7856(3)	-11940(3)	4319(4)	28(2)
C(68)	-8345(3)	-12236(3)	4252(4)	33(2)
C(69)	-8884(3)	-11914(3)	4246(4)	34(2)
C(70)	-8803(3)	-11381(3)	4314(3)	31(2)
C(71)	-9276(3)	-10986(2)	4384(3)	32(2)
C(72)	-9223(3)	-10431(3)	4136(4)	35(2)
C(73)	-8909(3)	-10226(3)	3584(4)	29(2)
C(74)	-8942(3)	-9664(3)	3561(4)	29(2)
C(75)	-9269(3)	-9440(3)	4079(4)	31(2)
C(76)	-9372(3)	-8887(3)	4256(3)	36(2)
C(77)	-8888(3)	-8493(3)	4259(4)	33(2)
C(78)	-8941(3)	-7950(3)	4221(4)	33(2)
C(79)	-8390(3)	-7664(3)	4255(4)	31(2)
C(80)	-7906(3)	-7981(3)	4322(4)	31(2)
C(81)	-8968(3)	-9366(3)	6187(4)	39(2)
C(82)	-8919(3)	-10601(3)	6191(4)	37(2)
C(83)	-8370(4)	-12836(3)	4173(5)	53(2)
C(84)	-9457(4)	-12199(3)	4196(4)	43(2)
C(85)	-8604(3)	-10563(3)	3080(4)	41(2)
C(86)	-8657(3)	-9331(3)	3022(4)	38(2)
C(87)	-9487(3)	-7646(3)	4141(4)	42(2)
C(88)	-8373(4)	-7062(2)	4209(5)	43(2)
C(89)	-6983(4)	-12761(3)	4864(4)	55(3)
C(90)	-6690(3)	-11600(3)	4726(5)	45(2)
C(91)	-6781(4)	-12303(3)	3508(4)	35(2)
C(92)	-6122(4)	-12401(4)	3581(4)	56(2)
C(93)	-7053(4)	-12802(3)	3219(4)	52(2)
C(94)	-6873(4)	-11815(3)	3051(4)	53(2)
C(95)	-6783(3)	-8413(3)	4718(4)	42(2)
C(96)	-6987(4)	-7236(3)	4905(5)	52(2)

C(97)	-6818(4)	-7675(3)	3522(4)	38(2)
C(98)	-6959(4)	-8142(3)	3057(4)	58(3)
C(99)	-6143(3)	-7614(3)	3591(4)	50(2)
C(100)	-7048(4)	-7146(3)	3261(4)	51(2)
C(101)	-6873(3)	-9750(3)	6202(4)	43(2)
C(102)	-6995(4)	-10307(3)	6346(4)	46(2)
C(103)	-7463(5)	-10293(3)	6819(4)	55(3)
C(104)	-7591(4)	-9755(3)	6947(4)	44(2)
C(105)	-7226(3)	-9434(2)	6572(3)	49(2)
C(106)	-6388(2)	-9599(3)	5750(3)	59(2)
C(107)	-6697(3)	-10801(3)	6129(4)	132(4)
C(108)	-7764(4)	-10764(3)	7169(4)	121(4)
C(109)	-8016(3)	-9541(3)	7435(3)	62(2)
C(110)	-7161(3)	-8839(2)	6594(3)	50(1)
C(111)	-10313(3)	-9547(3)	2962(5)	39(2)
C(112)	-10045(6)	-9955(3)	2608(6)	48(3)
C(113)	-10194(3)	-10458(3)	2896(5)	47(2)
C(114)	-10563(3)	-10335(3)	3428(5)	44(2)
C(115)	-10630(3)	-9797(3)	3464(4)	35(2)
C(116)	-10298(4)	-8971(3)	2806(4)	71(3)
C(117)	-9708(5)	-9887(3)	1968(5)	67(2)
C(118)	-10027(4)	-10990(3)	2635(4)	75(3)
C(119)	-10845(4)	-10741(3)	3868(4)	77(3)
C(120)	-11002(3)	-9500(3)	3952(4)	62(2)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table 3. Bond lengths (A) and angles (deg) for **9**

Fe(1)-C(41)	2.055(8)	Fe(1)-C(42)	2.07(1)
Fe(1)-C(45)	2.061(8)	Fe(1)-C(43)	2.072(8)
Fe(1)-C(3)	2.066(8)	Fe(1)-C(4)	2.088(8)
Fe(1)-C(2)	2.105(8)	Fe(1)-C(44)	2.11(1)
Fe(1)-C(5)	2.103(8)	Fe(1)-P(1)	2.257(3)
Fe(2)-C(54)	2.035(8)	Fe(2)-C(14)	2.047(8)
Fe(2)-C(13)	2.058(8)	Fe(2)-C(55)	2.062(8)
Fe(2)-C(53)	2.051(8)	Fe(2)-C(51)	2.063(8)
Fe(2)-C(15)	2.072(7)	Fe(2)-C(12)	2.088(8)
Fe(2)-C(52)	2.092(6)	Fe(2)-P(2)	2.331(3)
P(1)-C(5)	1.784(8)	P(1)-C(2)	1.798(7)
P(2)-C(15)	1.761(7)	P(2)-C(12)	1.777(8)
P(3)-C(10)	1.809(7)	P(3)-C(7)	1.830(8)
P(3)-C(11)	1.888(8)	P(4)-C(17)	1.790(7)
P(4)-C(20)	1.811(8)	P(4)-C(16)	1.89(1)
Si(1)-C(10)	1.872(8)	Si(1)-C(29)	1.879(7)
Si(1)-C(31)	1.89(1)	Si(1)-C(30)	1.899(8)
Si(2)-C(35)	1.887(8)	Si(2)-C(17)	1.90(1)
Si(2)-C(36)	1.886(7)	Si(2)-C(37)	1.90(1)
O(1)-C(1)	1.22(1)	O(2)-C(6)	1.208(8)
O(3)-C(11)	1.22(1)	O(4)-C(16)	1.25(1)
C(1)-C(2)	1.47(1)	C(1)-C(20)	1.50(1)
C(2)-C(3)	1.46(1)	C(3)-C(4)	1.41(1)
C(3)-C(21)	1.51(1)	C(4)-C(5)	1.46(1)
C(4)-C(22)	1.47(1)	C(5)-C(6)	1.51(1)
C(6)-C(7)	1.47(1)	C(7)-C(8)	1.37(1)
C(8)-C(9)	1.45(1)	C(8)-C(23)	1.50(1)
C(9)-C(10)	1.37(1)	C(9)-C(24)	1.50(1)
C(11)-C(12)	1.52(1)	C(12)-C(13)	1.44(1)
C(13)-C(14)	1.44(1)	C(13)-C(25)	1.50(1)
C(14)-C(15)	1.43(1)	C(14)-C(26)	1.50(1)
C(15)-C(16)	1.52(1)	C(17)-C(18)	1.34(1)
C(18)-C(19)	1.46(1)	C(18)-C(27)	1.50(1)
C(19)-C(20)	1.36(1)	C(19)-C(28)	1.51(1)
C(21)-H(21A)	0.9600	C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600	C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600	C(22)-H(22C)	0.9600
C(23)-H(23A)	0.9600	C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600	C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600	C(24)-H(24C)	0.9600
C(25)-H(25A)	0.9601	C(25)-H(25B)	0.9601
C(25)-H(25C)	0.9600	C(26)-H(26A)	0.9601
C(26)-H(26B)	0.9601	C(26)-H(26C)	0.9601
C(27)-H(27A)	0.9600	C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600	C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600	C(28)-H(28C)	0.9600
C(29)-H(29A)	0.9600	C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600	C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600	C(30)-H(30C)	0.9600
C(31)-C(33)	1.50(1)	C(31)-C(34)	1.50(1)
C(31)-C(32)	1.54(1)	C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600	C(32)-H(32C)	0.9600
C(33)-H(33A)	0.9601	C(33)-H(33B)	0.9601
C(33)-H(33C)	0.9601	C(34)-H(34A)	0.9602
C(34)-H(34B)	0.9602	C(34)-H(34C)	0.9602
C(35)-H(35A)	0.9600	C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600	C(36)-H(36A)	0.9600
C(36)-H(36B)	0.9600	C(36)-H(36C)	0.9600
C(37)-C(38)	1.50(1)	C(37)-C(39)	1.52(1)
C(37)-C(40)	1.52(1)	C(38)-H(38A)	0.9603
C(38)-H(38B)	0.9603	C(38)-H(38C)	0.9603

C(39)-H(39A)	0.9601	C(39)-H(39B)	0.9601
C(39)-H(39C)	0.9601	C(40)-H(40A)	0.9600
C(40)-H(40B)	0.9600	C(40)-H(40C)	0.9600
C(41)-C(45)	1.38(1)	C(41)-C(42)	1.43(2)
C(41)-C(46)	1.52(1)	C(42)-C(43)	1.40(1)
C(42)-C(47)	1.50(1)	C(43)-C(44)	1.46(1)
C(43)-C(48)	1.53(1)	C(44)-C(45)	1.45(1)
C(44)-C(49)	1.43(1)	C(45)-C(50)	1.54(1)
C(46)-H(46A)	0.9600	C(46)-H(46B)	0.9600
C(46)-H(46C)	0.9600	C(47)-H(47A)	0.9600
C(47)-H(47B)	0.9600	C(47)-H(47C)	0.9600
C(48)-H(48A)	0.9600	C(48)-H(48B)	0.9600
C(48)-H(48C)	0.9600	C(49)-H(49A)	0.9600
C(49)-H(49B)	0.9600	C(49)-H(49C)	0.9600
C(50)-H(50A)	0.9600	C(50)-H(50B)	0.9600
C(50)-H(50C)	0.9600	C(51)-C(52)	1.36(1)
C(51)-C(55)	1.42(1)	C(51)-C(56)	1.50(1)
C(52)-C(53)	1.37(1)	C(52)-C(57)	1.53(1)
C(53)-C(54)	1.38(1)	C(53)-C(58)	1.56(1)
C(54)-C(55)	1.43(1)	C(54)-C(59)	1.50(1)
C(55)-C(60)	1.45(1)	C(56)-H(56A)	0.9600
C(56)-H(56B)	0.9600	C(56)-H(56C)	0.9600
C(57)-H(57A)	0.9600	C(57)-H(57B)	0.9600
C(57)-H(57C)	0.9600	C(58)-H(58A)	0.9600
C(58)-H(58B)	0.9600	C(58)-H(58C)	0.9600
C(59)-H(59A)	0.9600	C(59)-H(59B)	0.9600
C(59)-H(59C)	0.9600	C(60)-H(60A)	0.9600
C(60)-H(60B)	0.9600	C(60)-H(60C)	0.9600
Fe(3)-C(103)	2.046(7)	Fe(3)-C(102)	2.078(8)
Fe(3)-C(104)	2.079(8)	Fe(3)-C(63)	2.068(7)
Fe(3)-C(101)	2.089(8)	Fe(3)-C(64)	2.085(7)
Fe(3)-C(62)	2.103(7)	Fe(3)-C(65)	2.115(7)
Fe(3)-C(105)	2.114(6)	Fe(3)-P(5)	2.338(3)
Fe(4)-C(112)	2.05(1)	Fe(4)-C(113)	2.062(8)
Fe(4)-C(74)	2.060(7)	Fe(4)-C(73)	2.072(7)
Fe(4)-C(72)	2.074(8)	Fe(4)-C(115)	2.078(7)
Fe(4)-C(111)	2.071(8)	Fe(4)-C(114)	2.080(8)
Fe(4)-C(75)	2.083(7)	Fe(4)-P(6)	2.257(3)
P(5)-C(65)	1.810(7)	P(5)-C(62)	1.809(7)
P(6)-C(72)	1.779(8)	P(6)-C(75)	1.792(8)
P(7)-C(67)	1.807(7)	P(7)-C(70)	1.814(8)
P(7)-C(66)	1.931(7)	P(8)-C(80)	1.822(7)
P(8)-C(77)	1.828(8)	P(8)-C(61)	1.940(8)
Si(3)-C(90)	1.847(8)	Si(3)-C(89)	1.85(1)
Si(3)-C(67)	1.879(7)	Si(3)-C(91)	1.90(1)
Si(4)-C(95)	1.851(8)	Si(4)-C(96)	1.85(1)
Si(4)-C(80)	1.856(8)	Si(4)-C(97)	1.92(1)
O(5)-C(61)	1.196(8)	O(6)-C(66)	1.205(8)
O(7)-C(71)	1.223(8)	O(8)-C(76)	1.263(8)
C(61)-C(62)	1.45(1)	C(62)-C(63)	1.43(1)
C(63)-C(64)	1.41(1)	C(63)-C(81)	1.51(1)
C(64)-C(65)	1.45(1)	C(64)-C(82)	1.50(1)
C(65)-C(66)	1.44(1)	C(67)-C(68)	1.36(1)
C(68)-C(69)	1.49(1)	C(68)-C(83)	1.52(1)
C(69)-C(70)	1.36(1)	C(69)-C(84)	1.51(1)
C(70)-C(71)	1.49(1)	C(71)-C(72)	1.49(1)
C(72)-C(73)	1.45(1)	C(73)-C(74)	1.41(1)
C(73)-C(85)	1.51(1)	C(74)-C(75)	1.42(1)
C(74)-C(86)	1.54(1)	C(75)-C(76)	1.46(1)
C(76)-C(77)	1.50(1)	C(77)-C(78)	1.37(1)
C(78)-C(79)	1.47(1)	C(78)-C(87)	1.49(1)
C(79)-C(80)	1.38(1)	C(79)-C(88)	1.515(8)
C(81)-H(81A)	0.9601	C(81)-H(81B)	0.9601

C(81)-H(81C)	0.9601	C(82)-H(82A)	0.9601
C(82)-H(82B)	0.9601	C(82)-H(82C)	0.9601
C(83)-H(83A)	0.9600	C(83)-H(83B)	0.9600
C(83)-H(83C)	0.9600	C(84)-H(84A)	0.9600
C(84)-H(84B)	0.9600	C(84)-H(84C)	0.9600
C(85)-H(85A)	0.9600	C(85)-H(85B)	0.9600
C(85)-H(85C)	0.9600	C(86)-H(86A)	0.9600
C(86)-H(86B)	0.9600	C(86)-H(86C)	0.9600
C(87)-H(87A)	0.9600	C(87)-H(87B)	0.9600
C(87)-H(87C)	0.9600	C(88)-H(88A)	0.9600
C(88)-H(88B)	0.9600	C(88)-H(88C)	0.9600
C(89)-H(89A)	0.9600	C(89)-H(89B)	0.9600
C(89)-H(89C)	0.9600	C(90)-H(90A)	0.9600
C(90)-H(90B)	0.9600	C(90)-H(90C)	0.9600
C(91)-C(93)	1.52(1)	C(91)-C(94)	1.56(1)
C(91)-C(92)	1.56(1)	C(92)-H(92A)	0.9601
C(92)-H(92B)	0.9601	C(92)-H(92C)	0.9601
C(93)-H(93A)	0.9600	C(93)-H(93B)	0.9600
C(93)-H(93C)	0.9600	C(94)-H(94A)	0.9602
C(94)-H(94B)	0.9602	C(94)-H(94C)	0.9602
C(95)-H(95A)	0.9600	C(95)-H(95B)	0.9600
C(95)-H(95C)	0.9600	C(96)-H(96A)	0.9600
C(96)-H(96B)	0.9600	C(96)-H(96C)	0.9600
C(97)-C(100)	1.53(1)	C(97)-C(98)	1.55(1)
C(97)-C(99)	1.58(1)	C(98)-H(98A)	0.9603
C(98)-H(98B)	0.9603	C(98)-H(98C)	0.9603
C(99)-H(99A)	0.9601	C(99)-H(99B)	0.9601
C(99)-H(99C)	0.9601	C(100)-H(10A)	0.9600
C(100)-H(10B)	0.9600	C(100)-H(10C)	0.9600
C(101)-C(105)	1.37(1)	C(101)-C(102)	1.46(1)
C(101)-C(106)	1.51(1)	C(102)-C(103)	1.46(1)
C(102)-C(107)	1.49(1)	C(103)-C(104)	1.41(1)
C(103)-C(108)	1.55(1)	C(104)-C(105)	1.40(1)
C(104)-C(109)	1.51(1)	C(105)-C(110)	1.502(7)
C(106)-H(10D)	0.9600	C(106)-H(10E)	0.9600
C(106)-H(10F)	0.9600	C(107)-H(10G)	0.9601
C(107)-H(10H)	0.9601	C(107)-H(10I)	0.9601
C(108)-H(10J)	0.9600	C(108)-H(10K)	0.9600
C(108)-H(10L)	0.9600	C(109)-H(10M)	0.9600
C(109)-H(10N)	0.9600	C(109)-H(10O)	0.9600
C(110)-H(11A)	0.9600	C(110)-H(11B)	0.9600
C(110)-H(11C)	0.9600	C(111)-C(112)	1.40(1)
C(111)-C(115)	1.42(1)	C(111)-C(116)	1.48(1)
C(112)-C(113)	1.44(1)	C(112)-C(117)	1.54(2)
C(113)-C(114)	1.43(1)	C(113)-C(118)	1.49(1)
C(114)-C(115)	1.36(1)	C(114)-C(119)	1.51(1)
C(115)-C(120)	1.52(1)	C(116)-H(11D)	0.9600
C(116)-H(11E)	0.9600	C(116)-H(11F)	0.9600
C(117)-H(11G)	0.9600	C(117)-H(11H)	0.9600
C(117)-H(11I)	0.9600	C(118)-H(11J)	0.9600
C(118)-H(11K)	0.9600	C(118)-H(11L)	0.9600
C(119)-H(11M)	0.9600	C(119)-H(11N)	0.9600
C(119)-H(11O)	0.9600	C(120)-H(12A)	0.9600
C(120)-H(12B)	0.9600	C(120)-H(12C)	0.9600

C(41)-Fe(1)-C(42)	40.7(4)	C(41)-Fe(1)-C(45)	39.0(4)
C(42)-Fe(1)-C(45)	66.9(3)	C(41)-Fe(1)-C(43)	67.4(3)
C(42)-Fe(1)-C(43)	39.6(3)	C(45)-Fe(1)-C(43)	67.2(4)
C(41)-Fe(1)-C(3)	136.3(3)	C(42)-Fe(1)-C(3)	176.5(3)
C(45)-Fe(1)-C(3)	109.7(3)	C(43)-Fe(1)-C(3)	140.2(3)
C(41)-Fe(1)-C(4)	172.8(4)	C(42)-Fe(1)-C(4)	143.0(3)
C(45)-Fe(1)-C(4)	133.8(4)	C(43)-Fe(1)-C(4)	112.0(3)

C(3)-Fe(1)-C(4)	39.8(4)	C(41)-Fe(1)-C(2)	110.8(3)
C(42)-Fe(1)-C(2)	139.0(4)	C(45)-Fe(1)-C(2)	111.3(3)
C(43)-Fe(1)-C(2)	178.2(3)	C(3)-Fe(1)-C(2)	41.0(3)
C(4)-Fe(1)-C(2)	69.8(3)	C(41)-Fe(1)-C(44)	67.8(4)
C(42)-Fe(1)-C(44)	68.1(4)	C(45)-Fe(1)-C(44)	40.6(3)
C(43)-Fe(1)-C(44)	40.9(3)	C(3)-Fe(1)-C(44)	109.7(4)
C(4)-Fe(1)-C(44)	106.8(4)	C(2)-Fe(1)-C(44)	138.6(3)
C(41)-Fe(1)-C(5)	146.3(4)	C(42)-Fe(1)-C(5)	114.2(3)
C(45)-Fe(1)-C(5)	172.5(4)	C(43)-Fe(1)-C(5)	108.5(3)
C(3)-Fe(1)-C(5)	69.3(3)	C(4)-Fe(1)-C(5)	40.9(3)
C(2)-Fe(1)-C(5)	73.1(4)	C(44)-Fe(1)-C(5)	132.2(3)
C(41)-Fe(1)-P(1)	107.9(3)	C(42)-Fe(1)-P(1)	104.4(3)
C(45)-Fe(1)-P(1)	139.3(3)	C(43)-Fe(1)-P(1)	131.9(3)
C(3)-Fe(1)-P(1)	77.9(2)	C(4)-Fe(1)-P(1)	77.9(2)
C(2)-Fe(1)-P(1)	48.5(2)	C(44)-Fe(1)-P(1)	172.3(3)
C(5)-Fe(1)-P(1)	48.2(2)	C(54)-Fe(2)-C(14)	127.5(4)
C(54)-Fe(2)-C(13)	161.7(4)	C(14)-Fe(2)-C(13)	41.0(4)
C(54)-Fe(2)-C(55)	40.9(4)	C(14)-Fe(2)-C(55)	103.1(4)
C(13)-Fe(2)-C(55)	121.5(4)	C(54)-Fe(2)-C(53)	39.6(4)
C(14)-Fe(2)-C(53)	167.1(3)	C(13)-Fe(2)-C(53)	151.0(4)
C(55)-Fe(2)-C(53)	66.9(4)	C(54)-Fe(2)-C(51)	66.8(3)
C(14)-Fe(2)-C(51)	113.5(3)	C(13)-Fe(2)-C(51)	102.7(3)
C(55)-Fe(2)-C(51)	40.1(4)	C(53)-Fe(2)-C(51)	64.8(4)
C(54)-Fe(2)-C(15)	110.7(3)	C(14)-Fe(2)-C(15)	40.6(3)
C(13)-Fe(2)-C(15)	69.6(3)	C(55)-Fe(2)-C(15)	116.1(3)
C(53)-Fe(2)-C(15)	134.9(4)	C(51)-Fe(2)-C(15)	148.0(3)
C(54)-Fe(2)-C(12)	157.7(4)	C(14)-Fe(2)-C(12)	69.8(3)
C(13)-Fe(2)-C(12)	40.6(3)	C(55)-Fe(2)-C(12)	158.9(4)
C(53)-Fe(2)-C(12)	122.5(3)	C(51)-Fe(2)-C(12)	123.0(3)
C(15)-Fe(2)-C(12)	72.1(3)	C(54)-Fe(2)-C(52)	66.1(3)
C(14)-Fe(2)-C(52)	146.7(3)	C(13)-Fe(2)-C(52)	115.6(3)
C(55)-Fe(2)-C(52)	66.4(3)	C(53)-Fe(2)-C(52)	38.6(3)
C(51)-Fe(2)-C(52)	38.1(3)	C(15)-Fe(2)-C(52)	172.6(3)
C(12)-Fe(2)-C(52)	108.2(3)	C(54)-Fe(2)-P(2)	117.9(3)
C(14)-Fe(2)-P(2)	76.2(2)	C(13)-Fe(2)-P(2)	76.3(2)
C(55)-Fe(2)-P(2)	152.6(3)	C(53)-Fe(2)-P(2)	108.5(3)
C(51)-Fe(2)-P(2)	164.4(2)	C(15)-Fe(2)-P(2)	46.7(2)
C(12)-Fe(2)-P(2)	47.0(2)	C(52)-Fe(2)-P(2)	128.0(2)
C(5)-P(1)-C(2)	88.8(5)	C(5)-P(1)-Fe(1)	61.4(3)
C(2)-P(1)-Fe(1)	61.3(3)	C(15)-P(2)-C(12)	87.6(5)
C(15)-P(2)-Fe(2)	58.9(3)	C(12)-P(2)-Fe(2)	59.3(3)
C(10)-P(3)-C(7)	92.0(3)	C(10)-P(3)-C(11)	102.1(3)
C(7)-P(3)-C(11)	96.5(3)	C(17)-P(4)-C(20)	91.1(4)
C(17)-P(4)-C(16)	105.1(4)	C(20)-P(4)-C(16)	96.1(4)
C(10)-Si(1)-C(29)	113.1(3)	C(10)-Si(1)-C(31)	111.8(4)
C(29)-Si(1)-C(31)	109.4(4)	C(10)-Si(1)-C(30)	104.6(3)
C(29)-Si(1)-C(30)	109.1(4)	C(31)-Si(1)-C(30)	108.6(4)
C(35)-Si(2)-C(17)	104.5(4)	C(35)-Si(2)-C(36)	109.3(5)
C(17)-Si(2)-C(36)	113.6(4)	C(35)-Si(2)-C(37)	108.2(4)
C(17)-Si(2)-C(37)	111.7(4)	C(36)-Si(2)-C(37)	109.3(4)
O(1)-C(1)-C(2)	119.9(7)	O(1)-C(1)-C(20)	120.0(7)
C(2)-C(1)-C(20)	119.5(7)	C(3)-C(2)-C(1)	131.5(7)
C(3)-C(2)-P(1)	112.8(5)	C(1)-C(2)-P(1)	115.6(6)
C(3)-C(2)-Fe(1)	68.1(4)	C(1)-C(2)-Fe(1)	129.6(6)
P(1)-C(2)-Fe(1)	70.1(3)	C(4)-C(3)-C(2)	113.0(5)
C(4)-C(3)-C(21)	122.6(5)	C(2)-C(3)-C(21)	124.4(7)
C(4)-C(3)-Fe(1)	70.9(3)	C(2)-C(3)-Fe(1)	70.9(4)
C(21)-C(3)-Fe(1)	127.0(6)	C(3)-C(4)-C(5)	110.9(5)
C(3)-C(4)-C(22)	123.1(5)	C(5)-C(4)-C(22)	126.0(7)
C(3)-C(4)-Fe(1)	69.3(3)	C(5)-C(4)-Fe(1)	70.1(4)
C(22)-C(4)-Fe(1)	127.1(6)	C(4)-C(5)-C(6)	129.1(7)
C(4)-C(5)-P(1)	114.4(5)	C(6)-C(5)-P(1)	116.5(6)
C(4)-C(5)-Fe(1)	69.0(4)	C(6)-C(5)-Fe(1)	129.4(6)

P(1)-C(5)-Fe(1)	70.4(3)	O(2)-C(6)-C(7)	121.6(6)
O(2)-C(6)-C(5)	119.0(6)	C(7)-C(6)-C(5)	118.6(7)
C(8)-C(7)-C(6)	124.6(7)	C(8)-C(7)-P(3)	108.7(6)
C(6)-C(7)-P(3)	126.6(5)	C(7)-C(8)-C(9)	114.3(7)
C(7)-C(8)-C(23)	125.9(7)	C(9)-C(8)-C(23)	119.7(6)
C(10)-C(9)-C(8)	116.3(7)	C(10)-C(9)-C(24)	125.1(7)
C(8)-C(9)-C(24)	118.6(7)	C(9)-C(10)-P(3)	108.3(6)
C(9)-C(10)-Si(1)	131.9(6)	P(3)-C(10)-Si(1)	119.4(4)
O(3)-C(11)-C(12)	121.6(7)	O(3)-C(11)-P(3)	123.6(5)
C(12)-C(11)-P(3)	114.6(5)	C(13)-C(12)-C(11)	122.8(7)
C(13)-C(12)-P(2)	115.2(5)	C(11)-C(12)-P(2)	122.0(6)
C(13)-C(12)-Fe(2)	68.6(4)	C(11)-C(12)-Fe(2)	129.2(5)
P(2)-C(12)-Fe(2)	73.7(3)	C(14)-C(13)-C(12)	110.5(5)
C(14)-C(13)-C(25)	124.6(5)	C(12)-C(13)-C(25)	124.3(6)
C(14)-C(13)-Fe(2)	69.1(3)	C(12)-C(13)-Fe(2)	70.8(5)
C(25)-C(13)-Fe(2)	133.9(5)	C(13)-C(14)-C(15)	110.7(5)
C(13)-C(14)-C(26)	123.6(5)	C(15)-C(14)-C(26)	124.9(6)
C(13)-C(14)-Fe(2)	69.9(3)	C(15)-C(14)-Fe(2)	70.7(5)
C(26)-C(14)-Fe(2)	134.3(5)	C(14)-C(15)-C(16)	122.4(6)
C(14)-C(15)-P(2)	116.0(5)	C(16)-C(15)-P(2)	121.5(6)
C(14)-C(15)-Fe(2)	68.8(4)	C(16)-C(15)-Fe(2)	128.0(5)
P(2)-C(15)-Fe(2)	74.4(3)	O(4)-C(16)-C(15)	123.1(7)
O(4)-C(16)-P(4)	121.9(6)	C(15)-C(16)-P(4)	114.9(5)
C(18)-C(17)-P(4)	109.6(6)	C(18)-C(17)-Si(2)	129.4(6)
P(4)-C(17)-Si(2)	120.6(4)	C(17)-C(18)-C(19)	115.8(6)
C(17)-C(18)-C(27)	126.2(7)	C(19)-C(18)-C(27)	117.9(7)
C(20)-C(19)-C(18)	112.8(7)	C(20)-C(19)-C(28)	126.7(8)
C(18)-C(19)-C(28)	120.5(6)	C(19)-C(20)-C(1)	123.9(8)
C(19)-C(20)-P(4)	110.1(6)	C(1)-C(20)-P(4)	126.0(6)
C(3)-C(21)-H(21A)	109.4	C(3)-C(21)-H(21B)	109.8
H(21A)-C(21)-H(21B)	109.5	C(3)-C(21)-H(21C)	109.2
H(21A)-C(21)-H(21C)	109.5	H(21B)-C(21)-H(21C)	109.5
C(4)-C(22)-H(22A)	109.1	C(4)-C(22)-H(22B)	109.9
H(22A)-C(22)-H(22B)	109.5	C(4)-C(22)-H(22C)	109.4
H(22A)-C(22)-H(22C)	109.5	H(22B)-C(22)-H(22C)	109.5
C(8)-C(23)-H(23A)	109.4	C(8)-C(23)-H(23B)	109.8
H(23A)-C(23)-H(23B)	109.5	C(8)-C(23)-H(23C)	109.2
H(23A)-C(23)-H(23C)	109.5	H(23B)-C(23)-H(23C)	109.5
C(9)-C(24)-H(24A)	109.2	C(9)-C(24)-H(24B)	109.6
H(24A)-C(24)-H(24B)	109.5	C(9)-C(24)-H(24C)	109.6
H(24A)-C(24)-H(24C)	109.5	H(24B)-C(24)-H(24C)	109.5
C(13)-C(25)-H(25A)	109.5	C(13)-C(25)-H(25B)	109.7
H(25A)-C(25)-H(25B)	109.5	C(13)-C(25)-H(25C)	109.3
H(25A)-C(25)-H(25C)	109.5	H(25B)-C(25)-H(25C)	109.5
C(14)-C(26)-H(26A)	109.6	C(14)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5	C(14)-C(26)-H(26C)	109.3
H(26A)-C(26)-H(26C)	109.5	H(26B)-C(26)-H(26C)	109.5
C(18)-C(27)-H(27A)	109.2	C(18)-C(27)-H(27B)	109.6
H(27A)-C(27)-H(27B)	109.5	C(18)-C(27)-H(27C)	109.7
H(27A)-C(27)-H(27C)	109.5	H(27B)-C(27)-H(27C)	109.5
C(19)-C(28)-H(28A)	109.2	C(19)-C(28)-H(28B)	109.8
H(28A)-C(28)-H(28B)	109.5	C(19)-C(28)-H(28C)	109.4
H(28A)-C(28)-H(28C)	109.5	H(28B)-C(28)-H(28C)	109.5
Si(1)-C(29)-H(29A)	109.5	Si(1)-C(29)-H(29B)	109.6
H(29A)-C(29)-H(29B)	109.5	Si(1)-C(29)-H(29C)	109.4
H(29A)-C(29)-H(29C)	109.5	H(29B)-C(29)-H(29C)	109.5
Si(1)-C(30)-H(30A)	109.6	Si(1)-C(30)-H(30B)	109.3
H(30A)-C(30)-H(30B)	109.5	Si(1)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5	H(30B)-C(30)-H(30C)	109.5
C(33)-C(31)-C(34)	109.8(8)	C(33)-C(31)-C(32)	108.7(8)
C(34)-C(31)-C(32)	106.9(8)	C(33)-C(31)-Si(1)	111.1(7)
C(34)-C(31)-Si(1)	108.6(6)	C(32)-C(31)-Si(1)	111.7(6)
C(31)-C(32)-H(32A)	109.4	C(31)-C(32)-H(32B)	109.3

H(32A)-C(32)-H(32B)	109.5	C(31)-C(32)-H(32C)	109.7
H(32A)-C(32)-H(32C)	109.5	H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5	C(31)-C(33)-H(33B)	109.0
H(33A)-C(33)-H(33B)	109.5	C(31)-C(33)-H(33C)	109.9
H(33A)-C(33)-H(33C)	109.5	H(33B)-C(33)-H(33C)	109.4
C(31)-C(34)-H(34A)	109.8	C(31)-C(34)-H(34B)	109.0
H(34A)-C(34)-H(34B)	109.4	C(31)-C(34)-H(34C)	109.7
H(34A)-C(34)-H(34C)	109.5	H(34B)-C(34)-H(34C)	109.5
Si(2)-C(35)-H(35A)	109.6	Si(2)-C(35)-H(35B)	109.3
H(35A)-C(35)-H(35B)	109.5	Si(2)-C(35)-H(35C)	109.6
H(35A)-C(35)-H(35C)	109.5	H(35B)-C(35)-H(35C)	109.5
Si(2)-C(36)-H(36A)	109.5	Si(2)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5	Si(2)-C(36)-H(36C)	109.4
H(36A)-C(36)-H(36C)	109.5	H(36B)-C(36)-H(36C)	109.5
C(38)-C(37)-C(39)	108.7(8)	C(38)-C(37)-C(40)	108(1)
C(39)-C(37)-C(40)	109(1)	C(38)-C(37)-Si(2)	109.8(6)
C(39)-C(37)-Si(2)	110.3(8)	C(40)-C(37)-Si(2)	111.4(7)
C(37)-C(38)-H(38A)	109.6	C(37)-C(38)-H(38B)	109.0
H(38A)-C(38)-H(38B)	109.5	C(37)-C(38)-H(38C)	109.8
H(38A)-C(38)-H(38C)	109.4	H(38B)-C(38)-H(38C)	109.4
C(37)-C(39)-H(39A)	109.9	C(37)-C(39)-H(39B)	109.1
H(39A)-C(39)-H(39B)	109.5	C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5	H(39B)-C(39)-H(39C)	109.5
C(37)-C(40)-H(40A)	109.6	C(37)-C(40)-H(40B)	109.4
H(40A)-C(40)-H(40B)	109.5	C(37)-C(40)-H(40C)	109.4
H(40A)-C(40)-H(40C)	109.5	H(40B)-C(40)-H(40C)	109.5
C(45)-C(41)-C(42)	108.1(6)	C(45)-C(41)-C(46)	125(1)
C(42)-C(41)-C(46)	126.9(7)	C(45)-C(41)-Fe(1)	70.7(5)
C(42)-C(41)-Fe(1)	70.0(4)	C(46)-C(41)-Fe(1)	128.0(6)
C(43)-C(42)-C(41)	107.7(6)	C(43)-C(42)-C(47)	127(1)
C(41)-C(42)-C(47)	124.8(7)	C(43)-C(42)-Fe(1)	70.4(5)
C(41)-C(42)-Fe(1)	69.3(3)	C(47)-C(42)-Fe(1)	127.0(6)
C(42)-C(43)-C(44)	109.4(7)	C(42)-C(43)-C(48)	124.0(8)
C(44)-C(43)-C(48)	126.6(8)	C(42)-C(43)-Fe(1)	69.9(5)
C(44)-C(43)-Fe(1)	70.9(5)	C(48)-C(43)-Fe(1)	126.8(6)
C(45)-C(44)-C(43)	104(1)	C(45)-C(44)-C(49)	130.2(8)
C(43)-C(44)-C(49)	126.0(7)	C(45)-C(44)-Fe(1)	68.0(5)
C(43)-C(44)-Fe(1)	68.2(5)	C(49)-C(44)-Fe(1)	128.2(8)
C(41)-C(45)-C(44)	110.9(7)	C(41)-C(45)-C(50)	127(1)
C(44)-C(45)-C(50)	122(1)	C(41)-C(45)-Fe(1)	70.3(5)
C(44)-C(45)-Fe(1)	71.5(5)	C(50)-C(45)-Fe(1)	125.7(6)
C(41)-C(46)-H(46A)	109.7	C(41)-C(46)-H(46B)	109.3
H(46A)-C(46)-H(46B)	109.5	C(41)-C(46)-H(46C)	109.4
H(46A)-C(46)-H(46C)	109.5	H(46B)-C(46)-H(46C)	109.5
C(42)-C(47)-H(47A)	109.6	C(42)-C(47)-H(47B)	109.2
H(47A)-C(47)-H(47B)	109.5	C(42)-C(47)-H(47C)	109.7
H(47A)-C(47)-H(47C)	109.5	H(47B)-C(47)-H(47C)	109.5
C(43)-C(48)-H(48A)	109.5	C(43)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5	C(43)-C(48)-H(48C)	109.4
H(48A)-C(48)-H(48C)	109.5	H(48B)-C(48)-H(48C)	109.5
C(44)-C(49)-H(49A)	109.2	C(44)-C(49)-H(49B)	109.6
H(49A)-C(49)-H(49B)	109.5	C(44)-C(49)-H(49C)	109.6
H(49A)-C(49)-H(49C)	109.5	H(49B)-C(49)-H(49C)	109.5
C(45)-C(50)-H(50A)	109.4	C(45)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5	C(45)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5	H(50B)-C(50)-H(50C)	109.5
C(52)-C(51)-C(55)	110.2(6)	C(52)-C(51)-C(56)	131.1(8)
C(55)-C(51)-C(56)	118.5(7)	C(52)-C(51)-Fe(2)	72.1(4)
C(55)-C(51)-Fe(2)	69.9(3)	C(56)-C(51)-Fe(2)	128.6(6)
C(53)-C(52)-C(51)	108.0(7)	C(53)-C(52)-C(57)	131.0(8)
C(51)-C(52)-C(57)	120.6(8)	C(53)-C(52)-Fe(2)	69.1(4)
C(51)-C(52)-Fe(2)	69.8(4)	C(57)-C(52)-Fe(2)	131.9(5)
C(52)-C(53)-C(54)	109.8(7)	C(52)-C(53)-C(58)	119(1)

C(54)-C(53)-C(58)	131(1)	C(52)-C(53)-Fe(2)	72.3(5)
C(54)-C(53)-Fe(2)	69.6(4)	C(58)-C(53)-Fe(2)	126.5(6)
C(53)-C(54)-C(55)	107.2(6)	C(53)-C(54)-C(59)	122(1)
C(55)-C(54)-C(59)	131(1)	C(53)-C(54)-Fe(2)	70.8(4)
C(55)-C(54)-Fe(2)	70.5(5)	C(59)-C(54)-Fe(2)	129.4(5)
C(51)-C(55)-C(54)	104.8(6)	C(51)-C(55)-C(60)	134.0(8)
C(54)-C(55)-C(60)	121(1)	C(51)-C(55)-Fe(2)	70.0(3)
C(54)-C(55)-Fe(2)	68.5(4)	C(60)-C(55)-Fe(2)	128.1(6)
C(51)-C(56)-H(56A)	109.7	C(51)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5	C(51)-C(56)-H(56C)	109.2
H(56A)-C(56)-H(56C)	109.5	H(56B)-C(56)-H(56C)	109.5
C(52)-C(57)-H(57A)	109.5	C(52)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5	C(52)-C(57)-H(57C)	109.4
H(57A)-C(57)-H(57C)	109.5	H(57B)-C(57)-H(57C)	109.5
C(53)-C(58)-H(58A)	109.7	C(53)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5	C(53)-C(58)-H(58C)	109.3
H(58A)-C(58)-H(58C)	109.5	H(58B)-C(58)-H(58C)	109.5
C(54)-C(59)-H(59A)	109.2	C(54)-C(59)-H(59B)	109.6
H(59A)-C(59)-H(59B)	109.5	C(54)-C(59)-H(59C)	109.6
H(59A)-C(59)-H(59C)	109.5	H(59B)-C(59)-H(59C)	109.5
C(55)-C(60)-H(60A)	109.2	C(55)-C(60)-H(60B)	109.5
H(60A)-C(60)-H(60B)	109.5	C(55)-C(60)-H(60C)	109.7
H(60A)-C(60)-H(60C)	109.5	H(60B)-C(60)-H(60C)	109.5
C(103)-Fe(3)-C(102)	41.4(4)	C(103)-Fe(3)-C(104)	39.9(4)
C(102)-Fe(3)-C(104)	67.7(3)	C(103)-Fe(3)-C(63)	125.3(4)
C(102)-Fe(3)-C(63)	165.6(3)	C(104)-Fe(3)-C(63)	105.3(3)
C(103)-Fe(3)-C(101)	68.0(3)	C(102)-Fe(3)-C(101)	40.9(3)
C(104)-Fe(3)-C(101)	65.8(3)	C(63)-Fe(3)-C(101)	149.3(3)
C(103)-Fe(3)-C(64)	105.7(3)	C(102)-Fe(3)-C(64)	130.0(3)
C(104)-Fe(3)-C(64)	114.1(3)	C(63)-Fe(3)-C(64)	39.8(4)
C(101)-Fe(3)-C(64)	170.8(3)	C(103)-Fe(3)-C(62)	161.8(4)
C(102)-Fe(3)-C(62)	154.1(3)	C(104)-Fe(3)-C(62)	124.8(3)
C(63)-Fe(3)-C(62)	40.1(3)	C(101)-Fe(3)-C(62)	118.8(3)
C(64)-Fe(3)-C(62)	69.3(3)	C(103)-Fe(3)-C(65)	113.9(3)
C(102)-Fe(3)-C(65)	108.5(3)	C(104)-Fe(3)-C(65)	145.5(3)
C(63)-Fe(3)-C(65)	69.6(3)	C(101)-Fe(3)-C(65)	134.7(3)
C(64)-Fe(3)-C(65)	40.5(3)	C(62)-Fe(3)-C(65)	74.3(3)
C(103)-Fe(3)-C(105)	66.5(3)	C(102)-Fe(3)-C(105)	66.7(2)
C(104)-Fe(3)-C(105)	39.0(3)	C(63)-Fe(3)-C(105)	116.5(3)
C(101)-Fe(3)-C(105)	38.1(3)	C(64)-Fe(3)-C(105)	146.8(3)
C(62)-Fe(3)-C(105)	107.5(2)	C(65)-Fe(3)-C(105)	172.7(3)
C(103)-Fe(3)-P(5)	149.7(3)	C(102)-Fe(3)-P(5)	114.5(3)
C(104)-Fe(3)-P(5)	166.6(2)	C(63)-Fe(3)-P(5)	75.3(2)
C(101)-Fe(3)-P(5)	106.6(2)	C(64)-Fe(3)-P(5)	75.3(2)
C(62)-Fe(3)-P(5)	47.7(2)	C(65)-Fe(3)-P(5)	47.6(2)
C(105)-Fe(3)-P(5)	128.4(2)	C(112)-Fe(4)-C(113)	41.0(3)
C(112)-Fe(4)-C(74)	107.3(4)	C(113)-Fe(4)-C(74)	133.1(3)
C(112)-Fe(4)-C(73)	110.6(4)	C(113)-Fe(4)-C(73)	108.4(3)
C(74)-Fe(4)-C(73)	40.1(3)	C(112)-Fe(4)-C(72)	139.9(4)
C(113)-Fe(4)-C(72)	110.9(3)	C(74)-Fe(4)-C(72)	69.4(3)
C(73)-Fe(4)-C(72)	40.8(3)	C(112)-Fe(4)-C(115)	66.5(4)
C(113)-Fe(4)-C(115)	66.5(3)	C(74)-Fe(4)-C(115)	144.3(3)
C(73)-Fe(4)-C(115)	174.8(3)	C(72)-Fe(4)-C(115)	138.9(3)
C(112)-Fe(4)-C(111)	39.8(4)	C(113)-Fe(4)-C(111)	67.9(4)
C(74)-Fe(4)-C(111)	112.1(3)	C(73)-Fe(4)-C(111)	140.2(3)
C(72)-Fe(4)-C(111)	178.5(3)	C(115)-Fe(4)-C(111)	40.0(3)
C(112)-Fe(4)-C(114)	67.2(4)	C(113)-Fe(4)-C(114)	40.3(3)
C(74)-Fe(4)-C(114)	173.4(4)	C(73)-Fe(4)-C(114)	137.0(3)
C(72)-Fe(4)-C(114)	112.0(3)	C(115)-Fe(4)-C(114)	38.2(4)
C(111)-Fe(4)-C(114)	66.5(3)	C(112)-Fe(4)-C(75)	130.7(3)
C(113)-Fe(4)-C(75)	171.0(4)	C(74)-Fe(4)-C(75)	40.2(3)
C(73)-Fe(4)-C(75)	69.7(3)	C(72)-Fe(4)-C(75)	73.7(4)
C(115)-Fe(4)-C(75)	115.5(3)	C(111)-Fe(4)-C(75)	107.6(3)

C(114)-Fe(4)-C(75)	146.2(4)	C(112)-Fe(4)-P(6)	171.5(3)
C(113)-Fe(4)-P(6)	140.2(3)	C(74)-Fe(4)-P(6)	77.0(2)
C(73)-Fe(4)-P(6)	77.5(2)	C(72)-Fe(4)-P(6)	48.3(2)
C(115)-Fe(4)-P(6)	105.6(3)	C(111)-Fe(4)-P(6)	131.9(3)
C(114)-Fe(4)-P(6)	108.9(3)	C(75)-Fe(4)-P(6)	48.6(2)
C(65)-P(5)-C(62)	89.5(4)	C(65)-P(5)-Fe(3)	59.7(2)
C(62)-P(5)-Fe(3)	59.3(2)	C(72)-P(6)-C(75)	88.5(5)
C(72)-P(6)-Fe(4)	60.5(3)	C(75)-P(6)-Fe(4)	60.6(3)
C(67)-P(7)-C(70)	92.1(3)	C(67)-P(7)-C(66)	105.3(3)
C(70)-P(7)-C(66)	94.3(3)	C(80)-P(8)-C(77)	91.8(3)
C(80)-P(8)-C(61)	103.2(3)	C(77)-P(8)-C(61)	96.0(3)
C(90)-Si(3)-C(89)	108.6(4)	C(90)-Si(3)-C(67)	105.0(3)
C(89)-Si(3)-C(67)	112.3(4)	C(90)-Si(3)-C(91)	110.0(4)
C(89)-Si(3)-C(91)	108.8(4)	C(67)-Si(3)-C(91)	111.9(4)
C(95)-Si(4)-C(96)	109.0(4)	C(95)-Si(4)-C(80)	104.9(4)
C(96)-Si(4)-C(80)	112.3(4)	C(95)-Si(4)-C(97)	109.8(4)
C(96)-Si(4)-C(97)	109.6(4)	C(80)-Si(4)-C(97)	111.1(4)
O(5)-C(61)-C(62)	125.9(7)	O(5)-C(61)-P(8)	119.5(5)
C(62)-C(61)-P(8)	114.5(5)	C(63)-C(62)-C(61)	124.0(6)
C(63)-C(62)-P(5)	112.3(5)	C(61)-C(62)-P(5)	123.6(5)
C(63)-C(62)-Fe(3)	68.6(4)	C(61)-C(62)-Fe(3)	129.6(5)
P(5)-C(62)-Fe(3)	73.0(2)	C(64)-C(63)-C(62)	113.5(4)
C(64)-C(63)-C(81)	123.6(5)	C(62)-C(63)-C(81)	122.7(6)
C(64)-C(63)-Fe(3)	70.8(3)	C(62)-C(63)-Fe(3)	71.3(4)
C(81)-C(63)-Fe(3)	129.8(6)	C(63)-C(64)-C(65)	112.7(5)
C(63)-C(64)-C(82)	124.4(5)	C(65)-C(64)-C(82)	122.8(6)
C(63)-C(64)-Fe(3)	69.4(3)	C(65)-C(64)-Fe(3)	70.9(4)
C(82)-C(64)-Fe(3)	129.8(6)	C(64)-C(65)-C(66)	124.0(6)
C(64)-C(65)-P(5)	111.8(5)	C(66)-C(65)-P(5)	124.1(6)
C(64)-C(65)-Fe(3)	68.7(4)	C(66)-C(65)-Fe(3)	128.7(5)
P(5)-C(65)-Fe(3)	72.6(3)	O(6)-C(66)-C(65)	126.3(7)
O(6)-C(66)-P(7)	120.5(5)	C(65)-C(66)-P(7)	113.2(5)
C(68)-C(67)-P(7)	109.7(6)	C(68)-C(67)-Si(3)	129.6(6)
P(7)-C(67)-Si(3)	120.6(4)	C(67)-C(68)-C(69)	113.9(6)
C(67)-C(68)-C(83)	125.7(8)	C(69)-C(68)-C(83)	120.3(7)
C(70)-C(69)-C(68)	114.6(7)	C(70)-C(69)-C(84)	126.5(7)
C(68)-C(69)-C(84)	118.9(6)	C(69)-C(70)-C(71)	124.3(7)
C(69)-C(70)-P(7)	109.3(6)	C(71)-C(70)-P(7)	126.4(5)
O(7)-C(71)-C(70)	120.2(6)	O(7)-C(71)-C(72)	117.5(6)
C(70)-C(71)-C(72)	122.0(6)	C(73)-C(72)-C(71)	130.1(7)
C(73)-C(72)-P(6)	114.2(5)	C(71)-C(72)-P(6)	115.6(6)
C(73)-C(72)-Fe(4)	69.5(4)	C(71)-C(72)-Fe(4)	131.4(5)
P(6)-C(72)-Fe(4)	71.2(3)	C(74)-C(73)-C(72)	110.7(5)
C(74)-C(73)-C(85)	124.0(5)	C(72)-C(73)-C(85)	125.3(7)
C(74)-C(73)-Fe(4)	69.5(3)	C(72)-C(73)-Fe(4)	69.7(4)
C(85)-C(73)-Fe(4)	126.0(5)	C(75)-C(74)-C(73)	113.4(5)
C(75)-C(74)-C(86)	123.8(6)	C(73)-C(74)-C(86)	122.8(5)
C(75)-C(74)-Fe(4)	70.8(4)	C(73)-C(74)-Fe(4)	70.4(3)
C(86)-C(74)-Fe(4)	126.5(5)	C(74)-C(75)-C(76)	130.6(7)
C(74)-C(75)-P(6)	113.2(5)	C(76)-C(75)-P(6)	116.1(6)
C(74)-C(75)-Fe(4)	69.0(4)	C(76)-C(75)-Fe(4)	131.7(5)
P(6)-C(75)-Fe(4)	70.8(3)	O(8)-C(76)-C(75)	120.5(6)
O(8)-C(76)-C(77)	118.8(6)	C(75)-C(76)-C(77)	120.6(6)
C(78)-C(77)-C(76)	126.2(7)	C(78)-C(77)-P(8)	109.8(6)
C(76)-C(77)-P(8)	123.9(5)	C(77)-C(78)-C(79)	114.0(7)
C(77)-C(78)-C(87)	126.2(7)	C(79)-C(78)-C(87)	119.8(6)
C(80)-C(79)-C(78)	115.5(6)	C(80)-C(79)-C(88)	124.0(7)
C(78)-C(79)-C(88)	120.5(7)	C(79)-C(80)-P(8)	108.6(5)
C(79)-C(80)-Si(4)	131.7(5)	P(8)-C(80)-Si(4)	119.5(4)
C(63)-C(81)-H(81A)	109.8	C(63)-C(81)-H(81B)	109.4
H(81A)-C(81)-H(81B)	109.5	C(63)-C(81)-H(81C)	109.3
H(81A)-C(81)-H(81C)	109.5	H(81B)-C(81)-H(81C)	109.5
C(64)-C(82)-H(82A)	109.3	C(64)-C(82)-H(82B)	109.4

H(82A)-C(82)-H(82B)	109.5	C(64)-C(82)-H(82C)	109.7
H(82A)-C(82)-H(82C)	109.5	H(82B)-C(82)-H(82C)	109.5
C(68)-C(83)-H(83A)	109.7	C(68)-C(83)-H(83B)	109.4
H(83A)-C(83)-H(83B)	109.5	C(68)-C(83)-H(83C)	109.2
H(83A)-C(83)-H(83C)	109.5	H(83B)-C(83)-H(83C)	109.5
C(69)-C(84)-H(84A)	109.7	C(69)-C(84)-H(84B)	109.1
H(84A)-C(84)-H(84B)	109.5	C(69)-C(84)-H(84C)	109.6
H(84A)-C(84)-H(84C)	109.5	H(84B)-C(84)-H(84C)	109.5
C(73)-C(85)-H(85A)	109.5	C(73)-C(85)-H(85B)	109.1
H(85A)-C(85)-H(85B)	109.5	C(73)-C(85)-H(85C)	109.8
H(85A)-C(85)-H(85C)	109.5	H(85B)-C(85)-H(85C)	109.5
C(74)-C(86)-H(86A)	109.1	C(74)-C(86)-H(86B)	109.5
H(86A)-C(86)-H(86B)	109.5	C(74)-C(86)-H(86C)	109.8
H(86A)-C(86)-H(86C)	109.5	H(86B)-C(86)-H(86C)	109.5
C(78)-C(87)-H(87A)	109.6	C(78)-C(87)-H(87B)	109.1
H(87A)-C(87)-H(87B)	109.5	C(78)-C(87)-H(87C)	109.7
H(87A)-C(87)-H(87C)	109.5	H(87B)-C(87)-H(87C)	109.5
C(79)-C(88)-H(88A)	109.7	C(79)-C(88)-H(88B)	109.3
H(88A)-C(88)-H(88B)	109.5	C(79)-C(88)-H(88C)	109.4
H(88A)-C(88)-H(88C)	109.5	H(88B)-C(88)-H(88C)	109.5
Si(3)-C(89)-H(89A)	109.5	Si(3)-C(89)-H(89B)	109.4
H(89A)-C(89)-H(89B)	109.5	Si(3)-C(89)-H(89C)	109.6
H(89A)-C(89)-H(89C)	109.5	H(89B)-C(89)-H(89C)	109.5
Si(3)-C(90)-H(90A)	109.4	Si(3)-C(90)-H(90B)	109.6
H(90A)-C(90)-H(90B)	109.5	Si(3)-C(90)-H(90C)	109.4
H(90A)-C(90)-H(90C)	109.5	H(90B)-C(90)-H(90C)	109.5
C(93)-C(91)-C(94)	110.6(8)	C(93)-C(91)-C(92)	108.3(7)
C(94)-C(91)-C(92)	108.5(7)	C(93)-C(91)-Si(3)	110.9(6)
C(94)-C(91)-Si(3)	110.8(5)	C(92)-C(91)-Si(3)	107.6(6)
C(91)-C(92)-H(92A)	109.8	C(91)-C(92)-H(92B)	109.4
H(92A)-C(92)-H(92B)	109.5	C(91)-C(92)-H(92C)	109.3
H(92A)-C(92)-H(92C)	109.5	H(92B)-C(92)-H(92C)	109.5
C(91)-C(93)-H(93A)	109.5	C(91)-C(93)-H(93B)	109.3
H(93A)-C(93)-H(93B)	109.5	C(91)-C(93)-H(93C)	109.6
H(93A)-C(93)-H(93C)	109.5	H(93B)-C(93)-H(93C)	109.5
C(91)-C(94)-H(94A)	109.4	C(91)-C(94)-H(94B)	109.9
H(94A)-C(94)-H(94B)	109.5	C(91)-C(94)-H(94C)	109.2
H(94A)-C(94)-H(94C)	109.5	H(94B)-C(94)-H(94C)	109.4
Si(4)-C(95)-H(95A)	109.4	Si(4)-C(95)-H(95B)	109.6
H(95A)-C(95)-H(95B)	109.5	Si(4)-C(95)-H(95C)	109.5
H(95A)-C(95)-H(95C)	109.5	H(95B)-C(95)-H(95C)	109.5
Si(4)-C(96)-H(96A)	109.5	Si(4)-C(96)-H(96B)	109.4
H(96A)-C(96)-H(96B)	109.5	Si(4)-C(96)-H(96C)	109.5
H(96A)-C(96)-H(96C)	109.5	H(96B)-C(96)-H(96C)	109.5
C(100)-C(97)-C(98)	111.4(8)	C(100)-C(97)-C(99)	107.1(7)
C(98)-C(97)-C(99)	109.8(7)	C(100)-C(97)-Si(4)	110.2(6)
C(98)-C(97)-Si(4)	110.2(6)	C(99)-C(97)-Si(4)	108.0(6)
C(97)-C(98)-H(98A)	109.4	C(97)-C(98)-H(98B)	109.2
H(98A)-C(98)-H(98B)	109.4	C(97)-C(98)-H(98C)	109.9
H(98A)-C(98)-H(98C)	109.5	H(98B)-C(98)-H(98C)	109.4
C(97)-C(99)-H(99A)	109.2	C(97)-C(99)-H(99B)	109.3
H(99A)-C(99)-H(99B)	109.5	C(97)-C(99)-H(99C)	109.9
H(99A)-C(99)-H(99C)	109.5	H(99B)-C(99)-H(99C)	109.5
C(97)-C(100)-H(10A)	109.6	C(97)-C(100)-H(10B)	109.3
H(10A)-C(100)-H(10B)	109.5	C(97)-C(100)-H(10C)	109.5
H(10A)-C(100)-H(10C)	109.5	H(10B)-C(100)-H(10C)	109.5
C(105)-C(101)-C(102)	109.0(6)	C(105)-C(101)-C(106)	130.0(7)
C(102)-C(101)-C(106)	120.8(6)	C(105)-C(101)-Fe(3)	71.9(5)
C(102)-C(101)-Fe(3)	69.1(3)	C(106)-C(101)-Fe(3)	128.7(5)
C(101)-C(102)-C(103)	104.9(6)	C(101)-C(102)-C(107)	130.4(8)
C(103)-C(102)-C(107)	124.6(8)	C(101)-C(102)-Fe(3)	70.0(3)
C(103)-C(102)-Fe(3)	68.1(5)	C(107)-C(102)-Fe(3)	129.8(5)
C(104)-C(103)-C(102)	107.8(6)	C(104)-C(103)-C(108)	123(1)

C(102)-C(103)-C(108)	128.9(8)	C(104)-C(103)-Fe(3)	71.3(4)
C(102)-C(103)-Fe(3)	70.4(4)	C(108)-C(103)-Fe(3)	126.2(6)
C(105)-C(104)-C(103)	108.7(7)	C(105)-C(104)-C(109)	123.9(7)
C(103)-C(104)-C(109)	127.3(7)	C(105)-C(104)-Fe(3)	71.8(5)
C(103)-C(104)-Fe(3)	68.8(3)	C(109)-C(104)-Fe(3)	128.5(6)
C(101)-C(105)-C(104)	109.5(6)	C(101)-C(105)-C(110)	122.1(7)
C(104)-C(105)-C(110)	128.0(7)	C(101)-C(105)-Fe(3)	70.0(4)
C(104)-C(105)-Fe(3)	69.2(4)	C(110)-C(105)-Fe(3)	132.0(4)
C(101)-C(106)-H(10D)	109.7	C(101)-C(106)-H(10E)	109.3
H(10D)-C(106)-H(10E)	109.5	C(101)-C(106)-H(10F)	109.4
H(10D)-C(106)-H(10F)	109.5	H(10E)-C(106)-H(10F)	109.5
C(102)-C(107)-H(10G)	109.3	C(102)-C(107)-H(10H)	109.4
H(10G)-C(107)-H(10H)	109.5	C(102)-C(107)-H(10I)	109.8
H(10G)-C(107)-H(10I)	109.5	H(10H)-C(107)-H(10I)	109.5
C(103)-C(108)-H(10J)	109.8	C(103)-C(108)-H(10K)	109.4
H(10J)-C(108)-H(10K)	109.5	C(103)-C(108)-H(10L)	109.3
H(10J)-C(108)-H(10L)	109.5	H(10K)-C(108)-H(10L)	109.5
C(104)-C(109)-H(10M)	109.7	C(104)-C(109)-H(10N)	109.4
H(10M)-C(109)-H(10N)	109.5	C(104)-C(109)-H(10O)	109.3
H(10M)-C(109)-H(10O)	109.5	H(10N)-C(109)-H(10O)	109.5
C(105)-C(110)-H(11A)	109.4	C(105)-C(110)-H(11B)	109.5
H(11A)-C(110)-H(11B)	109.5	C(105)-C(110)-H(11C)	109.5
H(11A)-C(110)-H(11C)	109.5	H(11B)-C(110)-H(11C)	109.5
C(112)-C(111)-C(115)	106.6(8)	C(112)-C(111)-C(116)	126(1)
C(115)-C(111)-C(116)	127.2(8)	C(112)-C(111)-Fe(4)	69.1(6)
C(115)-C(111)-Fe(4)	70.3(5)	C(116)-C(111)-Fe(4)	128.7(6)
C(111)-C(112)-C(113)	109(1)	C(111)-C(112)-C(117)	126.0(7)
C(113)-C(112)-C(117)	124.9(8)	C(111)-C(112)-Fe(4)	71.0(6)
C(113)-C(112)-Fe(4)	70.1(6)	C(117)-C(112)-Fe(4)	131(1)
C(114)-C(113)-C(112)	105.7(8)	C(114)-C(113)-C(118)	128.9(8)
C(112)-C(113)-C(118)	125(1)	C(114)-C(113)-Fe(4)	70.5(5)
C(112)-C(113)-Fe(4)	68.9(6)	C(118)-C(113)-Fe(4)	129.0(5)
C(115)-C(114)-C(113)	109.0(6)	C(115)-C(114)-C(119)	125.9(7)
C(113)-C(114)-C(119)	125.1(8)	C(115)-C(114)-Fe(4)	70.8(3)
C(113)-C(114)-Fe(4)	69.2(4)	C(119)-C(114)-Fe(4)	127.2(6)
C(114)-C(115)-C(111)	110.0(6)	C(114)-C(115)-C(120)	126.0(6)
C(111)-C(115)-C(120)	124.0(7)	C(114)-C(115)-Fe(4)	71.0(3)
C(111)-C(115)-Fe(4)	69.8(4)	C(120)-C(115)-Fe(4)	127.2(6)
C(111)-C(116)-H(11D)	109.4	C(111)-C(116)-H(11E)	109.5
H(11D)-C(116)-H(11E)	109.5	C(111)-C(116)-H(11F)	109.5
H(11D)-C(116)-H(11F)	109.5	H(11E)-C(116)-H(11F)	109.5
C(112)-C(117)-H(11G)	109.6	C(112)-C(117)-H(11H)	109.4
H(11G)-C(117)-H(11H)	109.5	C(112)-C(117)-H(11I)	109.4
H(11G)-C(117)-H(11I)	109.5	H(11H)-C(117)-H(11I)	109.5
C(113)-C(118)-H(11J)	109.5	C(113)-C(118)-H(11K)	109.5
H(11J)-C(118)-H(11K)	109.5	C(113)-C(118)-H(11L)	109.4
H(11J)-C(118)-H(11L)	109.5	H(11K)-C(118)-H(11L)	109.5
C(114)-C(119)-H(11M)	109.7	C(114)-C(119)-H(11N)	109.4
H(11M)-C(119)-H(11N)	109.5	C(114)-C(119)-H(11O)	109.3
H(11M)-C(119)-H(11O)	109.5	H(11N)-C(119)-H(11O)	109.5
C(115)-C(120)-H(12A)	109.3	C(115)-C(120)-H(12B)	109.4
H(12A)-C(120)-H(12B)	109.5	C(115)-C(120)-H(12C)	109.8
H(12A)-C(120)-H(12C)	109.5	H(12B)-C(120)-H(12C)	109.5

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **9**

atom	U11	U22	U33	U23	U13	U12
Fe(1)	27(1)	20(1)	30(1)	-1(1)	2(1)	-1(1)
Fe(2)	34(1)	33(1)	23(1)	0(1)	2(1)	1(1)
P(1)	30(1)	38(1)	29(1)	-1(1)	-4(1)	-1(1)
P(2)	33(1)	25(1)	25(1)	-1(1)	1(1)	-2(1)
P(3)	36(1)	25(1)	31(1)	-1(1)	0(1)	5(1)
P(4)	38(1)	24(1)	31(1)	0(1)	1(1)	-6(1)
Si(1)	31(1)	22(1)	32(1)	-2(1)	1(1)	2(1)
Si(2)	35(1)	26(1)	34(1)	4(1)	0(1)	-4(1)
O(1)	42(3)	44(3)	67(3)	23(2)	-26(2)	-12(2)
O(2)	48(3)	45(3)	100(4)	-44(3)	-37(3)	22(2)
O(3)	67(3)	27(2)	35(2)	-10(2)	-7(2)	12(2)
O(4)	84(4)	33(2)	33(3)	4(2)	1(2)	-19(2)
C(1)	56(5)	47(4)	37(4)	10(3)	4(3)	-15(3)
C(2)	21(3)	34(3)	31(3)	1(2)	-4(3)	-8(2)
C(3)	31(4)	47(4)	26(3)	9(3)	-3(3)	-7(3)
C(4)	30(4)	40(3)	26(3)	-6(2)	-3(3)	5(3)
C(5)	29(4)	30(3)	39(4)	-8(3)	-5(3)	10(3)
C(6)	43(4)	36(3)	39(4)	-15(3)	-7(3)	6(3)
C(7)	31(3)	30(3)	32(3)	-2(2)	-3(3)	5(3)
C(8)	36(4)	34(3)	26(3)	-4(2)	3(3)	-1(3)
C(9)	31(4)	35(3)	29(3)	7(2)	2(3)	1(3)
C(10)	43(4)	23(3)	30(4)	2(3)	-1(3)	-2(3)
C(11)	42(4)	21(3)	36(4)	1(2)	0(3)	3(3)
C(12)	44(4)	28(3)	28(4)	-1(3)	4(3)	5(3)
C(13)	47(4)	30(3)	21(3)	-3(2)	-1(3)	9(3)
C(14)	42(4)	30(4)	22(3)	0(3)	4(3)	-7(3)
C(15)	45(4)	17(3)	28(3)	5(2)	5(3)	-2(3)
C(16)	41(4)	29(3)	39(4)	3(3)	-2(3)	-2(3)
C(17)	47(4)	23(3)	33(4)	0(3)	-1(3)	2(3)
C(18)	41(4)	21(3)	31(3)	-5(2)	1(3)	-1(3)
C(19)	40(4)	35(4)	31(3)	-5(3)	2(3)	2(3)
C(20)	36(4)	37(3)	34(3)	2(3)	1(3)	-6(3)
C(21)	42(4)	34(3)	34(4)	2(3)	-5(3)	-13(3)
C(22)	42(5)	43(4)	38(4)	-6(3)	-9(3)	15(3)
C(23)	28(4)	47(4)	62(4)	-1(3)	0(3)	-4(3)
C(24)	33(4)	39(4)	64(5)	0(3)	8(3)	-6(3)
C(25)	43(5)	28(3)	39(4)	-4(3)	0(3)	5(3)
C(26)	49(5)	26(3)	40(5)	-1(3)	1(4)	-5(3)
C(27)	38(4)	24(3)	79(5)	-2(3)	1(4)	-4(3)
C(28)	32(4)	51(4)	66(5)	-7(3)	-4(3)	0(3)
C(29)	32(4)	41(4)	53(5)	-22(3)	1(4)	7(3)
C(30)	36(4)	33(4)	49(5)	2(3)	3(3)	-6(3)
C(31)	39(5)	36(4)	53(5)	5(3)	-6(4)	-3(3)
C(32)	110(8)	38(4)	62(6)	6(4)	-7(5)	-6(5)
C(33)	63(7)	50(5)	88(7)	-6(5)	-11(6)	6(5)
C(34)	59(5)	51(4)	35(4)	-6(3)	-8(3)	-7(4)
C(35)	47(5)	43(4)	49(5)	-6(3)	11(4)	6(4)
C(36)	51(5)	49(5)	83(7)	48(4)	-8(5)	-14(4)
C(37)	38(5)	43(4)	57(5)	-6(4)	-11(4)	2(3)
C(38)	70(6)	75(6)	37(4)	8(4)	-12(4)	-9(4)
C(39)	79(8)	71(7)	103(8)	31(6)	-28(7)	-24(6)
C(40)	160(10)	62(6)	58(6)	-18(4)	-24(6)	54(6)
C(41)	38(4)	48(4)	57(5)	18(3)	15(4)	18(3)
C(42)	38(4)	63(5)	38(4)	-9(3)	7(3)	-4(4)
C(43)	31(4)	28(3)	52(4)	5(3)	7(3)	-1(3)
C(44)	30(5)	56(4)	32(5)	0(3)	5(4)	-7(3)
C(45)	60(5)	26(4)	58(5)	-11(3)	32(4)	-6(3)
C(46)	64(6)	91(7)	170(10)	55(7)	38(6)	47(5)

C(47)	43(5)	150(10)	84(6)	-13(6)	2(4)	-36(5)
C(48)	88(6)	31(3)	103(6)	14(3)	28(5)	-11(3)
C(49)	60(6)	175(8)	29(5)	0(6)	11(4)	-20(7)
C(50)	150(10)	64(6)	140(10)	-67(6)	92(7)	-41(6)
C(51)	50(5)	64(5)	14(3)	-7(3)	4(3)	-4(4)
C(52)	63(5)	34(3)	53(4)	0(3)	27(3)	14(3)
C(53)	44(5)	101(7)	36(4)	15(5)	15(3)	9(5)
C(54)	82(7)	102(7)	54(6)	-57(5)	55(5)	-74(6)
C(55)	79(6)	43(4)	32(4)	17(3)	23(4)	22(4)
C(56)	124(3)	99(3)	82(2)	-6(2)	31(2)	0(3)
C(57)	124(3)	99(3)	82(2)	-6(2)	31(2)	0(3)
C(58)	124(3)	99(3)	82(2)	-6(2)	31(2)	0(3)
C(59)	124(3)	99(3)	82(2)	-6(2)	31(2)	0(3)
C(60)	124(3)	99(3)	82(2)	-6(2)	31(2)	0(3)
Fe(3)	38(1)	27(1)	25(1)	0(1)	-3(1)	-3(1)
Fe(4)	26(1)	25(1)	27(1)	-1(1)	1(1)	0(1)
P(5)	38(1)	25(1)	24(1)	0(1)	0(1)	-4(1)
P(6)	31(1)	33(1)	29(1)	-1(1)	4(1)	-3(1)
P(7)	31(1)	22(1)	31(1)	-1(1)	0(1)	2(1)
P(8)	38(1)	22(1)	32(1)	1(1)	1(1)	-6(1)
Si(3)	32(1)	26(1)	36(1)	1(1)	-1(1)	3(1)
Si(4)	34(1)	23(1)	38(1)	-1(1)	-3(1)	-2(1)
O(5)	70(3)	28(2)	35(3)	-5(2)	1(2)	-9(2)
O(6)	63(3)	31(2)	33(2)	5(2)	-4(2)	3(2)
O(7)	53(3)	47(3)	74(3)	22(2)	28(3)	14(2)
O(8)	49(3)	39(2)	83(4)	-16(2)	20(3)	-11(2)
C(61)	33(4)	30(3)	31(4)	-5(2)	3(3)	-6(3)
C(62)	30(3)	20(3)	22(3)	-3(2)	-2(3)	-1(2)
C(63)	31(4)	19(3)	34(4)	0(2)	-1(3)	6(3)
C(64)	27(4)	22(3)	34(4)	-2(3)	0(3)	-5(3)
C(65)	31(4)	31(3)	23(3)	1(2)	-2(3)	-3(3)
C(66)	30(3)	29(3)	26(3)	-7(2)	-6(2)	0(2)
C(67)	28(3)	20(3)	35(4)	1(2)	-1(3)	3(2)
C(68)	33(4)	30(3)	37(4)	3(3)	3(3)	-2(3)
C(69)	30(4)	42(4)	30(3)	4(3)	-1(3)	0(3)
C(70)	34(3)	29(3)	31(3)	5(2)	2(3)	2(3)
C(71)	25(3)	31(3)	38(3)	1(2)	8(3)	1(2)
C(72)	31(4)	40(4)	33(3)	6(3)	-1(3)	4(3)
C(73)	23(3)	33(4)	31(3)	-4(3)	-2(3)	1(3)
C(74)	24(3)	28(3)	33(4)	0(2)	-3(3)	-6(2)
C(75)	27(4)	39(4)	27(3)	-5(3)	-1(3)	-5(3)
C(76)	26(3)	37(3)	43(4)	-10(3)	14(3)	-12(3)
C(77)	35(4)	33(3)	29(3)	-3(3)	1(3)	-7(3)
C(78)	33(4)	28(3)	38(3)	2(2)	1(3)	-2(2)
C(79)	34(4)	19(3)	40(4)	-3(2)	-2(3)	-1(2)
C(80)	33(4)	22(3)	39(4)	1(3)	-5(3)	-11(3)
C(81)	41(4)	38(4)	37(4)	-3(3)	14(3)	7(3)
C(82)	42(4)	34(4)	36(4)	1(3)	14(3)	-18(3)
C(83)	55(5)	30(3)	72(5)	-12(3)	5(4)	-14(3)
C(84)	40(4)	48(4)	42(4)	1(3)	-1(3)	-4(3)
C(85)	35(4)	55(4)	32(4)	6(3)	8(3)	15(3)
C(86)	33(4)	46(4)	35(4)	2(3)	1(3)	-3(3)
C(87)	38(4)	43(4)	44(4)	2(3)	1(3)	-4(3)
C(88)	44(4)	17(3)	68(5)	4(3)	-2(3)	-3(3)
C(89)	65(6)	50(5)	50(5)	0(4)	-1(5)	9(4)
C(90)	40(5)	48(5)	48(5)	-3(4)	-5(4)	7(4)
C(91)	50(5)	24(3)	30(4)	1(3)	7(4)	6(3)
C(92)	38(5)	81(7)	49(5)	-4(4)	21(4)	14(4)
C(93)	63(5)	48(4)	46(4)	-25(3)	14(4)	-12(4)
C(94)	80(6)	38(4)	41(4)	7(3)	17(4)	-1(4)
C(95)	36(4)	49(5)	41(5)	3(3)	0(3)	5(3)
C(96)	49(6)	52(5)	54(5)	-2(4)	-3(4)	0(4)
C(97)	62(6)	22(3)	32(4)	0(3)	6(4)	-1(3)

C(98)	102(7)	36(4)	35(4)	-2(3)	2(4)	-16(4)
C(99)	43(5)	57(5)	49(5)	6(4)	20(4)	-3(4)
C(100)	66(5)	38(4)	49(4)	22(3)	9(4)	8(3)
C(101)	49(4)	37(3)	44(4)	15(3)	-18(3)	-12(3)
C(102)	64(5)	26(3)	49(4)	-13(3)	-33(4)	7(3)
C(103)	71(6)	47(4)	47(5)	26(4)	-33(5)	-28(4)
C(104)	50(5)	47(4)	36(4)	-11(3)	-9(3)	-8(3)
C(105)	68(5)	39(3)	40(3)	-10(3)	-19(3)	7(3)
C(106)	33(3)	103(5)	41(3)	20(3)	-5(2)	-7(3)
C(107)	133(7)	87(5)	177(8)	-97(5)	-133(6)	95(5)
C(108)	173(8)	104(6)	87(5)	88(4)	-87(5)	-111(6)
C(109)	66(4)	91(5)	28(3)	-21(3)	2(3)	-5(3)
C(110)	77(4)	28(3)	46(3)	1(2)	-23(3)	-27(3)
C(111)	37(4)	34(4)	44(4)	8(3)	-12(3)	-1(3)
C(112)	32(6)	77(6)	35(5)	-2(3)	-9(4)	-3(3)
C(113)	46(5)	36(4)	59(5)	-19(3)	-28(4)	15(3)
C(114)	29(4)	53(4)	50(5)	11(4)	-6(4)	-17(3)
C(115)	18(3)	47(4)	40(4)	1(3)	-4(3)	2(3)
C(116)	82(6)	27(3)	105(6)	11(3)	-42(4)	-13(3)
C(117)	41(5)	116(6)	43(5)	16(4)	6(3)	0(4)
C(118)	103(7)	43(4)	77(5)	-19(3)	-40(5)	10(4)
C(119)	80(7)	85(6)	64(5)	38(4)	-16(4)	-50(5)
C(120)	44(4)	85(6)	57(4)	-26(4)	6(3)	15(4)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table 5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **9**

atom	x	y	z	U(eq)
H(21A)	-11153.0010	-4608	2805	55
H(21B)	-11279	-4092.0002	2399	55
H(21C)	-10710	-4415	2281	55
H(22A)	-10743.0010	-5705.9995	2304	62
H(22B)	-11330	-5987	2457	62
H(22C)	-11164	-5459	2816	62
H(23A)	-12273	-7104	1383	69
H(23B)	-11925	-7600	1629	69
H(23C)	-12049	-7529	886	69
H(24A)	-10488	-8051	1212	68
H(24B)	-11094	-8061	876	68
H(24C)	-11049	-8026.0005	1634	68
H(25A)	-11289.9990	-5996	-823	55
H(25B)	-11549	-5477	-1130	55
H(25C)	-11805	-5704	-483.0000	55
H(26A)	-11519.9990	-4575	-1136	58
H(26B)	-11277	-4065	-794	58
H(26C)	-11796	-4374	-486	58
H(27A)	-10506.9990	-2044	1354	71
H(27B)	-11108	-2098	1694	71
H(27C)	-11073	-2033	939	71
H(28A)	-12054	-2597	912	75
H(28B)	-11944	-2542	1659	75
H(28C)	-12268	-3043	1386	75
H(29A)	-9606	-8095	731	63
H(29B)	-9039	-7817.9995	491	63
H(29C)	-9620	-7720.9995	122	63
H(30A)	-9381	-6516	299	58
H(30B)	-8832	-6630	721	58
H(30C)	-9330	-6274	998	58
H(32A)	-9361	-7907.9995	2623	105
H(32B)	-9520	-8122	1932	105
H(32C)	-9961	-7769	2317	105
H(33A)	-8490	-7070	1702	101
H(33B)	-8560	-7689	1638	101
H(33C)	-8511	-7427	2326	101
H(34A)	-9866	-6813	2346	72
H(34B)	-9271	-6545	2199	72
H(34C)	-9332	-6937	2787	72
H(35A)	-9318	-3746	942	69
H(35B)	-8800	-3369	773	69
H(35C)	-9304	-3445	276	69
H(36A)	-9080	-2177	528	92
H(36B)	-9640	-1923.0001	820	92
H(36C)	-9676	-2269	188	92
H(38A)	-9242	-3152	2786	91
H(38B)	-9212	-3513	2166	91
H(38C)	-9804	-3278	2392	91
H(39A)	-8508	-2550	2339	127
H(39B)	-8583	-2325	1634	127
H(39C)	-8463	-2934	1741	127
H(40A)	-9978	-2353	2386	141
H(40B)	-9584	-1958.0001	1999	141
H(40C)	-9383	-2177	2675	141
H(46A)	-13656	-4111	1814	160
H(46B)	-13479	-4435	1195	160
H(46C)	-13063	-4001	1476	160

H(47A)	-13313	-5890	1386	137
H(47B)	-13437.9990	-5343.0005	1048	137
H(47C)	-13857	-5558	1583	137
H(48A)	-13099	-6200	2843	111
H(48B)	-12424.9990	-6167	2832	111
H(48C)	-12766	-6273	2188	111
H(49A)	-12460.0010	-5091	3820	132
H(49B)	-11907.0010	-4893	3455	132
H(49C)	-12067	-5500	3452	132
H(50A)	-12423	-3811	2454	176
H(50B)	-12246	-4068	3118	176
H(50C)	-12878	-3865	3012	176
H(56A)	-10867	-5236	-1926	153
H(56B)	-10602	-5809.9995	-1901	153
H(56C)	-10365	-5391	-2399	153
H(57A)	-9437	-6224	-1550	153
H(57B)	-10036	-6287.9995	-1207	153
H(57C)	-9469	-6276.9995	-793	153
H(58A)	-9053	-5507	75	153
H(58B)	-8623	-5096	-231	153
H(58C)	-8688	-5666.0005	-535	153
H(59A)	-8903	-4104	-983.9999	153
H(59B)	-9072	-4247	-268	153
H(59C)	-9472	-3876	-682	153
H(60A)	-10059	-4161	-2098	153
H(60B)	-10203	-3931	-1410	153
H(60C)	-10653	-4290	-1773.0001	153
H(81A)	-9315	-9301	5947	58
H(81B)	-8791	-9033	6298	58
H(81C)	-9058	-9559	6576	58
H(82A)	-9002	-10423	6592	56
H(82B)	-8725	-10931	6279	56
H(82C)	-9273	-10671.9990	5965	56
H(83A)	-7991	-12983	4230	79
H(83B)	-8508	-12922	3746	79
H(83C)	-8625	-12984	4491	79
H(84A)	-9511	-12421	4571	65
H(84B)	-9462	-12416	3811	65
H(84C)	-9763	-11942	4174	65
H(85A)	-8687	-10427.0010	2655	61
H(85B)	-8735	-10925	3111	61
H(85C)	-8196	-10551	3155	61
H(86A)	-8841	-8989	2996	57
H(86B)	-8697	-9513	2614	57
H(86C)	-8256	-9284	3119	57
H(87A)	-9805	-7889.9995	4120	63
H(87B)	-9471	-7440.9995	3748	63
H(87C)	-9538	-7411	4504	63
H(88A)	-7992	-6937.9995	4312	64
H(88B)	-8644	-6912	4510	64
H(88C)	-8471	-6954	3776	64
H(89A)	-6957	-12656	5310	83
H(89B)	-6634	-12940	4739	83
H(89C)	-7304.0005	-12997	4808	83
H(90A)	-6830.0005	-11270	4550	68
H(90B)	-6286	-11634.0010	4635	68
H(90C)	-6751.0005	-11604	5186	68
H(92A)	-6059	-12697.0010	3867	84
H(92B)	-5942.9995	-12088	3757	84
H(92C)	-5959	-12479	3163	84
H(93A)	-6901	-12861	2791	78
H(93B)	-7463	-12757	3194	78
H(93C)	-6966	-13103	3489	78

H(94A)	-6696	-11884	2639	80
H(94B)	-6702	-11504	3242	80
H(94C)	-7278	-11756.0010	2990	80
H(95A)	-6918	-8464	5154	63
H(95B)	-6372	-8366	4721	63
H(95C)	-6880	-8719	4461	63
H(96A)	-7318	-7007	4909	77
H(96B)	-6659	-7043	4748	77
H(96C)	-6912	-7361	5337	77
H(98A)	-6772	-8083	2648	86
H(98B)	-7368	-8161	2992	86
H(98C)	-6824	-8470	3242	86
H(99A)	-5978	-7543	3173	75
H(99B)	-5984	-7937	3763	75
H(99C)	-6057.9995	-7324	3879	75
H(10A)	-6960	-6866.0005	3563	77
H(10B)	-7458	-7170	3206	77
H(10C)	-6871	-7070	2851	77
H(10D)	-6075	-9454	5996	88
H(10E)	-6523	-9337	5446	88
H(10F)	-6258.9995	-9909	5519	88
H(10G)	-6612	-10775	5674	199
H(10H)	-6941	-11102.9990	6205	199
H(10I)	-6344	-10843	6366	199
H(10J)	-7500	-10927	7465	182
H(10K)	-7887	-11022	6854	182
H(10L)	-8093	-10634	7403	182
H(10M)	-7827	-9496	7846	92
H(10N)	-8330	-9787	7481	92
H(10O)	-8160	-9203	7289	92
H(11A)	-7531	-8675	6538	76
H(11B)	-6907	-8726	6253	76
H(11C)	-7003	-8736	7006	76
H(11D)	-10614.0010	-8884	2524	107
H(11E)	-9941	-8887	2593	107
H(11F)	-10329	-8767	3199	107
H(11G)	-9956	-9968	1608	100
H(11H)	-9384	-10124	1965	100
H(11I)	-9576	-9526	1931	100
H(11J)	-9810	-11181	2956	112
H(11K)	-9795	-10944	2253	112
H(11L)	-10368	-11188	2527	112
H(11M)	-10774	-10648	4313	115
H(11N)	-10687	-11087	3782	115
H(11O)	-11253.0010	-10746	3789	115
H(12A)	-11384	-9458	3780	93
H(12B)	-10836.9990	-9155	4034	93
H(12C)	-11019	-9698	4350	93

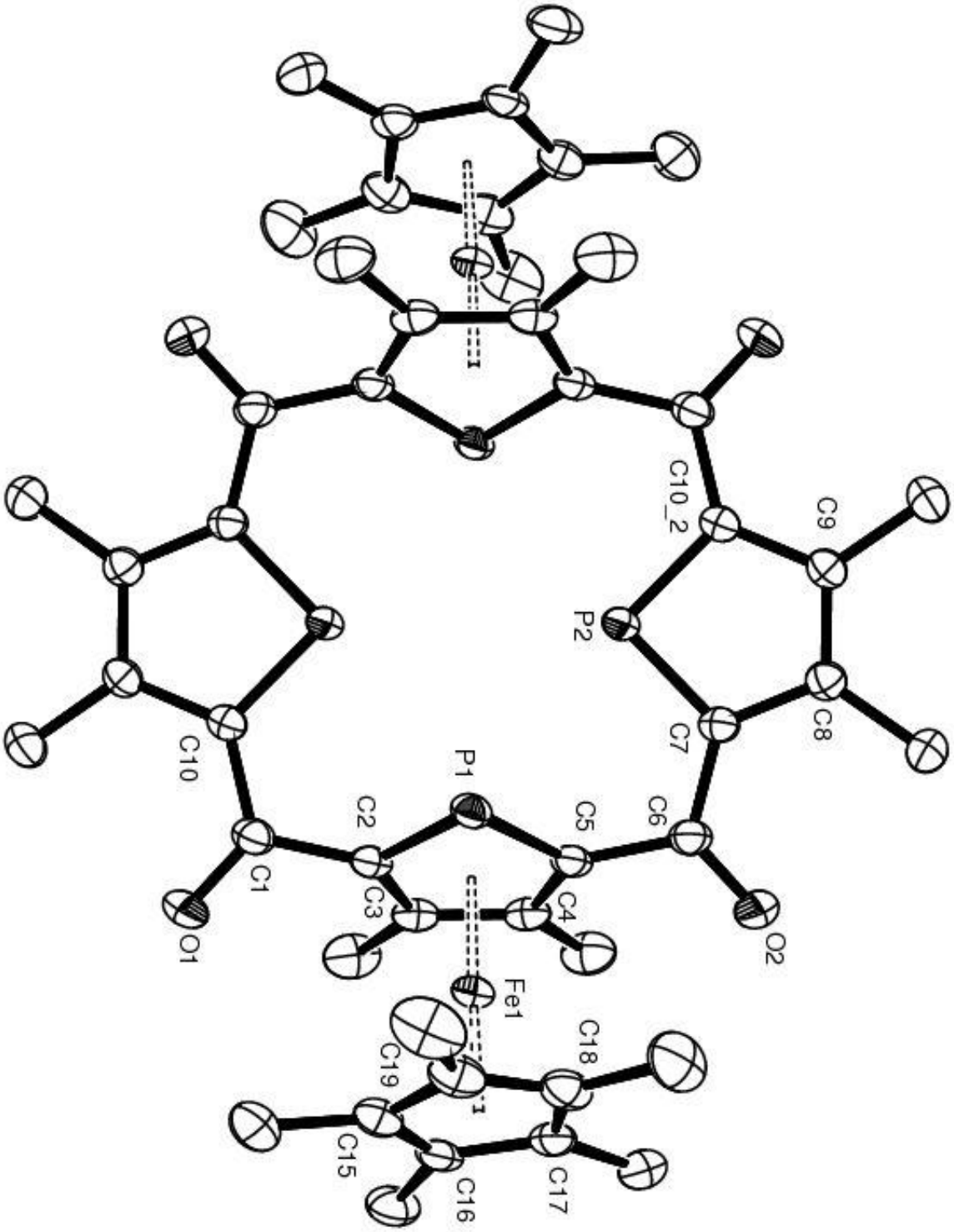
C10_2
C9
P2
C8
C7
C10
P1
C2
C5
C6
C1
C3
C4
O1
O2
Fe1
C18
C19
C15
C16
C17

Table 1. Crystal data for **10**

Compound	em485
Molecular formula	$C_{48}H_{54}Fe_2O_4P_4$,2($C_{16}H_{30}KN_2O_6$),2(C_2H_3N)
Molecular weight	1783.64
Crystal habit	Red Block
Crystal dimensions(mm)	0.40x0.30x0.26
Crystal system	triclinic
Space group	P-1
a(Å)	13.995(1)
b(Å)	14.050(1)
c(Å)	14.447(1)
α(°)	108.305(1)
β(°)	106.230(1)
γ(°)	109.092(1)
V(Å^3)	2305.8(3)
Z	1
d(g-cm^{-3})	1.285
F(000)	944
μ(cm^{-1})	0.538
Absorption corrections	multi-scan ; 0.8137 min, 0.8728 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	29.97
HKL ranges	-19 17 ; -19 19 ; -19 20
Reflections measured	28523
Unique data	13331
Rint	0.0214
Reflections used	10339
Criterion	I > 2σ(I)
Refinement type	Fsqd
Hydrogen atoms	constr
Parameters refined	526
Reflections / parameter	19
wR2	0.0999
R1	0.0358
Weights a, b	0.0498 ; 0.1565
GoF	1.059
difference peak / hole (e Å^{-3})	0.580(0.051) / -0.414(0.051)

Table 2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **10**

atom	x	y	z	U(eq)
Fe(1)	6549(1)	3560(1)	2718(1)	22(1)
P(1)	5301(1)	1824(1)	1306(1)	24(1)
P(2)	5155(1)	599(1)	-951(1)	24(1)
O(1)	6168(1)	1615(1)	4020(1)	47(1)
O(2)	6939(1)	3910(1)	372(1)	43(1)
C(1)	5897(1)	1180(1)	3037(1)	28(1)
C(2)	6222(1)	1902(1)	2488(1)	25(1)
C(3)	7370(1)	2594(1)	2787(1)	26(1)
C(4)	7515(1)	3046(1)	2046(1)	27(1)
C(5)	6468(1)	2698(1)	1194(1)	25(1)
C(6)	6391(1)	2944(1)	235(1)	28(1)
C(7)	5725(1)	1970(1)	-822(1)	23(1)
C(8)	5532(1)	1974(1)	-1850(1)	25(1)
C(9)	4947(1)	900(1)	-2702(1)	24(1)
C(10)	5322(1)	-32(1)	2354(1)	23(1)
C(11)	8323(1)	2746(1)	3720(1)	41(1)
C(12)	8648(1)	3711(1)	2115(1)	39(1)
C(13)	5897(2)	3052(1)	-1973(1)	38(1)
C(14)	4589(1)	643(1)	-3876(1)	34(1)
C(15)	6316(1)	4350(1)	4062(1)	31(1)
C(16)	7406(1)	4994(1)	4174(1)	29(1)
C(17)	7288(1)	5278(1)	3293(1)	30(1)
C(18)	6122(1)	4803(1)	2632(1)	33(1)
C(19)	5524(1)	4231(1)	3104(1)	35(1)
C(20)	6044(2)	3946(2)	4845(1)	43(1)
C(21)	8489(1)	5359(1)	5092(1)	39(1)
C(22)	8207(1)	5978(1)	3099(1)	42(1)
C(23)	5615(2)	4933(2)	1645(1)	52(1)
C(24)	4272(1)	3651(2)	2700(2)	53(1)
K(1)	40(1)	8924(1)	2241(1)	31(1)
O(3)	1678(1)	8546(1)	1671(1)	34(1)
O(4)	-553(1)	6937(1)	480(1)	31(1)
O(5)	-2136(1)	7215(1)	1281(1)	32(1)
O(6)	-1607(1)	9362(1)	2744(1)	32(1)
O(7)	706(1)	10861(1)	4108(1)	34(1)
O(8)	2235(1)	10723(1)	3198(1)	36(1)
N(1)	-963(2)	9698(2)	742(2)	66(1)
N(2)	920(2)	8100(2)	3697(1)	60(1)
C(25)	1300(1)	7663(1)	639(1)	39(1)
C(26)	337(1)	6657(1)	474(1)	38(1)
C(27)	-1504(1)	6016(1)	333(1)	36(1)
C(28)	-2436(1)	6335(1)	266(1)	36(1)
C(29)	-2969(1)	7589(1)	1270(1)	36(1)
C(30)	-2645(1)	8414(1)	2387(1)	38(1)
C(31)	-1214(1)	10154(1)	3826(1)	38(1)
C(32)	-177(1)	11162(1)	4107(1)	40(1)
C(33)	1713(1)	11802(1)	4391(1)	42(1)
C(34)	2577(1)	11424(2)	4301(1)	42(1)
C(35)	3048(1)	10369(2)	3037(1)	44(1)
C(36)	2580(1)	9549(2)	1880(1)	42(1)
C(37)	-1596(1)	10018(2)	823(1)	39(1)
C(38)	-2399(1)	10429(2)	937(1)	42(1)
C(39)	1557(2)	7790(2)	3605(1)	46(1)
C(40)	2395(2)	7417(2)	3476(1)	62(1)
N(3)	1585(2)	4423(2)	2279(2)	93(1)
C(41)	1439(2)	3528(3)	2001(2)	63(1)
C(42)	1257(2)	2383(2)	1633(2)	82(1)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table 3. Bond lengths (A) and angles (deg) for **10**

Fe(1)-C(18)	2.049(1)	Fe(1)-C(3)	2.052(1)
Fe(1)-C(17)	2.053(1)	Fe(1)-C(4)	2.055(1)
Fe(1)-C(19)	2.063(2)	Fe(1)-C(16)	2.066(1)
Fe(1)-C(15)	2.084(1)	Fe(1)-C(5)	2.103(1)
Fe(1)-C(2)	2.116(1)	Fe(1)-P(1)	2.2928(4)
P(1)-C(2)	1.775(1)	P(1)-C(5)	1.779(1)
P(2)-C(7)	1.752(1)	P(2)-C(10)#2	1.752(1)
O(1)-C(1)	1.240(2)	O(2)-C(6)	1.240(2)
C(1)-C(10)	1.457(2)	C(1)-C(2)	1.507(2)
C(2)-C(3)	1.427(2)	C(3)-C(4)	1.433(2)
C(3)-C(11)	1.507(2)	C(4)-C(5)	1.430(2)
C(4)-C(12)	1.510(2)	C(5)-C(6)	1.513(2)
C(6)-C(7)	1.460(2)	C(7)-C(8)	1.435(2)
C(8)-C(9)	1.387(2)	C(8)-C(13)	1.517(2)
C(9)-C(10)#2	1.439(2)	C(9)-C(14)	1.510(2)
C(10)-C(9)#2	1.439(2)	C(10)-P(2)#2	1.752(1)
C(11)-H(11A)	0.9800	C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800	C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800	C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800	C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800	C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800	C(14)-H(14C)	0.9800
C(15)-C(16)	1.428(2)	C(15)-C(19)	1.431(2)
C(15)-C(20)	1.500(2)	C(16)-C(17)	1.432(2)
C(16)-C(21)	1.503(2)	C(17)-C(18)	1.428(2)
C(17)-C(22)	1.500(2)	C(18)-C(19)	1.426(2)
C(18)-C(23)	1.501(2)	C(19)-C(24)	1.507(2)
C(20)-H(20A)	0.9800	C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800	C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800	C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800	C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800	C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800	C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800	C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800	K(1)-O(5)	2.780(1)
K(1)-O(3)	2.791(1)	K(1)-O(4)	2.793(1)
K(1)-O(6)	2.793(1)	K(1)-O(7)	2.806(1)
K(1)-O(8)	2.844(1)	K(1)-N(2)	2.880(2)
K(1)-N(1)	2.937(2)	O(3)-C(25)	1.418(2)
O(3)-C(36)	1.423(2)	O(4)-C(26)	1.425(2)
O(4)-C(27)	1.426(2)	O(5)-C(28)	1.426(2)
O(5)-C(29)	1.426(2)	O(6)-C(31)	1.419(2)
O(6)-C(30)	1.426(2)	O(7)-C(33)	1.422(2)
O(7)-C(32)	1.430(2)	O(8)-C(34)	1.420(2)
O(8)-C(35)	1.429(2)	N(1)-C(37)	1.134(2)
N(2)-C(39)	1.133(2)	C(25)-C(26)	1.495(2)
C(25)-H(25A)	0.9900	C(25)-H(25B)	0.9900
C(26)-H(26A)	0.9900	C(26)-H(26B)	0.9900
C(27)-C(28)	1.500(2)	C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900	C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900	C(29)-C(30)	1.492(2)
C(29)-H(29A)	0.9900	C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9900	C(30)-H(30B)	0.9900
C(31)-C(32)	1.497(2)	C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900	C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900	C(33)-C(34)	1.492(2)
C(33)-H(33A)	0.9900	C(33)-H(33B)	0.9900
C(34)-H(34A)	0.9900	C(34)-H(34B)	0.9900
C(35)-C(36)	1.495(2)	C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900	C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900	C(37)-C(38)	1.446(2)

C(38)-H(38A)	0.9800	C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800	C(39)-C(40)	1.466(3)
C(40)-H(40A)	0.9800	C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800	N(3)-C(41)	1.120(3)
C(41)-C(42)	1.433(4)	C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800	C(42)-H(42C)	0.9800

C(18)-Fe(1)-C(3)	163.92(6)	C(18)-Fe(1)-C(17)	40.73(6)
C(3)-Fe(1)-C(17)	125.89(6)	C(18)-Fe(1)-C(4)	125.96(6)
C(3)-Fe(1)-C(4)	40.83(5)	C(17)-Fe(1)-C(4)	104.88(6)
C(18)-Fe(1)-C(19)	40.58(6)	C(3)-Fe(1)-C(19)	153.61(6)
C(17)-Fe(1)-C(19)	68.24(6)	C(4)-Fe(1)-C(19)	165.34(6)
C(18)-Fe(1)-C(16)	68.29(6)	C(3)-Fe(1)-C(16)	107.11(5)
C(17)-Fe(1)-C(16)	40.69(5)	C(4)-Fe(1)-C(16)	116.00(6)
C(19)-Fe(1)-C(16)	67.86(6)	C(18)-Fe(1)-C(15)	68.20(6)
C(3)-Fe(1)-C(15)	118.97(5)	C(17)-Fe(1)-C(15)	68.20(6)
C(4)-Fe(1)-C(15)	150.79(5)	C(19)-Fe(1)-C(15)	40.36(5)
C(16)-Fe(1)-C(15)	40.25(6)	C(18)-Fe(1)-C(5)	105.55(5)
C(3)-Fe(1)-C(5)	69.55(5)	C(17)-Fe(1)-C(5)	113.49(5)
C(4)-Fe(1)-C(5)	40.22(5)	C(19)-Fe(1)-C(5)	129.16(5)
C(16)-Fe(1)-C(5)	147.35(6)	C(15)-Fe(1)-C(5)	168.99(5)
C(18)-Fe(1)-C(2)	154.91(6)	C(3)-Fe(1)-C(2)	40.02(5)
C(17)-Fe(1)-C(2)	163.33(5)	C(4)-Fe(1)-C(2)	69.46(5)
C(19)-Fe(1)-C(2)	120.76(6)	C(16)-Fe(1)-C(2)	126.44(5)
C(15)-Fe(1)-C(2)	108.66(5)	C(5)-Fe(1)-C(2)	72.91(5)
C(18)-Fe(1)-P(1)	112.75(4)	C(3)-Fe(1)-P(1)	75.84(4)
C(17)-Fe(1)-P(1)	148.34(4)	C(4)-Fe(1)-P(1)	76.04(4)
C(19)-Fe(1)-P(1)	102.82(4)	C(16)-Fe(1)-P(1)	165.14(4)
C(15)-Fe(1)-P(1)	125.31(4)	C(5)-Fe(1)-P(1)	47.51(4)
C(2)-Fe(1)-P(1)	47.26(3)	C(2)-P(1)-C(5)	89.73(6)
C(2)-P(1)-Fe(1)	61.13(4)	C(5)-P(1)-Fe(1)	60.66(4)
C(7)-P(2)-C(10)#2	91.07(6)	O(1)-C(1)-C(10)	123.7(1)
O(1)-C(1)-C(2)	120.5(1)	C(10)-C(1)-C(2)	115.7(1)
C(3)-C(2)-C(1)	120.8(1)	C(3)-C(2)-P(1)	113.0(1)
C(1)-C(2)-P(1)	125.4(1)	C(3)-C(2)-Fe(1)	67.59(7)
C(1)-C(2)-Fe(1)	137.3(1)	P(1)-C(2)-Fe(1)	71.61(5)
C(2)-C(3)-C(4)	112.4(1)	C(2)-C(3)-C(11)	123.5(1)
C(4)-C(3)-C(11)	123.9(1)	C(2)-C(3)-Fe(1)	72.39(8)
C(4)-C(3)-Fe(1)	69.69(7)	C(11)-C(3)-Fe(1)	129.9(1)
C(5)-C(4)-C(3)	111.8(1)	C(5)-C(4)-C(12)	125.0(1)
C(3)-C(4)-C(12)	123.0(1)	C(5)-C(4)-Fe(1)	71.72(8)
C(3)-C(4)-Fe(1)	69.48(8)	C(12)-C(4)-Fe(1)	130.9(1)
C(4)-C(5)-C(6)	122.4(1)	C(4)-C(5)-P(1)	113.1(1)
C(6)-C(5)-P(1)	124.2(1)	C(4)-C(5)-Fe(1)	68.07(7)
C(6)-C(5)-Fe(1)	134.1(1)	P(1)-C(5)-Fe(1)	71.84(5)
O(2)-C(6)-C(7)	123.6(1)	O(2)-C(6)-C(5)	120.3(1)
C(7)-C(6)-C(5)	115.9(1)	C(8)-C(7)-C(6)	126.8(1)
C(8)-C(7)-P(2)	111.7(1)	C(6)-C(7)-P(2)	121.2(1)
C(9)-C(8)-C(7)	112.8(1)	C(9)-C(8)-C(13)	124.5(1)
C(7)-C(8)-C(13)	122.6(1)	C(8)-C(9)-C(10)#2	112.7(1)
C(8)-C(9)-C(14)	124.7(1)	C(10)#2-C(9)-C(14)	122.5(1)
C(9)#2-C(10)-C(1)	126.7(1)	C(9)#2-C(10)-P(2)#2	111.6(1)
C(1)-C(10)-P(2)#2	121.7(1)	C(3)-C(11)-H(11A)	109.5
C(3)-C(11)-H(11B)	109.5	H(11A)-C(11)-H(11B)	109.5
C(3)-C(11)-H(11C)	109.5	H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5	C(4)-C(12)-H(12A)	109.5
C(4)-C(12)-H(12B)	109.5	H(12A)-C(12)-H(12B)	109.5
C(4)-C(12)-H(12C)	109.5	H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5	C(8)-C(13)-H(13A)	109.5
C(8)-C(13)-H(13B)	109.5	H(13A)-C(13)-H(13B)	109.5
C(8)-C(13)-H(13C)	109.5	H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5	C(9)-C(14)-H(14A)	109.5

C(9)-C(14)-H(14B)	109.5	H(14A)-C(14)-H(14B)	109.5
C(9)-C(14)-H(14C)	109.5	H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5	C(16)-C(15)-C(19)	107.5(1)
C(16)-C(15)-C(20)	126.5(1)	C(19)-C(15)-C(20)	125.9(1)
C(16)-C(15)-Fe(1)	69.22(8)	C(19)-C(15)-Fe(1)	69.05(8)
C(20)-C(15)-Fe(1)	130.5(1)	C(15)-C(16)-C(17)	108.3(1)
C(15)-C(16)-C(21)	125.6(1)	C(17)-C(16)-C(21)	126.0(1)
C(15)-C(16)-Fe(1)	70.53(8)	C(17)-C(16)-Fe(1)	69.14(8)
C(21)-C(16)-Fe(1)	128.3(1)	C(18)-C(17)-C(16)	107.8(1)
C(18)-C(17)-C(22)	125.1(1)	C(16)-C(17)-C(22)	127.1(1)
C(18)-C(17)-Fe(1)	69.50(8)	C(16)-C(17)-Fe(1)	70.16(8)
C(22)-C(17)-Fe(1)	127.2(1)	C(19)-C(18)-C(17)	108.0(1)
C(19)-C(18)-C(23)	126.1(1)	C(17)-C(18)-C(23)	125.9(2)
C(19)-C(18)-Fe(1)	70.24(8)	C(17)-C(18)-Fe(1)	69.77(8)
C(23)-C(18)-Fe(1)	127.9(1)	C(18)-C(19)-C(15)	108.4(1)
C(18)-C(19)-C(24)	126.0(1)	C(15)-C(19)-C(24)	125.5(2)
C(18)-C(19)-Fe(1)	69.18(8)	C(15)-C(19)-Fe(1)	70.59(8)
C(24)-C(19)-Fe(1)	128.4(1)	C(15)-C(20)-H(20A)	109.5
C(15)-C(20)-H(20B)	109.5	H(20A)-C(20)-H(20B)	109.5
C(15)-C(20)-H(20C)	109.5	H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5	C(16)-C(21)-H(21A)	109.5
C(16)-C(21)-H(21B)	109.5	H(21A)-C(21)-H(21B)	109.5
C(16)-C(21)-H(21C)	109.5	H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5	C(17)-C(22)-H(22A)	109.5
C(17)-C(22)-H(22B)	109.5	H(22A)-C(22)-H(22B)	109.5
C(17)-C(22)-H(22C)	109.5	H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5	C(18)-C(23)-H(23A)	109.5
C(18)-C(23)-H(23B)	109.5	H(23A)-C(23)-H(23B)	109.5
C(18)-C(23)-H(23C)	109.5	H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5	C(19)-C(24)-H(24A)	109.5
C(19)-C(24)-H(24B)	109.5	H(24A)-C(24)-H(24B)	109.5
C(19)-C(24)-H(24C)	109.5	H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5	O(5)-K(1)-O(3)	120.65(3)
O(5)-K(1)-O(4)	61.49(3)	O(3)-K(1)-O(4)	59.82(3)
O(5)-K(1)-O(6)	60.04(3)	O(3)-K(1)-O(6)	176.96(3)
O(4)-K(1)-O(6)	120.28(3)	O(5)-K(1)-O(7)	119.10(3)
O(3)-K(1)-O(7)	118.77(3)	O(4)-K(1)-O(7)	175.82(3)
O(6)-K(1)-O(7)	61.37(3)	O(5)-K(1)-O(8)	177.89(3)
O(3)-K(1)-O(8)	60.54(3)	O(4)-K(1)-O(8)	119.36(3)
O(6)-K(1)-O(8)	118.67(3)	O(7)-K(1)-O(8)	60.21(3)
O(5)-K(1)-N(2)	95.19(4)	O(3)-K(1)-N(2)	77.23(4)
O(4)-K(1)-N(2)	90.33(4)	O(6)-K(1)-N(2)	105.75(4)
O(7)-K(1)-N(2)	85.50(4)	O(8)-K(1)-N(2)	86.77(4)
O(5)-K(1)-N(1)	82.26(4)	O(3)-K(1)-N(1)	104.75(4)
O(4)-K(1)-N(1)	89.16(5)	O(6)-K(1)-N(1)	72.29(4)
O(7)-K(1)-N(1)	95.02(5)	O(8)-K(1)-N(1)	95.77(4)
N(2)-K(1)-N(1)	177.32(5)	C(25)-O(3)-C(36)	112.1(1)
C(25)-O(3)-K(1)	116.69(8)	C(36)-O(3)-K(1)	113.3(1)
C(26)-O(4)-C(27)	111.7(1)	C(26)-O(4)-K(1)	115.00(8)
C(27)-O(4)-K(1)	111.74(8)	C(28)-O(5)-C(29)	112.6(1)
C(28)-O(5)-K(1)	114.85(8)	C(29)-O(5)-K(1)	114.90(8)
C(31)-O(6)-C(30)	112.4(1)	C(31)-O(6)-K(1)	114.14(8)
C(30)-O(6)-K(1)	117.0(1)	C(33)-O(7)-C(32)	111.8(1)
C(33)-O(7)-K(1)	115.5(1)	C(32)-O(7)-K(1)	112.58(8)
C(34)-O(8)-C(35)	112.0(1)	C(34)-O(8)-K(1)	112.3(1)
C(35)-O(8)-K(1)	113.7(1)	C(37)-N(1)-K(1)	122.2(1)
C(39)-N(2)-K(1)	119.3(1)	O(3)-C(25)-C(26)	108.7(1)
O(3)-C(25)-H(25A)	110.0	C(26)-C(25)-H(25A)	110.0
O(3)-C(25)-H(25B)	110.0	C(26)-C(25)-H(25B)	110.0
H(25A)-C(25)-H(25B)	108.3	O(4)-C(26)-C(25)	108.3(1)
O(4)-C(26)-H(26A)	110.0	C(25)-C(26)-H(26A)	110.0
O(4)-C(26)-H(26B)	110.0	C(25)-C(26)-H(26B)	110.0
H(26A)-C(26)-H(26B)	108.4	O(4)-C(27)-C(28)	109.1(1)

O(4)-C(27)-H(27A)	109.9	C(28)-C(27)-H(27A)	109.9
O(4)-C(27)-H(27B)	109.9	C(28)-C(27)-H(27B)	109.9
H(27A)-C(27)-H(27B)	108.3	O(5)-C(28)-C(27)	109.3(1)
O(5)-C(28)-H(28A)	109.8	C(27)-C(28)-H(28A)	109.8
O(5)-C(28)-H(28B)	109.8	C(27)-C(28)-H(28B)	109.8
H(28A)-C(28)-H(28B)	108.3	O(5)-C(29)-C(30)	108.8(1)
O(5)-C(29)-H(29A)	109.9	C(30)-C(29)-H(29A)	109.9
O(5)-C(29)-H(29B)	109.9	C(30)-C(29)-H(29B)	109.9
H(29A)-C(29)-H(29B)	108.3	O(6)-C(30)-C(29)	109.3(1)
O(6)-C(30)-H(30A)	109.8	C(29)-C(30)-H(30A)	109.8
O(6)-C(30)-H(30B)	109.8	C(29)-C(30)-H(30B)	109.8
H(30A)-C(30)-H(30B)	108.3	O(6)-C(31)-C(32)	109.0(1)
O(6)-C(31)-H(31A)	109.9	C(32)-C(31)-H(31A)	109.9
O(6)-C(31)-H(31B)	109.9	C(32)-C(31)-H(31B)	109.9
H(31A)-C(31)-H(31B)	108.3	O(7)-C(32)-C(31)	110.1(1)
O(7)-C(32)-H(32A)	109.6	C(31)-C(32)-H(32A)	109.6
O(7)-C(32)-H(32B)	109.6	C(31)-C(32)-H(32B)	109.6
H(32A)-C(32)-H(32B)	108.2	O(7)-C(33)-C(34)	109.4(1)
O(7)-C(33)-H(33A)	109.8	C(34)-C(33)-H(33A)	109.8
O(7)-C(33)-H(33B)	109.8	C(34)-C(33)-H(33B)	109.8
H(33A)-C(33)-H(33B)	108.2	O(8)-C(34)-C(33)	108.5(1)
O(8)-C(34)-H(34A)	110.0	C(33)-C(34)-H(34A)	110.0
O(8)-C(34)-H(34B)	110.0	C(33)-C(34)-H(34B)	110.0
H(34A)-C(34)-H(34B)	108.4	O(8)-C(35)-C(36)	108.6(1)
O(8)-C(35)-H(35A)	110.0	C(36)-C(35)-H(35A)	110.0
O(8)-C(35)-H(35B)	110.0	C(36)-C(35)-H(35B)	110.0
H(35A)-C(35)-H(35B)	108.3	O(3)-C(36)-C(35)	108.8(1)
O(3)-C(36)-H(36A)	109.9	C(35)-C(36)-H(36A)	109.9
O(3)-C(36)-H(36B)	109.9	C(35)-C(36)-H(36B)	109.9
H(36A)-C(36)-H(36B)	108.3	N(1)-C(37)-C(38)	179.5(2)
C(37)-C(38)-H(38A)	109.5	C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5	C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5	H(38B)-C(38)-H(38C)	109.5
N(2)-C(39)-C(40)	178.2(2)	C(39)-C(40)-H(40A)	109.5
C(39)-C(40)-H(40B)	109.5	H(40A)-C(40)-H(40B)	109.5
C(39)-C(40)-H(40C)	109.5	H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5	N(3)-C(41)-C(42)	179.2(3)
C(41)-C(42)-H(42A)	109.5	C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5	C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5	H(42B)-C(42)-H(42C)	109.5

Estimated standard deviations are given in the parenthesis.
Symmetry operators ::
1: x, y, z 2: -x, -y, -z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **10**

atom	U11	U22	U33	U23	U13	U12
Fe(1)	21(1)	20(1)	18(1)	3(1)	5(1)	9(1)
P(1)	22(1)	22(1)	18(1)	4(1)	6(1)	6(1)
P(2)	27(1)	20(1)	18(1)	5(1)	9(1)	7(1)
O(1)	74(1)	30(1)	19(1)	6(1)	13(1)	14(1)
O(2)	58(1)	22(1)	32(1)	8(1)	19(1)	4(1)
C(1)	30(1)	25(1)	20(1)	6(1)	7(1)	11(1)
C(2)	26(1)	20(1)	19(1)	3(1)	7(1)	9(1)
C(3)	24(1)	21(1)	25(1)	3(1)	6(1)	11(1)
C(4)	24(1)	20(1)	29(1)	4(1)	12(1)	9(1)
C(5)	28(1)	19(1)	21(1)	4(1)	11(1)	8(1)
C(6)	31(1)	21(1)	26(1)	6(1)	14(1)	9(1)
C(7)	23(1)	21(1)	23(1)	7(1)	10(1)	9(1)
C(8)	25(1)	25(1)	26(1)	11(1)	13(1)	13(1)
C(9)	24(1)	28(1)	22(1)	10(1)	10(1)	13(1)
C(10)	21(1)	23(1)	20(1)	7(1)	8(1)	9(1)
C(11)	32(1)	37(1)	42(1)	11(1)	3(1)	19(1)
C(12)	28(1)	33(1)	46(1)	9(1)	18(1)	9(1)
C(13)	57(1)	28(1)	32(1)	16(1)	21(1)	19(1)
C(14)	43(1)	36(1)	24(1)	14(1)	13(1)	18(1)
C(15)	35(1)	29(1)	26(1)	6(1)	15(1)	18(1)
C(16)	34(1)	22(1)	19(1)	1(1)	6(1)	12(1)
C(17)	37(1)	20(1)	26(1)	4(1)	11(1)	13(1)
C(18)	42(1)	31(1)	27(1)	8(1)	11(1)	25(1)
C(19)	34(1)	36(1)	32(1)	7(1)	13(1)	22(1)
C(20)	53(1)	44(1)	35(1)	14(1)	26(1)	23(1)
C(21)	36(1)	32(1)	26(1)	2(1)	1(1)	10(1)
C(22)	54(1)	23(1)	38(1)	9(1)	20(1)	11(1)
C(23)	66(1)	60(1)	40(1)	24(1)	15(1)	45(1)
C(24)	36(1)	68(1)	50(1)	12(1)	17(1)	30(1)
K(1)	24(1)	30(1)	33(1)	8(1)	11(1)	13(1)
O(3)	27(1)	37(1)	31(1)	9(1)	15(1)	12(1)
O(4)	29(1)	27(1)	34(1)	11(1)	14(1)	12(1)
O(5)	27(1)	32(1)	33(1)	12(1)	11(1)	13(1)
O(6)	28(1)	36(1)	32(1)	13(1)	16(1)	16(1)
O(7)	33(1)	34(1)	36(1)	12(1)	14(1)	19(1)
O(8)	28(1)	39(1)	35(1)	9(1)	12(1)	16(1)
N(1)	74(1)	95(2)	89(1)	69(1)	56(1)	60(1)
N(2)	72(1)	79(1)	57(1)	41(1)	38(1)	47(1)
C(25)	35(1)	45(1)	32(1)	9(1)	19(1)	19(1)
C(26)	39(1)	35(1)	36(1)	8(1)	16(1)	21(1)
C(27)	37(1)	25(1)	37(1)	10(1)	15(1)	8(1)
C(28)	32(1)	30(1)	34(1)	11(1)	10(1)	7(1)
C(29)	24(1)	35(1)	47(1)	20(1)	13(1)	12(1)
C(30)	30(1)	43(1)	49(1)	23(1)	23(1)	18(1)
C(31)	41(1)	46(1)	35(1)	14(1)	21(1)	26(1)
C(32)	41(1)	40(1)	39(1)	10(1)	18(1)	27(1)
C(33)	38(1)	32(1)	40(1)	5(1)	14(1)	14(1)
C(34)	32(1)	41(1)	35(1)	4(1)	8(1)	13(1)
C(35)	23(1)	42(1)	52(1)	8(1)	15(1)	12(1)
C(36)	29(1)	44(1)	48(1)	13(1)	23(1)	14(1)
C(37)	40(1)	43(1)	43(1)	26(1)	21(1)	19(1)
C(38)	36(1)	41(1)	44(1)	16(1)	14(1)	19(1)
C(39)	59(1)	52(1)	31(1)	20(1)	18(1)	31(1)
C(40)	72(1)	80(2)	33(1)	17(1)	12(1)	52(1)
N(3)	92(2)	103(2)	49(1)	8(1)	20(1)	39(2)
C(41)	45(1)	88(2)	39(1)	24(1)	14(1)	18(1)
C(42)	56(1)	97(2)	70(2)	48(2)	13(1)	10(1)

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The anisotropic displacement factor exponent takes the form
 2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]
```

Table 5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **10**

atom	x	y	z	U(eq)
H(11A)	8085	2702	4289	61
H(11B)	8959	3484	4003	61
H(11C)	8544	2153	3476	61
H(12A)	8953	3198	1859	59
H(12B)	9153	4263	2865	59
H(12C)	8573	4103	1666	59
H(13A)	6707	3400	-1743	57
H(13B)	5701	3573	-1526	57
H(13C)	5517	2879	-2730	57
H(14A)	4830	1349	-3938	52
H(14B)	3773	212	-4260	52
H(14C)	4930	201	-4191	52
H(20A)	6717	4000	5350	64
H(20B)	5466	3160	4451	64
H(20C)	5770	4412	5245	64
H(21A)	9078	5438	4839	59
H(21B)	8402	4793	5364	59
H(21C)	8691	6082	5671	59
H(22A)	8288	6746	3340	62
H(22B)	8025	5650	2328	62
H(22C)	8910	5996	3502	62
H(23A)	4910	4255	1135	78
H(23B)	6132	5040	1306	78
H(23C)	5470	5588	1849	78
H(24A)	4013	4211	2948	80
H(24B)	4066	3100	2979	80
H(24C)	3923	3265	1911	80
H(25A)	1912	7475	589	46
H(25B)	1063	7902	75	46
H(26A)	91	6014	-223	46
H(26B)	563	6439	1057	46
H(27A)	-1313	5829	944	43
H(27B)	-1741	5345	-338.0000	43
H(28A)	-2578.0002	6591	-301	43
H(28B)	-3129	5673	74	43
H(29A)	-3702	6940	1005	43
H(29B)	-3034	7950	782	43
H(30A)	-3230.0002	8660	2399	45
H(30B)	-2570.9998	8054	2876	45
H(31A)	-1049	9811	4315	46
H(31B)	-1794	10384	3912	46
H(32A)	-328	11461	3576	47
H(32B)	51	11759	4828	47
H(33A)	1981	12370	5138	50
H(33B)	1575	12153	3904	50
H(34A)	3307	12084	4585	50
H(34B)	2658	11001	4727	50
H(35A)	3230	10010	3506	53
H(35B)	3743	11027	3226	53
H(36A)	2312	9876	1410	50
H(36B)	3167	9376	1727	50
H(38A)	-3070	10024	252	63
H(38B)	-2070	11236	1134	63
H(38C)	-2602	10307	1500	63
H(40A)	2064	6596	3186	92
H(40B)	3033	7763	4177	92
H(40C)	2649	7643	2976	92

H(42A)	1166	2084	886	123
H(42B)	582	1931	1672	123
H(42C)	1901	2352	2089	123

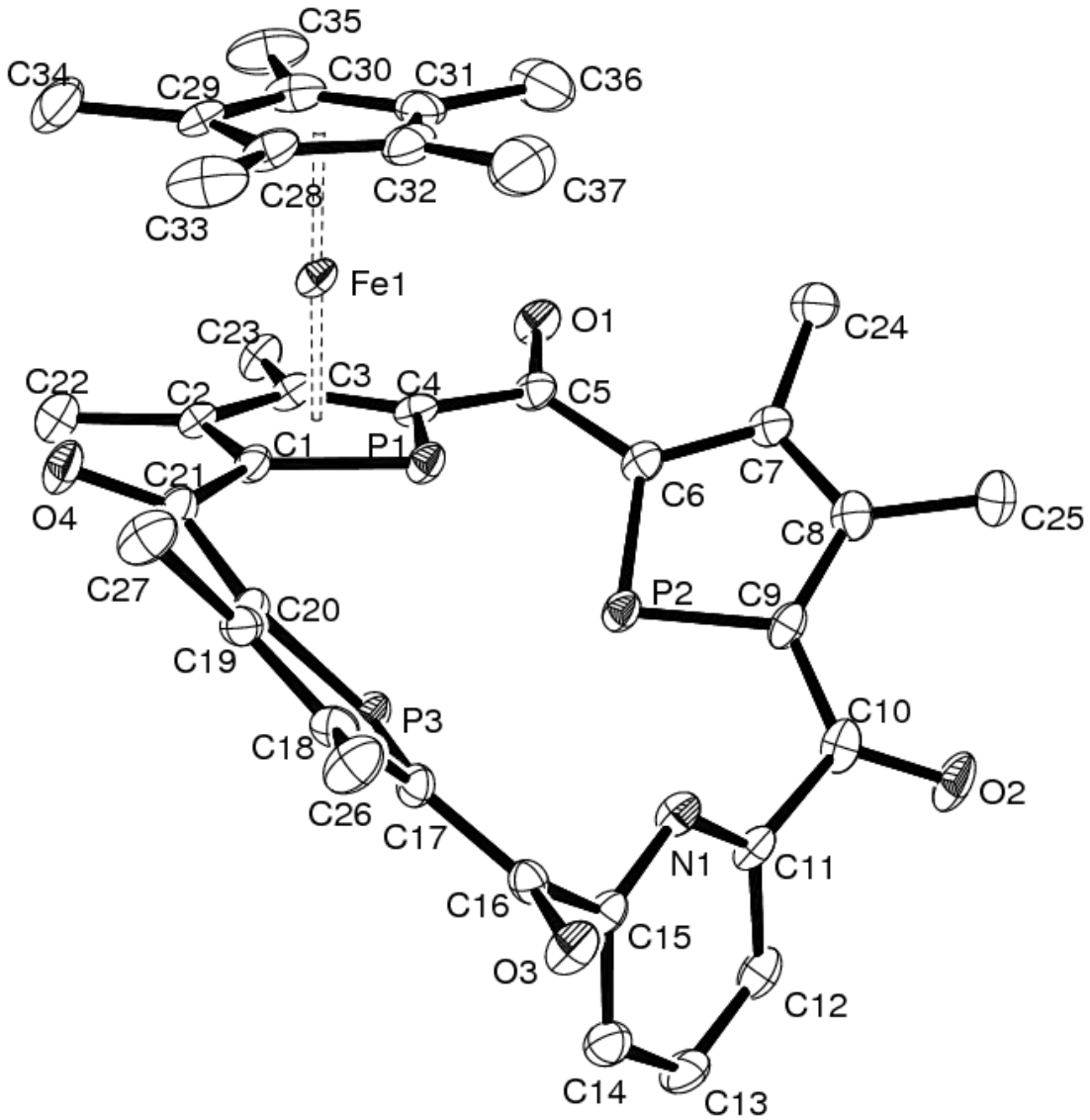

Table 1. Crystal data for **11**

Compound	**11**
Molecular formula	$C_{61}H_{84}FeK_2NO_{16}P_3,C_2H_3N$
Molecular weight	1355.31
Crystal habit	Red Plate
Crystal dimensions(mm)	0.22x0.18x0.02
Crystal system	monoclinic
Space group	$P2_1/c$
a(Å)	17.606(1)
b(Å)	16.733(1)
c(Å)	27.421(1)
α(°)	90.00
β(°)	125.457(2)
γ(°)	90.00
V(Å^3)	6580.2(6)
Z	4
d(g-cm^{-3})	1.368
F(000)	2864
μ(cm^{-1})	0.496
Absorption corrections	multi-scan ; 0.8987 min, 0.9902 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	25.02
HKL ranges	-20 19 ; -19 19 ; -31 32
Reflections measured	58153
Unique data	11464
Rint	0.0897
Reflections used	8811
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	constr
Parameters refined	796
Reflections / parameter	11
wR2	0.1646
R1	0.0968
Weights a, b	0.0105 ; 32.349
GoF	1.209
difference peak / hole (e Å^{-3})	0.641(0.081) / -0.595(0.081)
Flack's parameter	0.0(4).

This racemic compound appears in a non-centrosymmetric space group, so pseudoinversion centres are present

Table 2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **11**

atom	x	y	z	U(eq)
Fe(1)	6253(1)	5527(1)	2219(1)	29(1)
K(1)	10065(1)	350(1)	3864(1)	37(1)
K(2)	6197(1)	1124(1)	1020(1)	41(1)
P(1)	7346(1)	4555(1)	2514(1)	29(1)
P(2)	9326(1)	4484(1)	3115(1)	31(1)
P(3)	7427(1)	2977(1)	2093(1)	31(1)
O(1)	8512(3)	6696(2)	2947(2)	39(1)
O(2)	11582(3)	3411(3)	4426(2)	51(1)
O(3)	8377(3)	882(2)	2897(2)	40(1)
O(4)	4890(3)	3864(2)	1103(2)	40(1)
O(5)	9365(3)	1111(3)	4453(2)	43(1)
O(6)	11264(3)	1307(3)	4932(2)	46(1)
O(7)	12000(3)	599(3)	4363(2)	42(1)
O(8)	11121(3)	-775(2)	3690(2)	42(1)
O(9)	9277(3)	-1111(2)	3275(2)	43(1)
O(10)	8618(3)	-378(3)	3874(2)	42(1)
O(11)	4837(4)	-58(3)	819(3)	88(2)
O(12)	4297(3)	1385(3)	227(2)	54(1)
O(13)	5404(4)	2403(3)	117(4)	95(2)
O(14)	7199(3)	1802(3)	628(2)	54(1)
O(15)	7949(3)	543(3)	1442(2)	56(1)
O(16)	6680(3)	-504(3)	1385(2)	60(1)
N(1)	9509(3)	2597(3)	3279(2)	31(1)
C(1)	6335(4)	4553(3)	1765(2)	28(1)
C(2)	6181(4)	5294(3)	1459(3)	29(1)
C(3)	6899(4)	5859(3)	1820(3)	31(1)
C(4)	7588(4)	5549(3)	2405(3)	30(1)
C(5)	8451(4)	5955(4)	2914(3)	32(1)
C(6)	9187(4)	5415(3)	3346(3)	30(1)
C(7)	9841(4)	5541(3)	3974(3)	32(1)
C(8)	10425(4)	4879(4)	4260(3)	38(2)
C(9)	10246(4)	4247(3)	3857(3)	31(1)
C(10)	10781(4)	3544(4)	3974(3)	34(1)
C(11)	10379(4)	2874(3)	3508(3)	32(1)
C(12)	10936(4)	2543(4)	3358(3)	39(2)
C(13)	10606(4)	1922(4)	2956(3)	41(2)
C(14)	9729(4)	1616(4)	2734(3)	40(2)
C(15)	9210(4)	1973(3)	2905(3)	30(1)
C(16)	8289(4)	1574(3)	2711(3)	29(1)
C(17)	7431(4)	2012(3)	2343(2)	27(1)
C(18)	6518(4)	1778(3)	2173(3)	29(1)
C(19)	5861(4)	2375(3)	1862(3)	29(1)
C(20)	6235(4)	3074(3)	1786(2)	27(1)
C(21)	5734(4)	3828(4)	1512(3)	31(1)
C(22)	5397(4)	5431(4)	811(3)	42(2)
C(23)	6959(4)	6668(3)	1596(3)	38(2)
C(24)	9879(4)	6281(4)	4304(3)	42(2)
C(25)	11158(4)	4844(4)	4932(3)	48(2)
C(26)	6304(4)	1002(4)	2342(3)	45(2)
C(27)	4874(4)	2305(4)	1675(3)	45(2)
C(28)	5196(4)	5269(4)	2301(3)	42(2)
C(29)	4970(4)	5951(4)	1947(3)	37(2)
C(30)	5675(5)	6538(4)	2301(3)	44(2)
C(31)	6328(5)	6201(5)	2873(3)	49(2)
C(32)	6037(4)	5420(4)	2877(3)	45(2)
C(33)	4629(5)	4516(4)	2121(4)	63(2)
C(34)	4114(5)	6071(5)	1324(3)	63(2)

C(35)	5697(6)	7383(4)	2116(5)	74(3)
C(36)	7162(5)	6621(6)	3403(4)	88(3)
C(37)	6484(6)	4849(6)	3398(4)	84(3)
C(38)	9971(5)	1587(4)	4971(3)	47(2)
C(39)	10718(5)	1940(4)	4932(3)	53(2)
C(40)	12098(4)	1589(4)	5023(3)	49(2)
C(41)	12575(4)	895(4)	4957(3)	46(2)
C(42)	12464(4)	14(4)	4249(3)	53(2)
C(43)	11790(5)	-353(4)	3655(3)	49(2)
C(44)	10518(5)	-1263(4)	3175(3)	47(2)
C(45)	9867(5)	-1684(4)	3266(3)	46(2)
C(46)	8592(5)	-1485(4)	3319(3)	46(2)
C(47)	8029(4)	-851(4)	3354(3)	46(2)
C(48)	8099(4)	199(4)	3947(3)	47(2)
C(49)	8748(5)	650(4)	4515(3)	49(2)
C(50)	3984(6)	52(5)	375(4)	77(3)
C(51)	3657(5)	895(5)	201(5)	113(4)
C(52)	3954(6)	2092(6)	-16(6)	120(5)
C(53)	4660(6)	2672(5)	59(4)	80(3)
C(54)	6049(6)	2847(6)	224(6)	120(5)
C(55)	6990(6)	2575(5)	409(5)	84(3)
C(56)	8153(5)	1643(4)	982(4)	65(2)
C(57)	8342(5)	778(4)	1148(3)	55(2)
C(58)	8168(5)	-254(5)	1611(4)	80(3)
C(59)	7601(6)	-615(6)	1801(5)	102(4)
C(60)	6130(5)	-967(6)	1407(6)	138(6)
C(61)	5107(5)	-838(4)	960(4)	72(3)
N(2)	7504(8)	2866(7)	4356(5)	130(4)
C(62)	7779(7)	2940(6)	4087(4)	77(3)
C(63)	8160(10)	3043(8)	3760(5)	127(5)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table 3. Bond lengths (A) and angles (deg) for **11**

Fe(1)-C(28)	2.048(6)	Fe(1)-C(2)	2.049(6)
Fe(1)-C(29)	2.052(5)	Fe(1)-C(30)	2.053(6)
Fe(1)-C(31)	2.057(6)	Fe(1)-C(32)	2.058(6)
Fe(1)-C(3)	2.060(6)	Fe(1)-C(4)	2.097(5)
Fe(1)-C(1)	2.106(6)	Fe(1)-P(1)	2.278(2)
K(1)-O(3)	2.741(4)	K(1)-O(9)	2.811(4)
K(1)-O(10)	2.838(4)	K(1)-O(5)	2.839(4)
K(1)-O(7)	2.872(4)	K(1)-O(8)	2.874(4)
K(1)-O(6)	2.904(5)	K(1)-C(15)	3.458(6)
K(1)-C(14)	3.508(7)	K(1)-C(16)	3.534(6)
K(2)-O(15)	2.767(4)	K(2)-O(12)	2.768(5)
K(2)-O(14)	2.786(5)	K(2)-O(16)	2.856(5)
K(2)-O(11)	2.900(5)	K(2)-O(13)	2.942(6)
K(2)-C(18)	3.071(6)	K(2)-C(17)	3.307(6)
K(2)-C(19)	3.411(6)	K(2)-C(54)	3.54(1)
P(1)-C(1)	1.775(6)	P(1)-C(4)	1.785(6)
P(2)-C(6)	1.752(6)	P(2)-C(9)	1.759(6)
P(3)-C(17)	1.752(6)	P(3)-C(20)	1.757(5)
O(1)-C(5)	1.244(7)	O(2)-C(10)	1.244(7)
O(3)-C(16)	1.237(7)	O(4)-C(21)	1.238(6)
O(5)-C(49)	1.420(8)	O(5)-C(38)	1.425(8)
O(6)-C(40)	1.421(8)	O(6)-C(39)	1.430(8)
O(7)-C(41)	1.418(8)	O(7)-C(42)	1.420(8)
O(8)-C(43)	1.425(7)	O(8)-C(44)	1.431(8)
O(9)-C(46)	1.425(7)	O(9)-C(45)	1.425(7)
O(10)-C(48)	1.422(7)	O(10)-C(47)	1.422(8)
O(11)-C(50)	1.28(1)	O(11)-C(61)	1.37(1)
O(12)-C(52)	1.32(1)	O(12)-C(51)	1.36(1)
O(13)-C(54)	1.24(1)	O(13)-C(53)	1.30(1)
O(14)-C(55)	1.38(1)	O(14)-C(56)	1.394(8)
O(15)-C(57)	1.391(8)	O(15)-C(58)	1.39(1)
O(16)-C(60)	1.27(1)	O(16)-C(59)	1.35(1)
N(1)-C(15)	1.337(7)	N(1)-C(11)	1.356(7)
C(1)-C(2)	1.431(8)	C(1)-C(21)	1.490(8)
C(2)-C(3)	1.421(8)	C(2)-C(22)	1.507(8)
C(3)-C(4)	1.433(8)	C(3)-C(23)	1.515(8)
C(4)-C(5)	1.502(8)	C(5)-C(6)	1.456(8)
C(6)-C(7)	1.426(8)	C(7)-C(8)	1.401(8)
C(7)-C(24)	1.512(8)	C(8)-C(9)	1.43(1)
C(8)-C(25)	1.52(1)	C(9)-C(10)	1.423(8)
C(10)-C(11)	1.530(8)	C(11)-C(12)	1.380(8)
C(12)-C(13)	1.37(1)	C(12)-H(12)	0.9500
C(13)-C(14)	1.388(8)	C(13)-H(13)	0.9500
C(14)-C(15)	1.383(8)	C(14)-H(14)	0.9500
C(15)-C(16)	1.536(8)	C(16)-C(17)	1.438(8)
C(17)-C(18)	1.444(7)	C(18)-C(19)	1.385(8)
C(18)-C(26)	1.498(8)	C(19)-C(20)	1.416(8)
C(19)-C(27)	1.505(8)	C(20)-C(21)	1.472(8)
C(22)-H(22A)	0.9800	C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800	C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800	C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800	C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800	C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800	C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800	C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800	C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800	C(27)-H(27C)	0.9800
C(28)-C(29)	1.40(1)	C(28)-C(32)	1.43(1)
C(28)-C(33)	1.50(1)	C(29)-C(30)	1.43(1)
C(29)-C(34)	1.50(1)	C(30)-C(31)	1.42(1)
C(30)-C(35)	1.51(1)	C(31)-C(32)	1.41(1)

C(31)-C(36)	1.51(1)	C(32)-C(37)	1.50(1)
C(33)-H(33A)	0.9800	C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800	C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800	C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800	C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800	C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800	C(36)-H(36C)	0.9800
C(37)-H(37A)	0.9800	C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800	C(38)-C(39)	1.50(1)
C(38)-H(38A)	0.9900	C(38)-H(38B)	0.9900
C(39)-H(39A)	0.9900	C(39)-H(39B)	0.9900
C(40)-C(41)	1.50(1)	C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900	C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900	C(42)-C(43)	1.48(1)
C(42)-H(42A)	0.9900	C(42)-H(42B)	0.9900
C(43)-H(43A)	0.9900	C(43)-H(43B)	0.9900
C(44)-C(45)	1.48(1)	C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900	C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900	C(46)-C(47)	1.49(1)
C(46)-H(46A)	0.9900	C(46)-H(46B)	0.9900
C(47)-H(47A)	0.9900	C(47)-H(47B)	0.9900
C(48)-C(49)	1.50(1)	C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900	C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900	C(50)-C(51)	1.494(1)
C(50)-H(50A)	0.9900	C(50)-H(50B)	0.9900
C(51)-H(51A)	0.9900	C(51)-H(51B)	0.9900
C(52)-C(53)	1.494(1)	C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900	C(53)-H(53A)	0.9900
C(53)-H(53B)	0.9900	C(54)-C(55)	1.494(1)
C(54)-H(54A)	0.9900	C(54)-H(54B)	0.9900
C(55)-H(55A)	0.9900	C(55)-H(55B)	0.9900
C(56)-C(57)	1.495(1)	C(56)-H(56A)	0.9900
C(56)-H(56B)	0.9900	C(57)-H(57A)	0.9900
C(57)-H(57B)	0.9900	C(58)-C(59)	1.494(1)
C(58)-H(58A)	0.9900	C(58)-H(58B)	0.9900
C(59)-H(59A)	0.9900	C(59)-H(59B)	0.9900
C(60)-C(61)	1.494(1)	C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900	C(61)-H(61A)	0.9900
C(61)-H(61B)	0.9900	N(2)-C(62)	1.10(1)
C(62)-C(63)	1.41(1)	C(63)-H(63A)	0.9800
C(63)-H(63B)	0.9800	C(63)-H(63C)	0.9800

C(28)-Fe(1)-C(2)	123.2(3)	C(28)-Fe(1)-C(29)	39.9(2)
C(2)-Fe(1)-C(29)	106.8(2)	C(28)-Fe(1)-C(30)	67.7(2)
C(2)-Fe(1)-C(30)	121.7(3)	C(29)-Fe(1)-C(30)	40.8(3)
C(28)-Fe(1)-C(31)	67.8(3)	C(2)-Fe(1)-C(31)	157.7(3)
C(29)-Fe(1)-C(31)	68.1(3)	C(30)-Fe(1)-C(31)	40.4(3)
C(28)-Fe(1)-C(32)	40.7(3)	C(2)-Fe(1)-C(32)	160.3(3)
C(29)-Fe(1)-C(32)	67.9(3)	C(30)-Fe(1)-C(32)	67.6(3)
C(31)-Fe(1)-C(32)	40.0(3)	C(28)-Fe(1)-C(3)	158.9(3)
C(2)-Fe(1)-C(3)	40.5(2)	C(29)-Fe(1)-C(3)	123.0(2)
C(30)-Fe(1)-C(3)	107.4(2)	C(31)-Fe(1)-C(3)	122.7(3)
C(32)-Fe(1)-C(3)	158.4(3)	C(28)-Fe(1)-C(4)	160.0(3)
C(2)-Fe(1)-C(4)	69.5(2)	C(29)-Fe(1)-C(4)	157.7(2)
C(30)-Fe(1)-C(4)	121.1(2)	C(31)-Fe(1)-C(4)	106.4(2)
C(32)-Fe(1)-C(4)	122.7(2)	C(3)-Fe(1)-C(4)	40.3(2)
C(28)-Fe(1)-C(1)	106.3(2)	C(2)-Fe(1)-C(1)	40.3(2)
C(29)-Fe(1)-C(1)	119.4(2)	C(30)-Fe(1)-C(1)	155.6(3)
C(31)-Fe(1)-C(1)	161.4(3)	C(32)-Fe(1)-C(1)	124.2(3)
C(3)-Fe(1)-C(1)	69.3(2)	C(4)-Fe(1)-C(1)	72.9(2)
C(28)-Fe(1)-P(1)	116.4(2)	C(2)-Fe(1)-P(1)	76.6(2)
C(29)-Fe(1)-P(1)	154.2(2)	C(30)-Fe(1)-P(1)	156.8(2)

C(31)-Fe(1)-P(1)	117.9(2)	C(32)-Fe(1)-P(1)	100.0(2)
C(3)-Fe(1)-P(1)	76.6(2)	C(4)-Fe(1)-P(1)	48.0(2)
C(1)-Fe(1)-P(1)	47.5(2)	O(3)-K(1)-O(9)	80.3(1)
O(3)-K(1)-O(10)	70.9(1)	O(9)-K(1)-O(10)	59.1(1)
O(3)-K(1)-O(5)	79.6(1)	O(9)-K(1)-O(5)	119.0(1)
O(10)-K(1)-O(5)	59.9(1)	O(3)-K(1)-O(7)	137.3(1)
O(9)-K(1)-O(7)	117.0(1)	O(10)-K(1)-O(7)	151.8(1)
O(5)-K(1)-O(7)	116.8(1)	O(3)-K(1)-O(8)	119.7(1)
O(9)-K(1)-O(8)	59.1(1)	O(10)-K(1)-O(8)	113.0(1)
O(5)-K(1)-O(8)	157.6(1)	O(7)-K(1)-O(8)	58.1(1)
O(3)-K(1)-O(6)	122.8(1)	O(9)-K(1)-O(6)	152.4(1)
O(10)-K(1)-O(6)	111.0(1)	O(5)-K(1)-O(6)	58.7(1)
O(7)-K(1)-O(6)	58.1(1)	O(8)-K(1)-O(6)	111.5(1)
O(3)-K(1)-C(15)	42.3(1)	O(9)-K(1)-C(15)	113.2(1)
O(10)-K(1)-C(15)	110.3(1)	O(5)-K(1)-C(15)	86.5(1)
O(7)-K(1)-C(15)	97.0(1)	O(8)-K(1)-C(15)	115.3(1)
O(6)-K(1)-C(15)	94.3(1)	O(3)-K(1)-C(14)	54.3(1)
O(9)-K(1)-C(14)	104.1(2)	O(10)-K(1)-C(14)	125.1(1)
O(5)-K(1)-C(14)	109.0(1)	O(7)-K(1)-C(14)	83.1(1)
O(8)-K(1)-C(14)	92.5(1)	O(6)-K(1)-C(14)	102.1(2)
C(15)-K(1)-C(14)	22.9(1)	O(3)-K(1)-C(16)	17.5(1)
O(9)-K(1)-C(16)	96.0(1)	O(10)-K(1)-C(16)	85.6(1)
O(5)-K(1)-C(16)	78.3(1)	O(7)-K(1)-C(16)	122.1(1)
O(8)-K(1)-C(16)	123.6(1)	O(6)-K(1)-C(16)	109.3(1)
C(15)-K(1)-C(16)	25.4(1)	C(14)-K(1)-C(16)	41.6(1)
O(15)-K(2)-O(12)	158.3(2)	O(15)-K(2)-O(14)	60.2(1)
O(12)-K(2)-O(14)	112.3(2)	O(15)-K(2)-O(16)	59.0(1)
O(12)-K(2)-O(16)	113.9(2)	O(14)-K(2)-O(16)	113.3(2)
O(15)-K(2)-O(11)	115.9(2)	O(12)-K(2)-O(11)	58.0(2)
O(14)-K(2)-O(11)	147.3(2)	O(16)-K(2)-O(11)	57.5(2)
O(15)-K(2)-O(13)	118.5(2)	O(12)-K(2)-O(13)	57.1(2)
O(14)-K(2)-O(13)	58.4(2)	O(16)-K(2)-O(13)	152.6(2)
O(11)-K(2)-O(13)	113.6(2)	O(15)-K(2)-C(18)	101.5(2)
O(12)-K(2)-C(18)	99.8(2)	O(14)-K(2)-C(18)	118.2(2)
O(16)-K(2)-C(18)	98.1(2)	O(11)-K(2)-C(18)	94.5(2)
O(13)-K(2)-C(18)	108.8(2)	O(15)-K(2)-C(17)	80.5(2)
O(12)-K(2)-C(17)	121.1(2)	O(14)-K(2)-C(17)	94.6(2)
O(16)-K(2)-C(17)	99.9(2)	O(11)-K(2)-C(17)	117.4(2)
O(13)-K(2)-C(17)	106.6(2)	C(18)-K(2)-C(17)	25.8(1)
O(15)-K(2)-C(19)	121.4(2)	O(12)-K(2)-C(19)	80.2(1)
O(14)-K(2)-C(19)	114.1(2)	O(16)-K(2)-C(19)	118.8(2)
O(11)-K(2)-C(19)	95.7(2)	O(13)-K(2)-C(19)	86.5(2)
C(18)-K(2)-C(19)	24.0(1)	C(17)-K(2)-C(19)	40.9(1)
O(15)-K(2)-C(54)	102.1(2)	O(12)-K(2)-C(54)	76.3(2)
O(14)-K(2)-C(54)	42.7(2)	O(16)-K(2)-C(54)	153.4(2)
O(11)-K(2)-C(54)	133.0(2)	O(13)-K(2)-C(54)	19.5(2)
C(18)-K(2)-C(54)	104.4(3)	C(17)-K(2)-C(54)	94.4(2)
C(19)-K(2)-C(54)	86.4(2)	C(1)-P(1)-C(4)	89.1(3)
C(1)-P(1)-Fe(1)	61.1(2)	C(4)-P(1)-Fe(1)	60.7(2)
C(6)-P(2)-C(9)	90.6(3)	C(17)-P(3)-C(20)	90.3(3)
C(16)-O(3)-K(1)	120.6(4)	C(49)-O(5)-C(38)	111.5(5)
C(49)-O(5)-K(1)	116.1(4)	C(38)-O(5)-K(1)	119.8(4)
C(40)-O(6)-C(39)	112.4(5)	C(40)-O(6)-K(1)	115.6(4)
C(39)-O(6)-K(1)	108.2(4)	C(41)-O(7)-C(42)	112.1(5)
C(41)-O(7)-K(1)	117.2(4)	C(42)-O(7)-K(1)	118.0(4)
C(43)-O(8)-C(44)	112.7(5)	C(43)-O(8)-K(1)	109.1(4)
C(44)-O(8)-K(1)	110.9(3)	C(46)-O(9)-C(45)	111.6(5)
C(46)-O(9)-K(1)	119.5(4)	C(45)-O(9)-K(1)	118.3(3)
C(48)-O(10)-C(47)	111.4(5)	C(48)-O(10)-K(1)	111.3(3)
C(47)-O(10)-K(1)	111.4(4)	C(50)-O(11)-C(61)	115.3(6)
C(50)-O(11)-K(2)	117.7(5)	C(61)-O(11)-K(2)	119.0(4)
C(52)-O(12)-C(51)	113.0(6)	C(52)-O(12)-K(2)	121.9(5)
C(51)-O(12)-K(2)	122.1(4)	C(54)-O(13)-C(53)	122.5(7)

C(54)-O(13)-K(2)	108.3(6)	C(53)-O(13)-K(2)	107.8(5)
C(55)-O(14)-C(56)	113.0(5)	C(55)-O(14)-K(2)	118.7(4)
C(56)-O(14)-K(2)	115.5(4)	C(57)-O(15)-C(58)	109.2(5)
C(57)-O(15)-K(2)	117.9(4)	C(58)-O(15)-K(2)	120.2(4)
C(60)-O(16)-C(59)	116.9(6)	C(60)-O(16)-K(2)	121.2(5)
C(59)-O(16)-K(2)	113.3(5)	C(15)-N(1)-C(11)	117.4(5)
C(2)-C(1)-C(21)	126.2(5)	C(2)-C(1)-P(1)	113.4(4)
C(21)-C(1)-P(1)	120.3(4)	C(2)-C(1)-Fe(1)	67.7(3)
C(21)-C(1)-Fe(1)	129.2(4)	P(1)-C(1)-Fe(1)	71.3(2)
C(3)-C(2)-C(1)	112.3(5)	C(3)-C(2)-C(22)	123.8(5)
C(1)-C(2)-C(22)	123.7(5)	C(3)-C(2)-Fe(1)	70.2(3)
C(1)-C(2)-Fe(1)	72.0(3)	C(22)-C(2)-Fe(1)	130.2(4)
C(2)-C(3)-C(4)	111.9(5)	C(2)-C(3)-C(23)	123.7(5)
C(4)-C(3)-C(23)	124.3(5)	C(2)-C(3)-Fe(1)	69.3(3)
C(4)-C(3)-Fe(1)	71.2(3)	C(23)-C(3)-Fe(1)	130.2(4)
C(3)-C(4)-C(5)	128.3(5)	C(3)-C(4)-P(1)	113.3(4)
C(5)-C(4)-P(1)	118.4(4)	C(3)-C(4)-Fe(1)	68.5(3)
C(5)-C(4)-Fe(1)	128.3(4)	P(1)-C(4)-Fe(1)	71.4(2)
O(1)-C(5)-C(6)	124.1(5)	O(1)-C(5)-C(4)	121.1(5)
C(6)-C(5)-C(4)	114.7(5)	C(7)-C(6)-C(5)	127.3(5)
C(7)-C(6)-P(2)	112.5(4)	C(5)-C(6)-P(2)	120.2(4)
C(8)-C(7)-C(6)	112.1(5)	C(8)-C(7)-C(24)	123.2(6)
C(6)-C(7)-C(24)	124.5(5)	C(7)-C(8)-C(9)	113.0(5)
C(7)-C(8)-C(25)	122.8(6)	C(9)-C(8)-C(25)	124.2(6)
C(10)-C(9)-C(8)	128.2(5)	C(10)-C(9)-P(2)	119.5(5)
C(8)-C(9)-P(2)	111.7(4)	O(2)-C(10)-C(9)	126.3(6)
O(2)-C(10)-C(11)	114.2(5)	C(9)-C(10)-C(11)	119.5(5)
N(1)-C(11)-C(12)	122.1(6)	N(1)-C(11)-C(10)	119.2(5)
C(12)-C(11)-C(10)	118.6(5)	C(13)-C(12)-C(11)	120.0(6)
C(13)-C(12)-H(12)	120.0	C(11)-C(12)-H(12)	120.0
C(12)-C(13)-C(14)	118.5(6)	C(12)-C(13)-H(13)	120.8
C(14)-C(13)-H(13)	120.8	C(15)-C(14)-C(13)	118.5(6)
C(15)-C(14)-K(1)	76.5(4)	C(13)-C(14)-K(1)	105.1(4)
C(15)-C(14)-H(14)	120.8	C(13)-C(14)-H(14)	120.8
K(1)-C(14)-H(14)	88.5	N(1)-C(15)-C(14)	123.6(5)
N(1)-C(15)-C(16)	118.2(5)	C(14)-C(15)-C(16)	117.9(5)
N(1)-C(15)-K(1)	103.1(3)	C(14)-C(15)-K(1)	80.6(4)
C(16)-C(15)-K(1)	80.1(3)	O(3)-C(16)-C(17)	126.6(5)
O(3)-C(16)-C(15)	114.2(5)	C(17)-C(16)-C(15)	119.3(5)
O(3)-C(16)-K(1)	41.9(3)	C(17)-C(16)-K(1)	161.3(4)
C(15)-C(16)-K(1)	74.6(3)	C(16)-C(17)-C(18)	127.4(5)
C(16)-C(17)-P(3)	120.6(4)	C(18)-C(17)-P(3)	111.8(4)
C(16)-C(17)-K(2)	107.2(3)	C(18)-C(17)-K(2)	67.9(3)
P(3)-C(17)-K(2)	97.7(2)	C(19)-C(18)-C(17)	112.3(5)
C(19)-C(18)-C(26)	123.0(5)	C(17)-C(18)-C(26)	124.6(5)
C(19)-C(18)-K(2)	91.9(4)	C(17)-C(18)-K(2)	86.3(3)
C(26)-C(18)-K(2)	94.6(4)	C(18)-C(19)-C(20)	113.1(5)
C(18)-C(19)-C(27)	122.7(5)	C(20)-C(19)-C(27)	123.9(5)
C(18)-C(19)-K(2)	64.1(3)	C(20)-C(19)-K(2)	97.4(3)
C(27)-C(19)-K(2)	109.9(4)	C(19)-C(20)-C(21)	126.2(5)
C(19)-C(20)-P(3)	112.4(4)	C(21)-C(20)-P(3)	121.3(4)
O(4)-C(21)-C(20)	123.6(5)	O(4)-C(21)-C(1)	122.4(5)
C(20)-C(21)-C(1)	114.0(5)	C(2)-C(22)-H(22A)	109.5
C(2)-C(22)-H(22B)	109.5	H(22A)-C(22)-H(22B)	109.5
C(2)-C(22)-H(22C)	109.5	H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5	C(3)-C(23)-H(23A)	109.5
C(3)-C(23)-H(23B)	109.5	H(23A)-C(23)-H(23B)	109.5
C(3)-C(23)-H(23C)	109.5	H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5	C(7)-C(24)-H(24A)	109.5
C(7)-C(24)-H(24B)	109.5	H(24A)-C(24)-H(24B)	109.5
C(7)-C(24)-H(24C)	109.5	H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5	C(8)-C(25)-H(25A)	109.5
C(8)-C(25)-H(25B)	109.5	H(25A)-C(25)-H(25B)	109.5

C(8)-C(25)-H(25C)	109.5	H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5	C(18)-C(26)-H(26A)	109.5
C(18)-C(26)-H(26B)	109.5	H(26A)-C(26)-H(26B)	109.5
C(18)-C(26)-H(26C)	109.5	H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5	C(19)-C(27)-H(27A)	109.5
C(19)-C(27)-H(27B)	109.5	H(27A)-C(27)-H(27B)	109.5
C(19)-C(27)-H(27C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5	C(29)-C(28)-C(32)	108.6(6)
C(29)-C(28)-C(33)	126.1(7)	C(32)-C(28)-C(33)	125.3(7)
C(29)-C(28)-Fe(1)	70.2(3)	C(32)-C(28)-Fe(1)	70.0(3)
C(33)-C(28)-Fe(1)	127.9(5)	C(28)-C(29)-C(30)	107.6(6)
C(28)-C(29)-C(34)	126.5(6)	C(30)-C(29)-C(34)	125.8(6)
C(28)-C(29)-Fe(1)	69.9(3)	C(30)-C(29)-Fe(1)	69.6(3)
C(34)-C(29)-Fe(1)	129.0(5)	C(31)-C(30)-C(29)	107.8(6)
C(31)-C(30)-C(35)	125.6(7)	C(29)-C(30)-C(35)	126.5(7)
C(31)-C(30)-Fe(1)	70.0(4)	C(29)-C(30)-Fe(1)	69.6(3)
C(35)-C(30)-Fe(1)	128.5(5)	C(32)-C(31)-C(30)	108.2(6)
C(32)-C(31)-C(36)	125.4(8)	C(30)-C(31)-C(36)	126.2(8)
C(32)-C(31)-Fe(1)	70.0(4)	C(30)-C(31)-Fe(1)	69.7(4)
C(36)-C(31)-Fe(1)	128.9(5)	C(31)-C(32)-C(28)	107.7(6)
C(31)-C(32)-C(37)	127.2(7)	C(28)-C(32)-C(37)	125.0(7)
C(31)-C(32)-Fe(1)	70.0(4)	C(28)-C(32)-Fe(1)	69.3(4)
C(37)-C(32)-Fe(1)	128.8(5)	C(28)-C(33)-H(33A)	109.5
C(28)-C(33)-H(33B)	109.5	H(33A)-C(33)-H(33B)	109.5
C(28)-C(33)-H(33C)	109.5	H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5	C(29)-C(34)-H(34A)	109.5
C(29)-C(34)-H(34B)	109.5	H(34A)-C(34)-H(34B)	109.5
C(29)-C(34)-H(34C)	109.5	H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5	C(30)-C(35)-H(35A)	109.5
C(30)-C(35)-H(35B)	109.5	H(35A)-C(35)-H(35B)	109.5
C(30)-C(35)-H(35C)	109.5	H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5	C(31)-C(36)-H(36A)	109.5
C(31)-C(36)-H(36B)	109.5	H(36A)-C(36)-H(36B)	109.5
C(31)-C(36)-H(36C)	109.5	H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5	C(32)-C(37)-H(37A)	109.5
C(32)-C(37)-H(37B)	109.5	H(37A)-C(37)-H(37B)	109.5
C(32)-C(37)-H(37C)	109.5	H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5	O(5)-C(38)-C(39)	109.2(6)
O(5)-C(38)-H(38A)	109.8	C(39)-C(38)-H(38A)	109.8
O(5)-C(38)-H(38B)	109.8	C(39)-C(38)-H(38B)	109.8
H(38A)-C(38)-H(38B)	108.3	O(6)-C(39)-C(38)	109.0(5)
O(6)-C(39)-H(39A)	109.9	C(38)-C(39)-H(39A)	109.9
O(6)-C(39)-H(39B)	109.9	C(38)-C(39)-H(39B)	109.9
H(39A)-C(39)-H(39B)	108.3	O(6)-C(40)-C(41)	108.3(5)
O(6)-C(40)-H(40A)	110.0	C(41)-C(40)-H(40A)	110.0
O(6)-C(40)-H(40B)	110.0	C(41)-C(40)-H(40B)	110.0
H(40A)-C(40)-H(40B)	108.4	O(7)-C(41)-C(40)	109.4(5)
O(7)-C(41)-H(41A)	109.8	C(40)-C(41)-H(41A)	109.8
O(7)-C(41)-H(41B)	109.8	C(40)-C(41)-H(41B)	109.8
H(41A)-C(41)-H(41B)	108.2	O(7)-C(42)-C(43)	109.4(5)
O(7)-C(42)-H(42A)	109.8	C(43)-C(42)-H(42A)	109.8
O(7)-C(42)-H(42B)	109.8	C(43)-C(42)-H(42B)	109.8
H(42A)-C(42)-H(42B)	108.2	O(8)-C(43)-C(42)	107.2(6)
O(8)-C(43)-H(43A)	110.3	C(42)-C(43)-H(43A)	110.3
O(8)-C(43)-H(43B)	110.3	C(42)-C(43)-H(43B)	110.3
H(43A)-C(43)-H(43B)	108.5	O(8)-C(44)-C(45)	108.1(5)
O(8)-C(44)-H(44A)	110.1	C(45)-C(44)-H(44A)	110.1
O(8)-C(44)-H(44B)	110.1	C(45)-C(44)-H(44B)	110.1
H(44A)-C(44)-H(44B)	108.4	O(9)-C(45)-C(44)	109.0(5)
O(9)-C(45)-H(45A)	109.9	C(44)-C(45)-H(45A)	109.9
O(9)-C(45)-H(45B)	109.9	C(44)-C(45)-H(45B)	109.9
H(45A)-C(45)-H(45B)	108.3	O(9)-C(46)-C(47)	108.7(5)
O(9)-C(46)-H(46A)	110.0	C(47)-C(46)-H(46A)	110.0

O(9)-C(46)-H(46B)	110.0	C(47)-C(46)-H(46B)	110.0
H(46A)-C(46)-H(46B)	108.3	O(10)-C(47)-C(46)	109.5(5)
O(10)-C(47)-H(47A)	109.8	C(46)-C(47)-H(47A)	109.8
O(10)-C(47)-H(47B)	109.8	C(46)-C(47)-H(47B)	109.8
H(47A)-C(47)-H(47B)	108.2	O(10)-C(48)-C(49)	108.9(5)
O(10)-C(48)-H(48A)	109.9	C(49)-C(48)-H(48A)	109.9
O(10)-C(48)-H(48B)	109.9	C(49)-C(48)-H(48B)	109.9
H(48A)-C(48)-H(48B)	108.3	O(5)-C(49)-C(48)	108.9(6)
O(5)-C(49)-H(49A)	109.9	C(48)-C(49)-H(49A)	109.9
O(5)-C(49)-H(49B)	109.9	C(48)-C(49)-H(49B)	109.9
H(49A)-C(49)-H(49B)	108.3	O(11)-C(50)-C(51)	117.3(7)
O(11)-C(50)-H(50A)	108.0	C(51)-C(50)-H(50A)	108.0
O(11)-C(50)-H(50B)	108.0	C(51)-C(50)-H(50B)	108.0
H(50A)-C(50)-H(50B)	107.2	O(12)-C(51)-C(50)	113.5(7)
O(12)-C(51)-H(51A)	108.9	C(50)-C(51)-H(51A)	108.9
O(12)-C(51)-H(51B)	108.9	C(50)-C(51)-H(51B)	108.9
H(51A)-C(51)-H(51B)	107.7	O(12)-C(52)-C(53)	114.3(7)
O(12)-C(52)-H(52A)	108.7	C(53)-C(52)-H(52A)	108.7
O(12)-C(52)-H(52B)	108.7	C(53)-C(52)-H(52B)	108.7
H(52A)-C(52)-H(52B)	107.6	O(13)-C(53)-C(52)	119.3(7)
O(13)-C(53)-H(53A)	107.5	C(52)-C(53)-H(53A)	107.5
O(13)-C(53)-H(53B)	107.5	C(52)-C(53)-H(53B)	107.5
H(53A)-C(53)-H(53B)	107.0	O(13)-C(54)-C(55)	125.4(8)
O(13)-C(54)-K(2)	52.2(5)	C(55)-C(54)-K(2)	82.6(5)
O(13)-C(54)-H(54A)	106.0	C(55)-C(54)-H(54A)	106.0
K(2)-C(54)-H(54A)	93.9	O(13)-C(54)-H(54B)	106.0
C(55)-C(54)-H(54B)	106.0	K(2)-C(54)-H(54B)	154.4
H(54A)-C(54)-H(54B)	106.3	O(14)-C(55)-C(54)	113.3(6)
O(14)-C(55)-H(55A)	108.9	C(54)-C(55)-H(55A)	108.9
O(14)-C(55)-H(55B)	108.9	C(54)-C(55)-H(55B)	108.9
H(55A)-C(55)-H(55B)	107.7	O(14)-C(56)-C(57)	111.2(6)
O(14)-C(56)-H(56A)	109.4	C(57)-C(56)-H(56A)	109.4
O(14)-C(56)-H(56B)	109.4	C(57)-C(56)-H(56B)	109.4
H(56A)-C(56)-H(56B)	108.0	O(15)-C(57)-C(56)	110.7(6)
O(15)-C(57)-H(57A)	109.5	C(56)-C(57)-H(57A)	109.5
O(15)-C(57)-H(57B)	109.5	C(56)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	108.1	O(15)-C(58)-C(59)	113.1(6)
O(15)-C(58)-H(58A)	109.0	C(59)-C(58)-H(58A)	109.0
O(15)-C(58)-H(58B)	109.0	C(59)-C(58)-H(58B)	109.0
H(58A)-C(58)-H(58B)	107.8	O(16)-C(59)-C(58)	111.6(7)
O(16)-C(59)-H(59A)	109.3	C(58)-C(59)-H(59A)	109.3
O(16)-C(59)-H(59B)	109.3	C(58)-C(59)-H(59B)	109.3
H(59A)-C(59)-H(59B)	108.0	O(16)-C(60)-C(61)	117.6(8)
O(16)-C(60)-H(60A)	107.9	C(61)-C(60)-H(60A)	107.9
O(16)-C(60)-H(60B)	107.9	C(61)-C(60)-H(60B)	107.9
H(60A)-C(60)-H(60B)	107.2	O(11)-C(61)-C(60)	115.2(7)
O(11)-C(61)-H(61A)	108.5	C(60)-C(61)-H(61A)	108.5
O(11)-C(61)-H(61B)	108.5	C(60)-C(61)-H(61B)	108.5
H(61A)-C(61)-H(61B)	107.5	N(2)-C(62)-C(63)	178(1)
C(62)-C(63)-H(63A)	109.5	C(62)-C(63)-H(63B)	109.5
H(63A)-C(63)-H(63B)	109.5	C(62)-C(63)-H(63C)	109.5
H(63A)-C(63)-H(63C)	109.5	H(63B)-C(63)-H(63C)	109.5

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **11**

atom	U11	U22	U33	U23	U13	U12
Fe(1)	21(1)	28(1)	37(1)	2(1)	16(1)	2(1)
K(1)	29(1)	35(1)	43(1)	-1(1)	19(1)	2(1)
K(2)	32(1)	40(1)	47(1)	6(1)	22(1)	4(1)
P(1)	21(1)	25(1)	34(1)	0(1)	12(1)	-1(1)
P(2)	21(1)	29(1)	34(1)	-2(1)	10(1)	-1(1)
P(3)	21(1)	30(1)	36(1)	1(1)	14(1)	-2(1)
O(1)	32(2)	27(2)	51(3)	-1(2)	20(2)	-2(2)
O(2)	22(2)	37(3)	52(3)	0(2)	-2(2)	-1(2)
O(3)	29(2)	27(2)	54(3)	4(2)	19(2)	-2(2)
O(4)	20(2)	38(2)	41(3)	2(2)	6(2)	0(2)
O(5)	42(2)	40(3)	47(3)	0(2)	26(2)	2(2)
O(6)	43(3)	36(3)	59(3)	-5(2)	29(2)	-4(2)
O(7)	29(2)	39(2)	48(3)	-1(2)	17(2)	1(2)
O(8)	40(2)	39(2)	53(3)	-2(2)	31(2)	0(2)
O(9)	34(2)	32(2)	58(3)	-1(2)	25(2)	2(2)
O(10)	35(2)	39(2)	53(3)	-1(2)	25(2)	3(2)
O(11)	35(3)	57(4)	113(5)	23(3)	9(3)	-10(3)
O(12)	35(3)	55(3)	54(3)	9(3)	16(2)	10(2)
O(13)	64(4)	43(3)	179(7)	23(4)	72(5)	9(3)
O(14)	46(3)	45(3)	69(3)	14(3)	33(3)	2(2)
O(15)	36(3)	52(3)	83(4)	15(3)	36(3)	17(2)
O(16)	49(3)	42(3)	85(4)	17(3)	36(3)	4(2)
N(1)	26(3)	25(3)	40(3)	3(2)	18(2)	0(2)
C(1)	20(3)	29(3)	31(3)	-1(3)	13(3)	1(2)
C(2)	23(3)	32(3)	33(3)	2(3)	16(3)	5(2)
C(3)	24(3)	28(3)	42(4)	5(3)	19(3)	6(2)
C(4)	26(3)	26(3)	42(4)	-1(3)	23(3)	1(2)
C(5)	24(3)	32(4)	41(4)	-2(3)	20(3)	-3(3)
C(6)	21(3)	29(3)	39(3)	-2(3)	16(3)	-5(2)
C(7)	22(3)	30(3)	42(4)	-5(3)	18(3)	-6(3)
C(8)	27(3)	44(4)	37(4)	-3(3)	15(3)	-10(3)
C(9)	20(3)	30(3)	35(3)	7(3)	12(3)	-1(2)
C(10)	22(3)	35(3)	36(4)	6(3)	12(3)	-10(3)
C(11)	22(3)	26(3)	41(4)	7(3)	14(3)	4(2)
C(12)	23(3)	42(4)	46(4)	9(3)	15(3)	1(3)
C(13)	29(3)	52(4)	50(4)	6(3)	27(3)	11(3)
C(14)	37(3)	34(3)	43(4)	-1(3)	21(3)	3(3)
C(15)	25(3)	26(3)	36(3)	7(3)	16(3)	3(2)
C(16)	29(3)	27(3)	26(3)	-5(3)	13(3)	-5(2)
C(17)	21(3)	27(3)	27(3)	-2(2)	11(3)	-3(2)
C(18)	30(3)	24(3)	38(4)	-8(3)	22(3)	-7(2)
C(19)	23(3)	30(3)	33(3)	-8(3)	15(3)	-3(2)
C(20)	19(3)	34(3)	26(3)	-5(3)	11(2)	0(2)
C(21)	23(3)	35(3)	32(3)	-1(3)	13(3)	-1(3)
C(22)	32(3)	44(4)	44(4)	5(3)	18(3)	2(3)
C(23)	29(3)	33(3)	44(4)	8(3)	17(3)	2(3)
C(24)	32(3)	44(4)	47(4)	-10(3)	22(3)	-8(3)
C(25)	34(4)	58(4)	35(4)	-1(3)	9(3)	-3(3)
C(26)	31(3)	39(4)	63(5)	6(3)	26(3)	-1(3)
C(27)	32(3)	36(4)	66(5)	3(3)	28(4)	-3(3)
C(28)	32(3)	37(4)	66(5)	2(3)	34(4)	4(3)
C(29)	26(3)	42(4)	48(4)	4(3)	25(3)	11(3)
C(30)	47(4)	28(3)	75(5)	-6(3)	46(4)	-2(3)
C(31)	35(4)	65(5)	54(5)	-26(4)	30(4)	-5(4)
C(32)	39(4)	55(4)	52(4)	9(4)	33(4)	13(3)
C(33)	66(5)	38(4)	116(7)	-9(4)	70(5)	-10(4)
C(34)	31(4)	85(6)	64(5)	8(5)	22(4)	14(4)
C(35)	94(7)	35(4)	140(10)	9(5)	91(7)	12(4)

C(36)	47(5)	140(10)	85(7)	-62(6)	41(5)	-29(5)
C(37)	91(7)	121(8)	66(6)	40(6)	60(6)	46(6)
C(38)	45(4)	46(4)	45(4)	-3(3)	24(3)	8(3)
C(39)	55(4)	36(4)	55(5)	-8(3)	25(4)	2(3)
C(40)	40(4)	42(4)	49(4)	-3(3)	16(3)	-8(3)
C(41)	25(3)	45(4)	49(4)	5(3)	11(3)	0(3)
C(42)	31(4)	53(4)	72(5)	1(4)	28(4)	5(3)
C(43)	47(4)	47(4)	66(5)	-3(4)	40(4)	0(3)
C(44)	49(4)	46(4)	46(4)	-6(3)	27(4)	3(3)
C(45)	47(4)	38(4)	55(5)	-9(3)	31(4)	3(3)
C(46)	44(4)	34(4)	58(5)	-2(3)	29(4)	-1(3)
C(47)	38(4)	34(4)	65(5)	-1(3)	29(4)	-1(3)
C(48)	36(4)	49(4)	64(5)	5(4)	35(4)	4(3)
C(49)	50(4)	47(4)	61(5)	8(4)	40(4)	9(3)
C(50)	54(5)	73(6)	95(7)	-4(5)	37(5)	-12(5)
C(51)	27(4)	140(10)	130(10)	60(8)	20(5)	0(5)
C(52)	79(7)	96(8)	200(10)	80(10)	90(10)	53(6)
C(53)	88(7)	51(5)	74(6)	23(5)	31(5)	33(5)
C(54)	75(7)	67(6)	180(10)	76(7)	49(8)	17(6)
C(55)	92(7)	54(5)	140(10)	22(6)	86(7)	4(5)
C(56)	43(4)	70(5)	88(6)	6(5)	41(5)	-2(4)
C(57)	32(4)	77(6)	53(5)	0(4)	24(4)	9(4)
C(58)	50(5)	68(6)	114(8)	28(5)	44(5)	31(4)
C(59)	53(5)	71(6)	130(10)	43(6)	24(6)	20(5)
C(60)	74(7)	50(6)	180(10)	49(7)	12(8)	-6(5)
C(61)	93(7)	36(4)	109(8)	-1(5)	71(6)	-10(4)
N(2)	150(10)	150(10)	130(10)	-27(7)	103(8)	-54(8)
C(62)	94(7)	72(6)	78(7)	0(5)	59(6)	-1(5)
C(63)	160(10)	160(10)	120(10)	85(8)	120(10)	110(10)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table 5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **11**

atom	x	y	z	U(eq)
H(12)	11548	2743	3533	47
H(13)	10970	1708	2834	49
H(14)	9491	1171	2470	47
H(22A)	5589	5251	558	64
H(22B)	5246	6002	743	64
H(22C)	4847	5129	710	64
H(23A)	7363	7021	1938	56
H(23B)	6334	6901	1341	56
H(23C)	7218	6603	1364	56
H(24A)	9393	6656	4019	63
H(24B)	10492	6534	4498	63
H(24C)	9778	6132	4608	63
H(25A)	11680	5194	5040	72
H(25B)	11382	4293	5050	72
H(25C)	10884	5021	5139	72
H(26A)	6375	1066	2721	68
H(26B)	6736	590	2386	68
H(26C)	5662	842	2028	68
H(27A)	4582	1830	1423	67
H(27B)	4522	2782	1448	67
H(27C)	4875	2257	2031	67
H(33A)	4160	4571	2204	95
H(33B)	5040	4065	2350	95
H(33C)	4318	4421	1693	95
H(34A)	3614	6290	1342	94
H(34B)	3915	5558	1114	94
H(34C)	4252	6445	1110	94
H(35A)	5414	7397	1685	112
H(35B)	6345	7567	2337	112
H(35C)	5346	7734	2205	112
H(36A)	7410	7008	3261	132
H(36B)	7644	6227	3662	132
H(36C)	6971	6900	3630	132
H(37A)	7160	4935	3653	126
H(37B)	6348	4298	3249	126
H(37C)	6233	4943	3632	126
H(38A)	10258	1253	5335	56
H(38B)	9612	2019	4996	56
H(39A)	10431	2258	4560	63
H(39B)	11120	2298	5277	63
H(40A)	12512	1825	5428	59
H(40B)	11950	2007	4724	59
H(41A)	13182	1069	5049	55
H(41B)	12692	467	5243	55
H(42A)	12732	-403	4564	64
H(42B)	12980	266	4257	64
H(43A)	11480	65	3342	59
H(43B)	12115	-724.0001	3552	59
H(44A)	10889	-1656	3125	57
H(44B)	10164	-928	2811	57
H(45A)	9486	-2071	2937	55
H(45B)	10224	-1982	3648	55
H(46A)	8899	-1825	3682	55
H(46B)	8183	-1826.9999	2965	55
H(47A)	7726	-510	2992	55
H(47B)	7534	-1101	3370	55
H(48A)	7613	-70	3963	56

H(48B)	7787	572	3603	56
H(49A)	8388	1005	4600	58
H(49B)	9109	271	4853	58
H(50A)	3582	-215	469	93
H(50B)	3883	-223	22	93
H(51A)	3080	901	-211	136
H(51B)	3502	1108	469	136
H(52A)	3653	2325	165	145
H(52B)	3465	2019	-449	145
H(53A)	4337	3034	-292	96
H(53B)	4869	3001	414	96
H(54A)	6161	3220	539	143
H(54B)	5794	3173	-141	143
H(55A)	7021	2610	61	101
H(55B)	7468	2940	722	101
H(56A)	8462	1971	1350	78
H(56B)	8419	1793	761	78
H(57A)	8079	452	782	66
H(57B)	9024	686	1412	66
H(58A)	8837	-295	1946	96
H(58B)	8065	-564	1271	96
H(59A)	7733	-1195	1869	122
H(59B)	7783	-371.0000	2184	122
H(60A)	6271	-924	1812	166
H(60B)	6274	-1522	1361	166
H(61A)	4904	-1127	588	87
H(61B)	4777	-1079	1118	87
H(63A)	8506	3547	3877	190
H(63B)	7655	3055	3331	190
H(63C)	8581	2597	3843	190