Supporting Information

Ring-Opening Reaction of Phosphorus-Bridged [1]ferrocenophane via Ring Slippage from η^5- to η^1-Cp

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Experimental Section

General Remarks. All reactions were carried out under an atmosphere of dry nitrogen using Schlenk tube techniques. All solvents were dried and purified by distillation: ether and THF were distilled from sodium/benzophenone and hexane was distilled from sodium metal. These purified solvents were stored under an N_2 atmosphere. Other reagents were used as received. **3a**, **3b**, and **3c** were prepared according to previously described methods.

NMR spectra were recorded on a JEOL LA-300 spectrometer. ^{1}H and ^{13}C NMR chemical shifts were reported relative to Me_4Si and were determined by reference to the residual solvent peaks. ^{31}P NMR chemical shifts were reported relative to H_3PO_4 (85%) used as an external reference. Elemental analyses were performed with a Perkin-Elmer 2400CHN elemental analyzer.

Photolysis was carried out with Pyrex-glass-filtered emission from a 400W mercury arc lamp (Riko-Kagaku Sangyo UVL-400P). The emission-lines used and their relative intensities (in parenthesis) were as follows: 577.0 (69), 546.1 (82), 435.8 (69), 404.7 (42), 365.0 (100), 334.1 (7), 312.6 (38), and 302.2 (9). Gel permeation chromatography (GPC) analyses were run on a JASCO LC-2000 GPC-System using two Shodex KF803L columns (exclusion limit: 4×10^6) connected sequentially. The molecular weights were estimated based on a comparison to polystyrene standards.

[Fe{(η^5-C_5H_4)(η^1-C_5H_4)P(S)Ph}{P(OMe)$_3$}$_2$] (4a). **3a** (103 mg, 0.318mmol), THF (30 mL), and $P(OMe)_3$ (0.40 mL, 3.39 mmol) were added to a Pyrex Schlenk tube, and the solution was irradiated with the 400W mercury arc lamp at 0 °C for 10 min. The solvent and the excess $P(OMe)_3$ were removed *in vacuo*. To the residue dissolved in THF was added hexane to form precipitates, which were collected by filtration and washed with hexane. The product obtained was dried *in vacuo* to give an orange powder. Yield: 176 mg (97% based on **3a**). ^{1}H NMR (300.4 MHz, $CDCl_3$): δ = 2.86 (d, $^{2}J_{HH}$ = 24.2 Hz, 1H, CH_2), 2.99 (d, $^{2}J_{HH}$ = 24.2 Hz, 1H, CH_2), 3.54 (d, $^{3}J_{PH}$ = 11.0 Hz, 9H, $P(OMe)_3$), 3.59 (d, $^{3}J_{PH}$ = 10.6 Hz, 9H, $P(OMe)_3$), 4.11 (m, 1H, η^5-Cp), 4.22 (m, 1H, η^5-Cp), 4.38 (m, 1H, η^5-Cp), 5.79 (m, 1H, η^5-Cp), 6.45 (m, 2H, η^1-Cp), 7.35-7.52 (m, 3H, Ph), 7.91 (m, 2H, Ph). $^{13}C\{^{1}H\}$ NMR (75.45 MHz, $CDCl_3$): δ = 51.4 (d, $^{2}J_{PC}$ = 4 Hz, $P(OMe)_3$), 52.0 (d, $^{2}J_{PC}$ = 7 Hz, $P(OMe)_3$), 57.8 (d, $^{3}J_{PC}$ = 24 Hz, CH_2), 78.9 (dd, J_{PC} = 10

and 7 Hz, η^5-Cp), 79.6 (d, J_{PC} = 11 Hz, η^5-Cp), 84.5 (dd, J_{PC} = 12 and 6 Hz, η^5-Cp), 86.3 (d, J_{PC} = 10 Hz, η^5-Cp), 106.7 (d, J_{PC} = 91 Hz, ipso-η^1-Cp-P), 114.4 (dd, J_{PC} = 98 and 19 Hz, ipso-η^5-Cp-P), 128.3 (d, J_{PC} = 12 Hz, Ph), 131.0 (d, J_{PC} = 3 Hz, Ph), 131.4 (d, J_{PC} = 11 Hz, Ph), 131.4 (d, J_{PC} = 24 Hz, η^1-Cp), 135.7 (d, J_{PC} = 13 Hz, η^1-Cp), 151.5 (d, J_{PC} = 109 Hz, ipso-Ph), 199.0 (dt, J_{PC} = 29 and 39 Hz, ipso-η^1-Cp-Fe). $^{31}P\{^1H\}$ NMR (121.5 MHz, $CDCl_3$): δ = 33.9 (d, $^3J_{PP}$ = 4 Hz, P(S)Ph), 186.1 (dd, $^3J_{PP}$ = 4 Hz, $^2J_{PP}$ = 151 Hz, $P(OMe)_3$), 194.4 (d, $^2J_{PP}$ = 152 Hz, $P(OMe)_3$). Anal. Calcd for $C_{22}H_{31}FeP_3S$: C, 46.17; H, 5.46. Found: C, 46.23; H, 5.28.

[Fe{(η^5-C_5H_4)(η^1-C_5H_4)PPh}{$P(OMe)_3$}$_2$] (4b). **3b** (170 mg, 0.582 mmol), THF (15 mL), and $P(OMe)_3$ (0.80 mL, 6.78 mmol) were added to a Pyrex Schlenk tube, and the solution was irradiated with the 400W mercury arc lamp at 0 °C for 15 min. The solvent and the excess $P(OMe)_3$ were removed *in vacuo*. Only $^{31}P\{^1H\}$ NMR spectrum was measured for a thus-obtained reddish wax, which was a mixture of two isomers. $^{31}P\{^1H\}$ NMR (121.5 MHz, $CDCl_3$): for one isomer, δ = -16.3 (d, $^3J_{PP}$ = 7 Hz, PPh), 189.9 (dd, $^3J_{PP}$ = 7 Hz, $^2J_{PP}$ = 152 Hz, $P(OMe)_3$), 193.6 (d, $^2J_{PP}$ = 152 Hz, $P(OMe)_3$), and for the orther isomer, δ = -44.6 (s), 183.3 (d, $^2J_{PP}$ = 165 Hz, $P(OMe)_3$), 188.5 (d, $^2J_{PP}$ = 164 Hz, $P(OMe)_3$).

[Fe{(η^5-C_5H_4)(η^1-C_5H_4)PMes}{$P(OMe)_3$}$_2$] (4c). **3c** (25 mg, 0.075 mmol), THF (10 mL), and $P(OMe)_3$ (0.20 mL, 1.70 mmol) were added to a Pyrex Schlenk tube, and the solution was irradiated with the 400W mercury arc lamp at 0 °C for 10 min. The solvent and the excess $P(OMe)_3$ were removed *in vacuo*. Only $^{31}P\{^1H\}$ NMR spectrum was measured for a thus-obtained reddish powder, which was a mixture of two isomers. $^{31}P\{^1H\}$ NMR (121.5 MHz, $CDCl_3$): for one isomer, δ = -20.7 (d, $^3J_{PP}$ = 7 Hz, PMes), 188.8 (dd, $^3J_{PP}$ = 7 Hz, $^2J_{PP}$ = 156 Hz, $P(OMe)_3$), 194.2 (d, $^2J_{PP}$ = 158 Hz, $P(OMe)_3$), and for the orther isomer, δ = -49.8 (s), 183.4 (d, $^2J_{PP}$ = 165 Hz, $P(OMe)_3$), 188.0 (d, $^2J_{PP}$ = 165 Hz, $P(OMe)_3$).

[Fe{(η^5-C_5H_4) P(S) (C_5H_4)Ph}(PMe_3)$_3$] (5). **3a** (57 mg, 0.176mmol), THF (10 mL), and PMe_3 (0.46 M ether solution, 3 mL, 1.38 mmol) were added to a Pyrex Schlenk tube, and the solution was irradiated with the 400W mercury arc lamp at 0 °C for 10 min.

Reduction of a volume of the thus-obtained solution *in vacuo* gave yellow precipitates, which was separated by decantation and washed with a small amount of THF. After workup, 77 mg (79 %) of **5** was obtained. ^{1}H NMR (300.4 MHz, CD_3COCD_3): δ = 1.46 (m, 27H, PMe_3), 4.33 (br, 1H, η^5-Cp), 4.53 (br, 1H, η^5-Cp), 4.86 (br, 1H, η^5-Cp), 4.97 (br, 1H, η^5-Cp), 5.78 (m, 2H, Cp$^-$), 6.12 (m, 2H, Cp$^-$), 7.10-7.18 (m, 3H, Ph), 7.57 (m, 2H, Ph). ^{13}C{^{1}H} NMR (75.45 MHz, CD_3COCD_3): δ = 23.0 (m, PMe_3), 76.3 (d, J_{PC} = 6 Hz, η^5-Cp), 80.0 (d, J_{PC} = 8 Hz, η^5-Cp), 86.7 (d, J_{PC} = 10 Hz, η^5-Cp), 87.4 (d, J_{PC} = 11 Hz, η^5-Cp), 88.7 (d, J_{PC} = 104 Hz, ipso-Cp$^-$-P), 96.2 (brd, J_{PC} = 111 Hz, ipso-η^5-Cp-P), 109.9 (d, J_{PC} = 18 Hz, Cp$^-$), 114.6 (d, J_{PC} = 16 Hz, Cp$^-$), 127.3 (d, J_{PC} = 12 Hz, Ph), 128.8 (s, Ph), 129.9 (d, J_{PC} = 11 Hz, Ph), 143.5 (d, J_{PC} = 85 Hz, ipso-Ph). ^{31}P{^{1}H} NMR (121.5 MHz, CD_3COCD_3): δ = 26.0 (s, P(S)Ph), 23.4 (s, PMe_3).

Polymerization of 3a by Photolysis. A solution of **3a** (200 mg, 0.62 mmol) in THF (15 mL) was irradiated with the mercury arc lamp for 15 min at 0 °C. The solvent of the resulting solution was removed *in vacuo* to give a polymer of **3a** in an almost quantitative yield ($Mw = 4.8 \times 10^4$, $Mn = 2.9 \times 10^4$, $Mw/Mn = 1.63$). ^{31}P{^{1}H} NMR (δ, in THF) (relative intensities are in parentheses): 37.3 (94), 30.9 (6).

Polymerization of 4a by Thermolysis. A solution of **4a** (144 mg, 0.25 mmol) in THF (6 mL) was refluxed for 24h. After the solvent was removed *in vacuo*, the residue was washed with ether and dried to give yellow powder (34 mg, 0.11 mmol, 44 %). ^{31}P{^{1}H} NMR (δ, in THF) (relative intensities are in parentheses): 37.7(80), 36.7(10), and 34.5(10) ppm. GPC analysis showed that the product is an oligomer having a molecular weight in a range of 300-10000 (Mw = 730, Mn = 1640, Mw/Mn = 2.23).

X-ray crystallography. A suitable crystal of **4a** was mounted on a glass fiber. All measurements were made on a Mac Science DIP2030 imaging plate area detector. The data were collected to a maximum 2θ value of 55.8°. Cell parameters and intensities for the reflection were estimated using the program packages of MacDENZO. A total of 3386 reflections were collected, and 3259 reflections (I> 0.00σ(I)) were used for the final refinement. The structure was solved by direct methods and expanded using Fourier techniques. Non-hydrogen atoms were refined anisotropically. Hydrogen

atoms were located at ideal positions. All calculations were performed using a teXsan crystallographic software package from the Molecular Structure Corporation. Details of data collection and refinement were listed in Table 1, and bond distances and angles, atomic coordinates, and anisotropic thermal parameters were listed in Table 2, 3, 4, and 5, respectively.

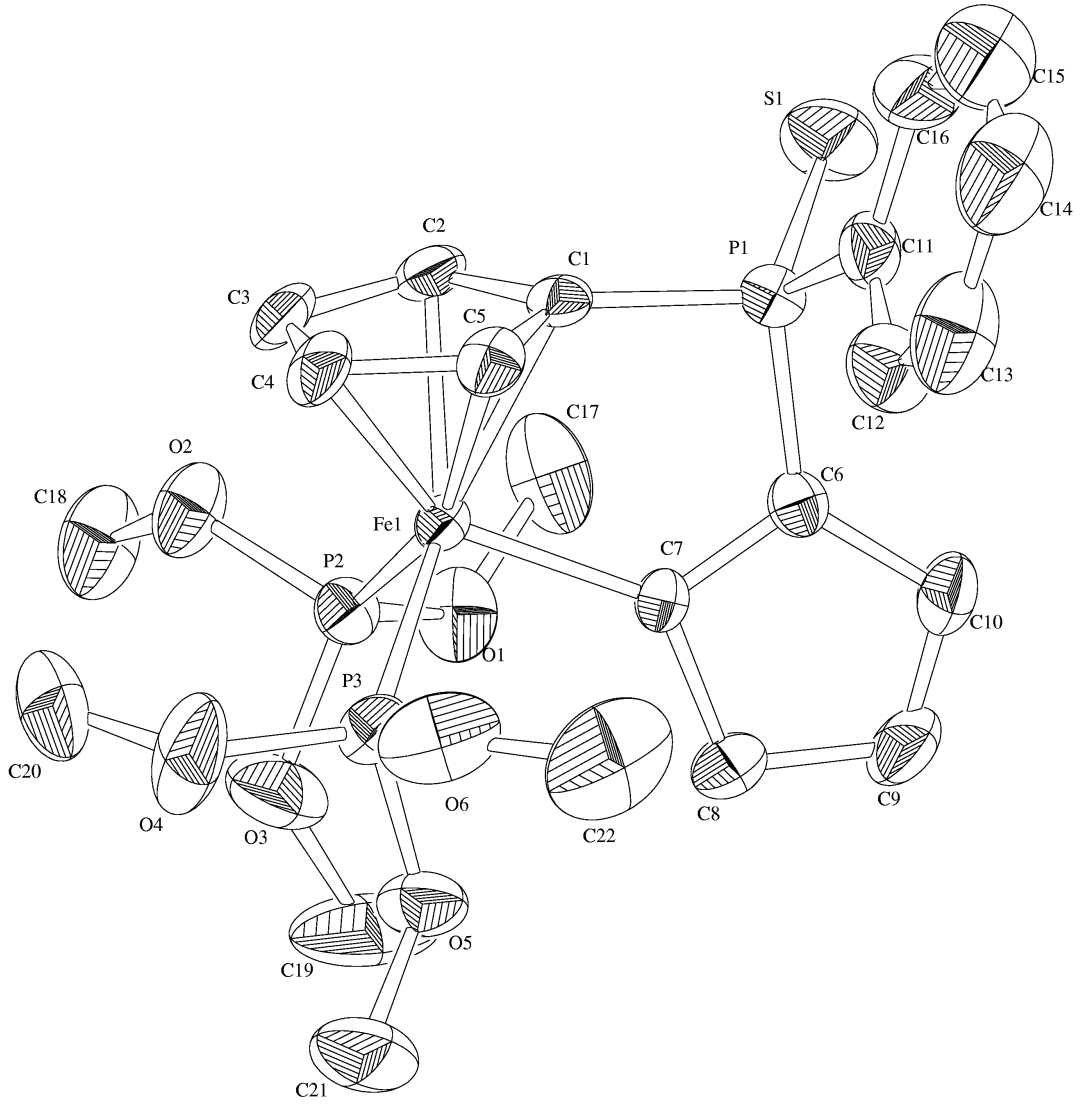

Figure S1. ORTEP drawing of **4a** at 50 % probability.

Table 1. Experimental Data for **4a**.

A. Crystal Data

Empirical Formula	$C_{22}H_{31}FeO_6P_3S$
Formula Weight	572.31
Crystal Color, Habit	pale yellow, plate
Crystal Dimensions	0.40 X 0.25 X 0.15 mm
Crystal System	orthorhombic
Lattice Type	F-centered
Lattice Parameters	a = 14.6900(1) Å b = 60.5050(7) Å c = 11.7620(1) Å V = 10454.3(2) Å ^{3}
Space Group	Fdd2 (#43)
Z value	16
D_{calc}	1.454 g/cm^3
F_{000}	4768.00
μ(MoKα)	8.75 cm^{-1}

B. Intensity Measurements

Diffractometer	Mac Science DIP2030 Imaging Plate
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Temperature	-73.0 ^{o}C
Data Images	180 exposures at 5.0 minutes
Oscillation Range	1.0^o
$2\theta_{max}$	55.6^o
No. of Reflections Measured	Total: 3386
Corrections	Lorentz-polarization Secondary Extinction (coefficient: 2.00490e-07)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	$1/\sigma^2(Fo) = 4Fo^2/\sigma^2(Fo^2)$
p-factor	0.0980
Anomalous Dispersion	All non-hydrogen atoms
No. of Observations (I>0.00σ(I), 2θ < 55.59^o)	3259
No. Variables	299
Reflection/Parameter Ratio	10.90
Residuals: R; Rw	0.038 ; 0.067
Residuals: R1	0.037
No. of Reflections to calc R1	3224
Goodness of Fit Indicator	1.32
Max Shift/Error in Final Cycle	0.054
Maximum peak in Final Diff. Map	0.38 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.47 e$^-$/Å^3

Table 2. Bond Lengths (Å)

atom	atom	distance	atom	atom	distance
Fe(1)	P(2)	2.130(2)	Fe(1)	P(3)	2.129(2)
Fe(1)	C(1)	2.105(6)	Fe(1)	C(2)	2.120(6)
Fe(1)	C(3)	2.148(6)	Fe(1)	C(4)	2.149(7)
Fe(1)	C(5)	2.119(6)	Fe(1)	C(7)	1.954(6)
S(1)	P(1)	1.966(3)	P(1)	C(1)	1.800(7)
P(1)	C(6)	1.757(7)	P(1)	C(11)	1.825(8)
P(2)	O(1)	1.609(6)	P(2)	O(2)	1.604(6)
P(2)	O(3)	1.599(6)	P(3)	O(4)	1.587(7)
P(3)	O(5)	1.593(6)	P(3)	O(6)	1.633(7)
O(1)	C(17)	1.44(1)	O(2)	C(18)	1.440(9)
O(3)	C(19)	1.45(2)	O(4)	C(20)	1.39(1)
O(5)	C(21)	1.454(10)	O(6)	C(22)	1.43(2)
C(1)	C(2)	1.438(9)	C(1)	C(5)	1.411(9)
C(2)	C(3)	1.41(1)	C(3)	C(4)	1.40(1)
C(4)	C(5)	1.425(10)	C(6)	C(7)	1.372(8)
C(6)	C(10)	1.480(9)	C(7)	C(8)	1.534(9)
C(8)	C(9)	1.46(1)	C(9)	C(10)	1.34(1)
C(11)	C(12)	1.37(1)	C(11)	C(16)	1.39(1)
C(12)	C(13)	1.37(1)	C(13)	C(14)	1.40(2)
C(14)	C(15)	1.35(2)	C(15)	C(16)	1.41(2)
C(2)	H(1)	0.99	C(3)	H(2)	0.94
C(4)	H(3)	0.91	C(5)	H(4)	0.95
C(8)	H(5)	0.96	C(8)	H(6)	0.98
C(9)	H(7)	1.01	C(10)	H(8)	0.99
C(12)	H(9)	1.01	C(13)	H(10)	0.99
C(14)	H(11)	0.93	C(15)	H(12)	0.93
C(16)	H(13)	0.99	C(17)	H(14)	0.93
C(17)	H(15)	1.01	C(17)	H(16)	0.92
C(18)	H(17)	0.96	C(18)	H(18)	0.90
C(18)	H(19)	1.02	C(19)	H(20)	0.98
C(19)	H(21)	0.98	C(19)	H(22)	0.96
C(20)	H(23)	0.93	C(20)	H(24)	0.92
C(20)	H(25)	1.02	C(21)	H(26)	0.93
C(21)	H(27)	0.93	C(21)	H(28)	1.04
C(22)	H(29)	0.89	C(22)	H(30)	1.02
C(22)	H(31)	1.01			

Table 5. Bond Angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
P(2)	Fe(1)	P(3)	95.67(7)	P(2)	Fe(1)	C(1)	129.4(2)
P(2)	Fe(1)	C(2)	95.6(2)	P(2)	Fe(1)	C(3)	95.0(2)
P(2)	Fe(1)	C(4)	126.5(2)	P(2)	Fe(1)	C(5)	159.7(2)
P(2)	Fe(1)	C(7)	93.3(2)	P(3)	Fe(1)	C(1)	134.9(2)
P(3)	Fe(1)	C(2)	153.3(2)	P(3)	Fe(1)	C(3)	116.1(2)
P(3)	Fe(1)	C(4)	89.4(2)	P(3)	Fe(1)	C(5)	97.9(2)
P(3)	Fe(1)	C(7)	95.3(2)	C(1)	Fe(1)	C(2)	39.8(2)
C(1)	Fe(1)	C(3)	65.5(3)	C(1)	Fe(1)	C(4)	64.9(3)
C(1)	Fe(1)	C(5)	39.0(3)	C(1)	Fe(1)	C(7)	84.2(3)
C(2)	Fe(1)	C(3)	38.7(3)	C(2)	Fe(1)	C(4)	64.5(3)
C(2)	Fe(1)	C(5)	65.9(3)	C(2)	Fe(1)	C(7)	108.1(3)
C(3)	Fe(1)	C(4)	38.1(3)	C(3)	Fe(1)	C(5)	65.4(3)
C(3)	Fe(1)	C(7)	146.4(3)	C(4)	Fe(1)	C(5)	39.0(3)
C(4)	Fe(1)	C(7)	139.3(3)	C(5)	Fe(1)	C(7)	100.4(3)
S(1)	P(1)	C(1)	113.7(2)	S(1)	P(1)	C(6)	117.7(2)
S(1)	P(1)	C(11)	113.3(3)	C(1)	P(1)	C(6)	97.9(3)
C(1)	P(1)	C(11)	103.7(3)	C(6)	P(1)	C(11)	108.7(3)
Fe(1)	P(2)	O(1)	120.8(2)	Fe(1)	P(2)	O(2)	111.5(2)
Fe(1)	P(2)	O(3)	122.3(3)	O(1)	P(2)	O(2)	103.6(3)
O(1)	P(2)	O(3)	96.0(4)	O(2)	P(2)	O(3)	99.2(4)
Fe(1)	P(3)	O(4)	119.6(3)	Fe(1)	P(3)	O(5)	117.5(2)
Fe(1)	P(3)	O(6)	117.2(3)	O(4)	P(3)	O(5)	102.7(5)
O(4)	P(3)	O(6)	93.7(5)	O(5)	P(3)	O(6)	102.3(3)
P(2)	O(1)	C(17)	120.2(6)	P(2)	O(2)	C(18)	123.7(6)
P(2)	O(3)	C(19)	125.8(9)	P(3)	O(4)	C(20)	127.0(7)
P(3)	O(5)	C(21)	122.8(7)	P(3)	O(6)	C(22)	119.4(8)
Fe(1)	C(1)	P(1)	114.9(3)	Fe(1)	C(1)	C(2)	70.7(3)
Fe(1)	C(1)	C(5)	71.0(3)	P(1)	C(1)	C(2)	125.0(5)
P(1)	C(1)	C(5)	125.8(5)	C(2)	C(1)	C(5)	108.1(6)
Fe(1)	C(2)	C(1)	69.5(3)	Fe(1)	C(2)	C(3)	71.7(4)
C(1)	C(2)	C(3)	107.6(6)	Fe(1)	C(3)	C(2)	69.6(3)
Fe(1)	C(3)	C(4)	71.0(4)	C(2)	C(3)	C(4)	108.0(6)
Fe(1)	C(4)	C(3)	70.9(4)	Fe(1)	C(4)	C(5)	69.4(3)
C(3)	C(4)	C(5)	109.2(6)	Fe(1)	C(5)	C(1)	70.0(3)
Fe(1)	C(5)	C(4)	71.6(4)	C(1)	C(5)	C(4)	107.1(6)
P(1)	C(6)	C(7)	118.3(5)	P(1)	C(6)	C(10)	129.2(5)
C(7)	C(6)	C(10)	112.2(6)	Fe(1)	C(7)	C(6)	123.9(5)
Fe(1)	C(7)	C(8)	132.8(5)	C(6)	C(7)	C(8)	103.4(5)
C(7)	C(8)	C(9)	106.9(6)	C(8)	C(9)	C(10)	110.0(6)
C(6)	C(10)	C(9)	107.6(6)	P(1)	C(11)	C(12)	120.9(6)
P(1)	C(11)	C(16)	119.7(7)	C(12)	C(11)	C(16)	119.4(8)
C(11)	C(12)	C(13)	121.1(9)	C(12)	C(13)	C(14)	120(1)
C(13)	C(14)	C(15)	118.9(10)	C(14)	C(15)	C(16)	121(1)
C(11)	C(16)	C(15)	118(1)				

Table 4. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Fe(1)	0.74029(3)	0.050847(6)	0.950(1)	2.024(8)
S(1)	0.42399(8)	0.05312(2)	0.898(1)	4.92(3)
P(1)	0.53374(5)	0.07125(1)	0.917(1)	2.73(1)
P(2)	0.77789(5)	0.02096(1)	0.867(1)	2.55(1)
P(3)	0.87120(6)	0.06569(1)	0.940(1)	2.97(2)
O(1)	0.7207(2)	0.01183(5)	0.761(1)	3.93(5)
O(2)	0.7792(2)	0.00065(4)	0.954(1)	3.92(6)
O(3)	0.8760(2)	0.01784(5)	0.809(1)	5.07(7)
O(4)	0.9480(2)	0.05796(7)	1.024(1)	7.3(1)
O(5)	0.9197(2)	0.06589(5)	0.820(1)	3.97(6)
O(6)	0.8800(3)	0.09135(6)	0.981(1)	5.52(7)
C(1)	0.6135(2)	0.06019(5)	1.018(1)	2.48(4)
C(2)	0.6285(2)	0.03718(5)	1.040(1)	2.97(5)
C(3)	0.7077(2)	0.03518(5)	1.109(1)	3.09(5)
C(4)	0.7414(3)	0.05670(6)	1.131(1)	3.10(6)
C(5)	0.6842(2)	0.07231(5)	1.074(1)	2.75(5)
C(6)	0.6085(2)	0.07334(5)	0.801(1)	2.47(5)
C(7)	0.6946(2)	0.06429(4)	0.811(1)	2.16(4)
C(8)	0.7360(3)	0.06747(7)	0.692(1)	3.42(7)
C(9)	0.6662(3)	0.07828(8)	0.623(1)	4.14(7)
C(10)	0.5906(3)	0.08180(6)	0.685(1)	3.56(6)
C(11)	0.5087(2)	0.09890(6)	0.970(1)	3.31(6)
C(12)	0.5696(3)	0.11603(6)	0.954(1)	4.34(8)
C(13)	0.5554(5)	0.13668(7)	1.000(1)	5.8(1)
C(14)	0.4774(6)	0.1406(1)	1.063(1)	7.3(2)
C(15)	0.4147(5)	0.1238(1)	1.078(1)	7.1(1)
C(16)	0.4288(4)	0.10257(8)	1.031(1)	5.5(1)
C(17)	0.6230(3)	0.01030(8)	0.768(1)	5.22(10)
C(18)	0.8002(4)	-0.02166(6)	0.920(1)	5.2(1)
C(19)	0.8982(5)	0.0210(1)	0.692(1)	7.1(1)
C(20)	0.9601(3)	0.0367(1)	1.067(1)	6.1(1)
C(21)	1.0124(3)	0.0732(1)	0.806(1)	6.0(1)
C(22)	0.8389(6)	0.10807(7)	0.915(1)	7.4(2)
H(1)	0.5910	0.0253	1.0127	3.6
H(2)	0.7332	0.0218	1.1345	3.7
H(3)	0.7935	0.0602	1.1731	3.7
H(4)	0.6904	0.0879	1.0734	3.3
H(5)	0.7888	0.0765	0.6947	4.1
H(6)	0.7518	0.0536	0.6582	4.1
H(7)	0.6733	0.0822	0.5431	5.0
H(8)	0.5359	0.0885	0.6569	4.3
H(9)	0.6230	0.1135	0.9083	5.2
H(10)	0.5989	0.1482	0.9869	6.9
H(11)	0.4673	0.1549	1.0938	8.8
H(12)	0.3614	0.1266	1.1197	8.5
H(13)	0.3849	0.0911	1.0384	6.6
H(14)	0.6069	0.0007	0.8268	6.3
H(15)	0.5997	0.0046	0.6967	6.3

Table 4. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(16)	0.5984	0.0246	0.7796	6.3
H(17)	0.8605	-0.0222	0.8884	6.3
H(18)	0.7964	-0.0311	0.9827	6.3
H(19)	0.7585	-0.0264	0.8620	6.3
H(20)	0.9609	0.0180	0.6780	8.5
H(21)	0.8627	0.0112	0.6444	8.5
H(22)	0.8852	0.0358	0.6684	8.5
H(23)	0.9086	0.0327	1.1095	7.3
H(24)	1.0131	0.0364	1.1117	7.3
H(25)	0.9670	0.0266	1.0041	7.3
H(26)	1.0175	0.0881	0.8285	7.3
H(27)	1.0515	0.0642	0.8490	7.3
H(28)	1.0293	0.0721	0.7266	7.3
H(29)	0.8510	0.1220	0.9467	9.0
H(30)	0.8629	0.1077	0.8384	9.0
H(31)	0.7750	0.1057	0.9108	9.0

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 5. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	0.0290(2)	0.0254(2)	0.0226(2)	0.0003(1)	0.0002(2)	0.0015(1)
S(1)	0.0409(5)	0.0731(7)	0.0730(7)	-0.0206(4)	-0.0030(5)	0.0048(6)
P(1)	0.0300(3)	0.0380(4)	0.0358(4)	0.0007(3)	0.0014(3)	0.0018(3)
P(2)	0.0353(3)	0.0277(3)	0.0338(4)	0.0023(3)	0.0015(3)	-0.0024(3)
P(3)	0.0381(4)	0.0416(4)	0.0332(4)	-0.0126(3)	-0.0061(3)	0.0035(3)
O(1)	0.064(2)	0.045(1)	0.041(1)	0.006(1)	-0.009(1)	-0.013(1)
O(2)	0.077(2)	0.030(1)	0.042(1)	0.005(1)	-0.005(2)	0.0008(9)
O(3)	0.046(1)	0.061(2)	0.086(2)	0.007(1)	0.023(2)	-0.005(2)
O(4)	0.058(2)	0.116(3)	0.101(3)	-0.041(2)	-0.049(2)	0.064(3)
O(5)	0.037(1)	0.067(2)	0.047(1)	-0.015(1)	0.006(1)	-0.002(1)
O(6)	0.087(2)	0.054(1)	0.069(2)	-0.031(2)	0.011(2)	-0.017(1)
C(1)	0.034(1)	0.034(1)	0.026(1)	0.0045(9)	0.0093(9)	0.0016(10)
C(2)	0.042(1)	0.036(1)	0.035(2)	-0.001(1)	0.011(1)	0.011(1)
C(3)	0.051(2)	0.039(1)	0.027(1)	0.004(1)	0.007(1)	0.012(1)
C(4)	0.051(2)	0.048(1)	0.019(1)	0.005(1)	-0.003(1)	0.002(1)
C(5)	0.048(2)	0.033(1)	0.023(1)	0.004(1)	0.003(1)	-0.0040(9)
C(6)	0.031(1)	0.030(1)	0.032(1)	0.0012(9)	-0.0026(10)	-0.0017(10)
C(7)	0.031(1)	0.027(1)	0.0241(10)	-0.0017(9)	-0.0033(9)	0.0006(8)
C(8)	0.047(2)	0.054(2)	0.029(1)	0.001(1)	0.006(1)	0.003(1)
C(9)	0.063(2)	0.066(2)	0.028(1)	-0.006(2)	-0.006(1)	0.015(1)
C(10)	0.050(2)	0.050(2)	0.035(1)	0.004(1)	-0.011(1)	0.009(1)
C(11)	0.044(1)	0.044(1)	0.038(2)	0.020(1)	0.002(1)	0.003(1)
C(12)	0.060(2)	0.038(2)	0.068(3)	0.006(1)	0.000(2)	-0.005(2)
C(13)	0.108(4)	0.043(2)	0.068(3)	0.018(2)	-0.017(3)	-0.005(2)
C(14)	0.145(5)	0.064(3)	0.068(4)	0.055(3)	0.018(4)	0.000(3)
C(15)	0.116(5)	0.081(3)	0.074(3)	0.058(3)	0.030(4)	0.000(3)
C(16)	0.072(3)	0.068(2)	0.067(3)	0.039(2)	0.037(2)	0.018(2)
C(17)	0.063(2)	0.059(2)	0.077(3)	0.004(2)	-0.034(2)	-0.025(2)
C(18)	0.100(4)	0.029(1)	0.070(3)	0.017(2)	-0.008(3)	0.001(2)
C(19)	0.099(4)	0.080(3)	0.092(3)	-0.011(3)	0.062(4)	-0.029(3)
C(20)	0.049(2)	0.103(3)	0.081(4)	0.013(3)	-0.020(3)	0.021(3)
C(21)	0.041(2)	0.105(4)	0.084(4)	-0.017(2)	0.011(2)	0.009(3)
C(22)	0.131(6)	0.033(2)	0.118(6)	-0.011(2)	0.024(4)	0.000(2)

The general temperature factor expression:
$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$