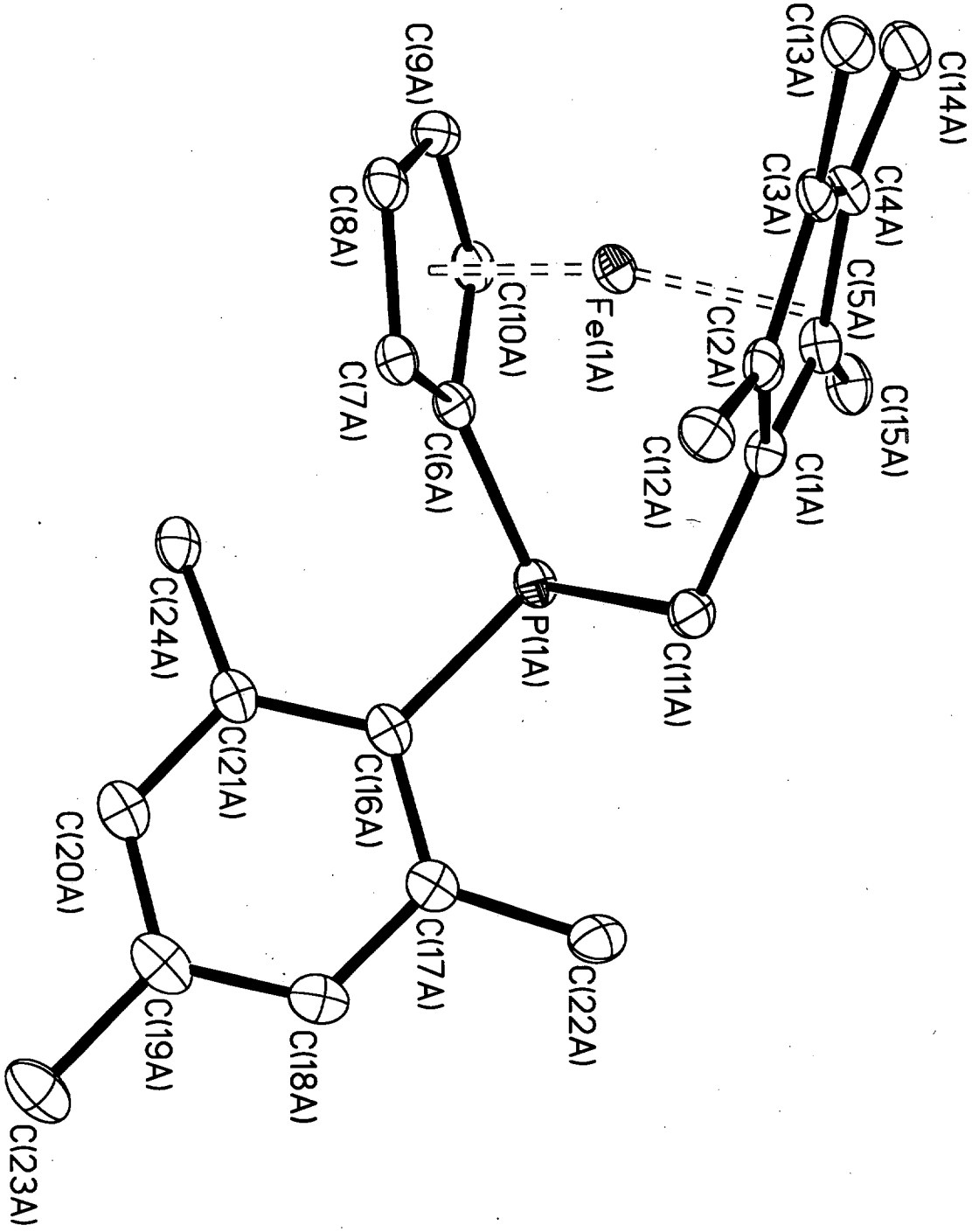
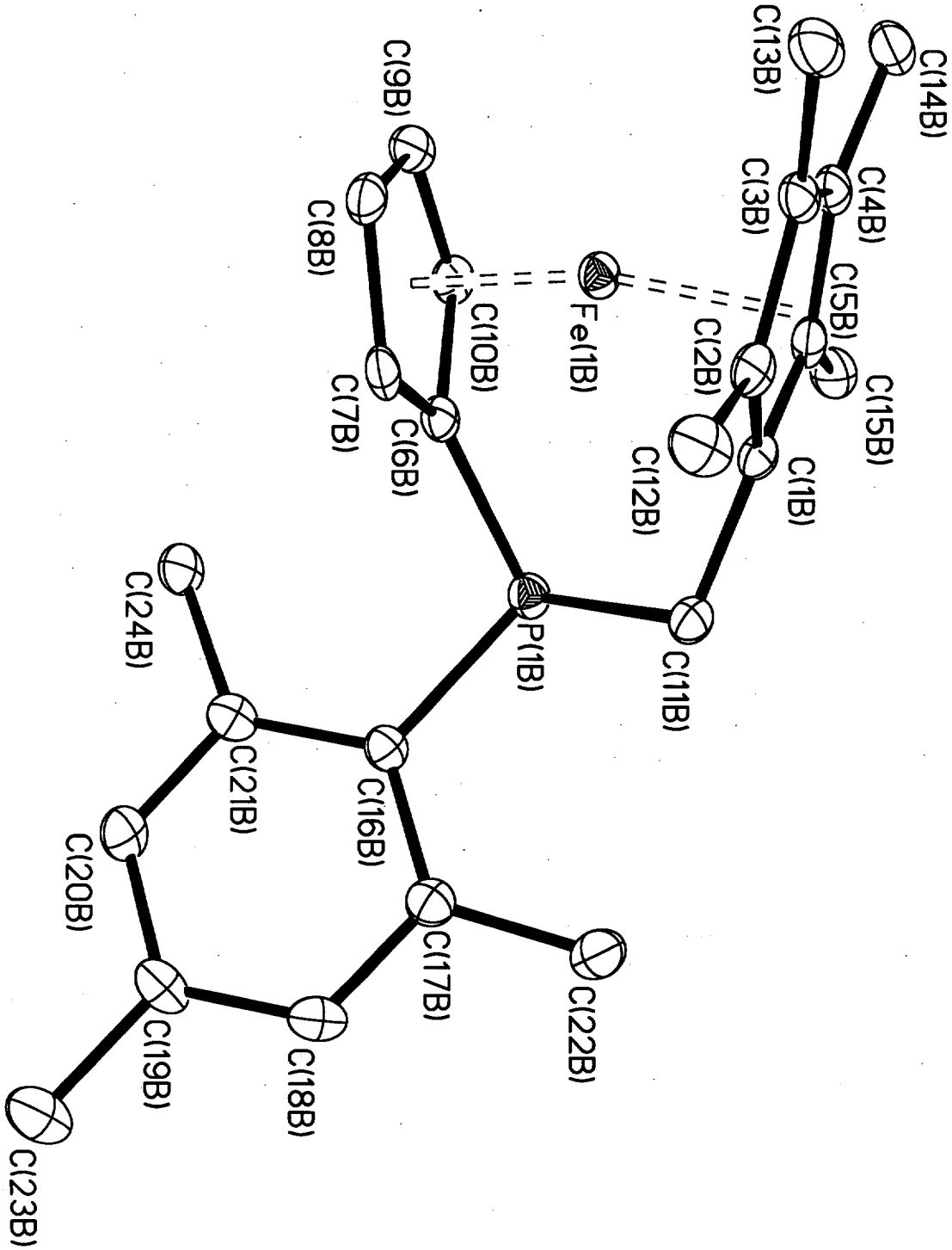
© 2001 American Chemical Society, J. Am. Chem. Soc., Resendes ja002750e Supporting Info Page 41

Supp Material for Compound 8b.




C(14B)
C(13B)
C(4B)
C(3B)
C(5B)
C(15B)
C(2B)
C(1B)
C(12B)
C(9B)
C(8B)
Fe(1B)
C(10B)
C(7B)
C(6B)
P(1B)
C(11B)
C(24B)
C(21B)
C(16B)
C(17B)
C(22B)
C(20B)
C(19B)
C(18B)
C(23B)

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

- 6.2332 (0.0092) x + 12.6426 (0.0382) y + 9.0778 (0.0235) z = 5.0114 (0.0240)

* 0.0120 (0.0020) C1A
* -0.0043 (0.0019) C2A
* -0.0051 (0.0020) C3A
* 0.0126 (0.0020) C4A
* -0.0151 (0.0020) C5A

Rms deviation of fitted atoms = 0.0107

- 6.2226 (0.0092) x + 17.4763 (0.0336) y + 4.5670 (0.0263) z = 11.0080 (0.0221)

Angle to previous plane (with approximate esd) = 18.06 ( 0.20 )

* -0.0079 (0.0019) C6A
* 0.0047 (0.0020) C7A
* 0.0003 (0.0020) C8A
* -0.0053 (0.0020) C9A
* 0.0082 (0.0020) C10A

Rms deviation of fitted atoms = 0.0060

5.5728 (0.0103) x + 20.3347 (0.0298) y - 2.8256 (0.0267) z = 7.6506 (0.0293)

Angle to previous plane (with approximate esd) = 87.53 ( 0.10 )

* 0.0087 (0.0019) C1B
* -0.0090 (0.0020) C2B
* 0.0058 (0.0020) C3B
* -0.0003 (0.0020) C4B
* -0.0052 (0.0019) C5B

Rms deviation of fitted atoms = 0.0066

5.9407 (0.0097) x + 19.0356 (0.0317) y + 2.5531 (0.0266) z = 6.5509 (0.0319)

Angle to previous plane (with approximate esd) = 18.28 ( 0.19 )

* -0.0096 (0.0019) C6B
* 0.0081 (0.0019) C7B
* -0.0035 (0.0020) C8B
* -0.0026 (0.0020) C9B
* 0.0076 (0.0020) C10B

Rms deviation of fitted atoms = 0.0068

Table 1. Crystal data and structure refinement for k9954.

| | | |
|---|---|---|
| Identification code | k9954 | |
| Empirical formula | C24 H29 Fe P | |
| Formula weight | 404.29 | |
| Temperature | 100.0(1) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P2(1)/c | |
| Unit cell dimensions | a = 8.4879(3) Å | $\alpha = 90°$. |
| | b = 27.4428(11) Å | $\beta = 91.899(2)°$. |
| | c = 17.3725(4) Å | $\gamma = 90°$. |
| Volume | 4044.4(2) $Å^3$ | |
| Z | 8 | |
| Density (calculated) | 1.328 $Mg/m^3$ | |
| Absorption coefficient | 0.830 $mm^{-1}$ | |
| F(000) | 1712 | |
| Crystal size | 0.30 x 0.27 x 0.12 $mm^3$ | |
| Theta range for data collection | 4.17 to 26.07°. | |
| Index ranges | $0<=h<=10$, $0<=k<=33$, $-21<=l<=21$ | |
| Reflections collected | 35655 | |
| Independent reflections | 7954 [R(int) = 0.100] | |
| Completeness to theta = 26.07° | 99.1 % | |
| Absorption correction | multi-scan (Denzo-SMN) | |
| Max. and min. transmission | 0.9070 and 0.7889 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 7954 / 0 / 483 | |
| Goodness-of-fit on $F^2$ | 0.959 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0480, wR2 = 0.0978 | |
| R indices (all data) | R1 = 0.1004, wR2 = 0.1087 | |
| Largest diff. peak and hole | 0.582 and -0.290 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for k9954. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Fe(1A) | 2257(1) | 6058(1) | 424(1) | 25(1) |
| P(1A) | 2174(1) | 6990(1) | -643(1) | 26(1) |
| C(1A) | 3378(4) | 6039(1) | -557(2) | 26(1) |
| C(2A) | 2649(4) | 5574(1) | -428(2) | 25(1) |
| C(3A) | 3285(4) | 5379(1) | 279(2) | 26(1) |
| C(4A) | 4405(4) | 5721(1) | 591(2) | 28(1) |
| C(5A) | 4503(4) | 6122(1) | 69(2) | 29(1) |
| C(6A) | 1216(4) | 6687(1) | 155(2) | 26(1) |
| C(7A) | 88(4) | 6300(1) | 127(2) | 26(1) |
| C(8A) | 34(4) | 6083(1) | 874(2) | 28(1) |
| C(9A) | 1119(4) | 6336(1) | 1371(2) | 29(1) |
| C(10A) | 1826(4) | 6709(1) | 937(2) | 27(1) |
| C(11A) | 2843(4) | 6418(1) | -1150(2) | 28(1) |
| C(12A) | 1393(4) | 5335(1) | -928(2) | 28(1) |
| C(13A) | 2941(4) | 4889(1) | 613(2) | 33(1) |
| C(14A) | 5385(4) | 5655(1) | 1316(2) | 41(1) |
| C(15A) | 5635(4) | 6542(1) | 149(2) | 37(1) |
| C(16A) | 533(4) | 7235(1) | -1258(2) | 26(1) |
| C(17A) | 741(4) | 7295(1) | -2055(2) | 28(1) |
| C(18A) | -465(4) | 7505(1) | -2509(2) | 35(1) |
| C(19A) | -1868(4) | 7658(1) | -2202(2) | 37(1) |
| C(20A) | -2007(4) | 7627(1) | -1412(2) | 34(1) |
| C(21A) | -821(4) | 7430(1) | -934(2) | 28(1) |
| C(22A) | 2245(4) | 7168(1) | -2446(2) | 37(1) |
| C(23A) | -3169(5) | 7873(1) | -2715(2) | 49(1) |
| C(24A) | -1041(4) | 7479(1) | -75(2) | 33(1) |
| Fe(1B) | -8103(1) | 5933(1) | -6123(1) | 24(1) |
| P(1B) | -7726(1) | 6204(1) | -4359(1) | 27(1) |
| C(1B) | -8993(4) | 5489(1) | -5345(2) | 25(1) |
| C(2B) | -8301(4) | 5208(1) | -5940(2) | 27(1) |
| C(3B) | -9086(4) | 5330(1) | -6659(2) | 25(1) |

Table 3. Bond lengths [Å] and angles [°] for k9954.

| | |
|---|---|
| Fe(1A)-C(1A) | 1.980(3) |
| Fe(1A)-C(6A) | 1.988(3) |
| Fe(1A)-C(7A) | 2.009(3) |
| Fe(1A)-C(2A) | 2.025(3) |
| Fe(1A)-C(5A) | 2.031(3) |
| Fe(1A)-C(10A) | 2.034(3) |
| Fe(1A)-C(4A) | 2.056(3) |
| Fe(1A)-C(8A) | 2.067(3) |
| Fe(1A)-C(3A) | 2.077(3) |
| Fe(1A)-C(9A) | 2.080(3) |
| P(1A)-C(6A) | 1.829(3) |
| P(1A)-C(16A) | 1.854(3) |
| P(1A)-C(11A) | 1.896(3) |
| C(1A)-C(2A) | 1.437(4) |
| C(1A)-C(5A) | 1.441(4) |
| C(1A)-C(11A) | 1.524(4) |
| C(2A)-C(3A) | 1.430(4) |
| C(2A)-C(12A) | 1.504(4) |
| C(3A)-C(4A) | 1.431(4) |
| C(3A)-C(13A) | 1.496(4) |
| C(4A)-C(5A) | 1.431(4) |
| C(4A)-C(14A) | 1.496(4) |
| C(5A)-C(15A) | 1.503(5) |
| C(6A)-C(7A) | 1.431(4) |
| C(6A)-C(10A) | 1.439(4) |
| C(7A)-C(8A) | 1.429(4) |
| C(8A)-C(9A) | 1.423(4) |
| C(9A)-C(10A) | 1.418(4) |
| C(16A)-C(21A) | 1.403(4) |
| C(16A)-C(17A) | 1.410(4) |
| C(17A)-C(18A) | 1.395(5) |
| C(17A)-C(22A) | 1.507(5) |
| C(18A)-C(19A) | 1.385(5) |
| C(19A)-C(20A) | 1.383(5) |

| | | | | |
|---|---|---|---|---|
| C(4B) | -10284(4) | 5677(1) | -6504(2) | 26(1) |
| C(5B) | -10257(4) | 5779(1) | -5698(2) | 26(1) |
| C(6B) | -6960(4) | 6322(1) | -5317(2) | 24(1) |
| C(7B) | -5864(4) | 6047(1) | -5751(2) | 26(1) |
| C(8B) | -6016(4) | 6194(1) | -6538(2) | 28(1) |
| C(9B) | -7176(4) | 6564(1) | -6592(2) | 30(1) |
| C(10B) | -7746(4) | 6648(1) | -5851(2) | 27(1) |
| C(11B) | -8327(4) | 5546(1) | -4530(2) | 28(1) |
| C(12B) | -6949(4) | 4851(1) | -5858(2) | 35(1) |
| C(13B) | -8745(4) | 5108(1) | -7422(2) | 34(1) |
| C(14B) | -11482(4) | 5883(1) | -7076(2) | 33(1) |
| C(15B) | -11364(4) | 6115(1) | -5311(2) | 34(1) |
| C(16B) | -5948(4) | 6187(1) | -3708(2) | 25(1) |
| C(17B) | -5849(4) | 5872(1) | -3064(2) | 29(1) |
| C(18B) | -4548(4) | 5899(1) | -2562(2) | 32(1) |
| C(19B) | -3331(4) | 6221(1) | -2663(2) | 32(1) |
| C(20B) | -3480(4) | 6546(1) | -3274(2) | 32(1) |
| C(21B) | -4771(4) | 6544(1) | -3786(2) | 29(1) |
| C(22B) | -7149(4) | 5528(1) | -2864(2) | 42(1) |
| C(23B) | -1925(5) | 6244(1) | -2101(2) | 48(1) |
| C(24B) | -4892(4) | 6952(1) | -4371(2) | 35(1) |

| | |
|---|---|
| C(19A)-C(23A) | 1.516(5) |
| C(20A)-C(21A) | 1.392(4) |
| C(21A)-C(24A) | 1.516(4) |
| Fe(1B)-C(6B) | 1.987(3) |
| Fe(1B)-C(1B) | 1.988(3) |
| Fe(1B)-C(7B) | 2.011(3) |
| Fe(1B)-C(2B) | 2.024(3) |
| Fe(1B)-C(10B) | 2.037(3) |
| Fe(1B)-C(5B) | 2.039(3) |
| Fe(1B)-C(3B) | 2.062(3) |
| Fe(1B)-C(8B) | 2.063(3) |
| Fe(1B)-C(4B) | 2.069(3) |
| Fe(1B)-C(9B) | 2.078(3) |
| P(1B)-C(6B) | 1.835(3) |
| P(1B)-C(16B) | 1.857(3) |
| P(1B)-C(11B) | 1.897(3) |
| C(1B)-C(2B) | 1.431(4) |
| C(1B)-C(5B) | 1.456(4) |
| C(1B)-C(11B) | 1.515(4) |
| C(2B)-C(3B) | 1.435(4) |
| C(2B)-C(12B) | 1.511(4) |
| C(3B)-C(4B) | 1.425(4) |
| C(3B)-C(13B) | 1.496(4) |
| C(4B)-C(5B) | 1.428(4) |
| C(4B)-C(14B) | 1.509(4) |
| C(5B)-C(15B) | 1.491(4) |
| C(6B)-C(7B) | 1.430(4) |
| C(6B)-C(10B) | 1.437(4) |
| C(7B)-C(8B) | 1.428(4) |
| C(8B)-C(9B) | 1.414(5) |
| C(9B)-C(10B) | 1.409(4) |
| C(16B)-C(21B) | 1.410(4) |
| C(16B)-C(17B) | 1.413(4) |
| C(17B)-C(18B) | 1.386(4) |
| C(17B)-C(22B) | 1.501(5) |
| C(18B)-C(19B) | 1.375(5) |

| | |
|---|---|
| C(19B)-C(20B) | 1.388(4) |
| C(19B)-C(23B) | 1.518(4) |
| C(20B)-C(21B) | 1.389(4) |
| C(21B)-C(24B) | 1.513(4) |

| | |
|---|---|
| C(1A)-Fe(1A)-C(6A) | 92.46(13) |
| C(1A)-Fe(1A)-C(7A) | 104.49(13) |
| C(6A)-Fe(1A)-C(7A) | 41.96(12) |
| C(1A)-Fe(1A)-C(2A) | 42.04(12) |
| C(6A)-Fe(1A)-C(2A) | 118.64(12) |
| C(7A)-Fe(1A)-C(2A) | 101.51(13) |
| C(1A)-Fe(1A)-C(5A) | 42.08(12) |
| C(6A)-Fe(1A)-C(5A) | 105.48(14) |
| C(7A)-Fe(1A)-C(5A) | 139.01(13) |
| C(2A)-Fe(1A)-C(5A) | 69.88(13) |
| C(1A)-Fe(1A)-C(10A) | 119.91(13) |
| C(6A)-Fe(1A)-C(10A) | 41.91(12) |
| C(7A)-Fe(1A)-C(10A) | 69.29(13) |
| C(2A)-Fe(1A)-C(10A) | 158.76(12) |
| C(5A)-Fe(1A)-C(10A) | 103.93(13) |
| C(1A)-Fe(1A)-C(4A) | 70.12(12) |
| C(6A)-Fe(1A)-C(4A) | 143.97(14) |
| C(7A)-Fe(1A)-C(4A) | 170.31(13) |
| C(2A)-Fe(1A)-C(4A) | 69.01(12) |
| C(5A)-Fe(1A)-C(4A) | 41.00(13) |
| C(10A)-Fe(1A)-C(4A) | 120.30(13) |
| C(1A)-Fe(1A)-C(8A) | 142.81(12) |
| C(6A)-Fe(1A)-C(8A) | 69.90(13) |
| C(7A)-Fe(1A)-C(8A) | 41.02(12) |
| C(2A)-Fe(1A)-C(8A) | 118.16(13) |
| C(5A)-Fe(1A)-C(8A) | 171.83(13) |
| C(10A)-Fe(1A)-C(8A) | 68.07(13) |
| C(4A)-Fe(1A)-C(8A) | 141.07(13) |
| C(1A)-Fe(1A)-C(3A) | 69.85(13) |
| C(6A)-Fe(1A)-C(3A) | 159.35(12) |
| C(7A)-Fe(1A)-C(3A) | 130.54(13) |

| | |
|---|---|
| C(2A)-Fe(1A)-C(3A) | 40.78(12) |
| C(5A)-Fe(1A)-C(3A) | 68.84(13) |
| C(10A)-Fe(1A)-C(3A) | 157.45(12) |
| C(4A)-Fe(1A)-C(3A) | 40.50(12) |
| C(8A)-Fe(1A)-C(3A) | 117.88(13) |
| C(1A)-Fe(1A)-C(9A) | 160.01(14) |
| C(6A)-Fe(1A)-C(9A) | 69.75(12) |
| C(7A)-Fe(1A)-C(9A) | 68.69(12) |
| C(2A)-Fe(1A)-C(9A) | 155.61(13) |
| C(5A)-Fe(1A)-C(9A) | 132.38(13) |
| C(10A)-Fe(1A)-C(9A) | 40.30(12) |
| C(4A)-Fe(1A)-C(9A) | 119.10(12) |
| C(8A)-Fe(1A)-C(9A) | 40.14(12) |
| C(3A)-Fe(1A)-C(9A) | 129.26(13) |
| C(6A)-P(1A)-C(16A) | 104.91(15) |
| C(6A)-P(1A)-C(11A) | 97.08(14) |
| C(16A)-P(1A)-C(11A) | 105.24(14) |
| C(2A)-C(1A)-C(5A) | 107.6(3) |
| C(2A)-C(1A)-C(11A) | 126.2(3) |
| C(5A)-C(1A)-C(11A) | 125.2(3) |
| C(2A)-C(1A)-Fe(1A) | 70.66(17) |
| C(5A)-C(1A)-Fe(1A) | 70.85(17) |
| C(11A)-C(1A)-Fe(1A) | 115.0(2) |
| C(3A)-C(2A)-C(1A) | 108.3(3) |
| C(3A)-C(2A)-C(12A) | 124.9(3) |
| C(1A)-C(2A)-C(12A) | 126.8(3) |
| C(3A)-C(2A)-Fe(1A) | 71.56(17) |
| C(1A)-C(2A)-Fe(1A) | 67.30(17) |
| C(12A)-C(2A)-Fe(1A) | 125.3(2) |
| C(2A)-C(3A)-C(4A) | 107.8(3) |
| C(2A)-C(3A)-C(13A) | 126.7(3) |
| C(4A)-C(3A)-C(13A) | 125.4(3) |
| C(2A)-C(3A)-Fe(1A) | 67.66(17) |
| C(4A)-C(3A)-Fe(1A) | 68.97(18) |
| C(13A)-C(3A)-Fe(1A) | 132.1(2) |
| C(3A)-C(4A)-C(5A) | 108.5(3) |

| | |
|---|---|
| C(3A)-C(4A)-C(14A) | 125.7(3) |
| C(5A)-C(4A)-C(14A) | 125.7(3) |
| C(3A)-C(4A)-Fe(1A) | 70.53(18) |
| C(5A)-C(4A)-Fe(1A) | 68.55(18) |
| C(14A)-C(4A)-Fe(1A) | 129.7(2) |
| C(4A)-C(5A)-C(1A) | 107.7(3) |
| C(4A)-C(5A)-C(15A) | 125.5(3) |
| C(1A)-C(5A)-C(15A) | 126.7(3) |
| C(4A)-C(5A)-Fe(1A) | 70.46(18) |
| C(1A)-C(5A)-Fe(1A) | 67.07(18) |
| C(15A)-C(5A)-Fe(1A) | 130.0(2) |
| C(7A)-C(6A)-C(10A) | 106.4(3) |
| C(7A)-C(6A)-P(1A) | 128.8(2) |
| C(10A)-C(6A)-P(1A) | 122.7(2) |
| C(7A)-C(6A)-Fe(1A) | 69.79(18) |
| C(10A)-C(6A)-Fe(1A) | 70.77(17) |
| P(1A)-C(6A)-Fe(1A) | 111.59(16) |
| C(8A)-C(7A)-C(6A) | 108.7(3) |
| C(8A)-C(7A)-Fe(1A) | 71.68(18) |
| C(6A)-C(7A)-Fe(1A) | 68.25(18) |
| C(9A)-C(8A)-C(7A) | 108.0(3) |
| C(9A)-C(8A)-Fe(1A) | 70.42(19) |
| C(7A)-C(8A)-Fe(1A) | 67.30(17) |
| C(10A)-C(9A)-C(8A) | 107.8(3) |
| C(10A)-C(9A)-Fe(1A) | 68.13(17) |
| C(8A)-C(9A)-Fe(1A) | 69.44(17) |
| C(9A)-C(10A)-C(6A) | 109.1(3) |
| C(9A)-C(10A)-Fe(1A) | 71.57(18) |
| C(6A)-C(10A)-Fe(1A) | 67.32(17) |
| C(1A)-C(11A)-P(1A) | 109.8(2) |
| C(21A)-C(16A)-C(17A) | 118.6(3) |
| C(21A)-C(16A)-P(1A) | 121.1(2) |
| C(17A)-C(16A)-P(1A) | 119.5(2) |
| C(18A)-C(17A)-C(16A) | 119.3(3) |
| C(18A)-C(17A)-C(22A) | 117.2(3) |
| C(16A)-C(17A)-C(22A) | 123.4(3) |

| | |
|---|---|
| C(19A)-C(18A)-C(17A) | 122.1(3) |
| C(20A)-C(19A)-C(18A) | 117.8(3) |
| C(20A)-C(19A)-C(23A) | 121.5(3) |
| C(18A)-C(19A)-C(23A) | 120.7(3) |
| C(19A)-C(20A)-C(21A) | 122.1(3) |
| C(20A)-C(21A)-C(16A) | 119.6(3) |
| C(20A)-C(21A)-C(24A) | 116.3(3) |
| C(16A)-C(21A)-C(24A) | 123.9(3) |
| C(6B)-Fe(1B)-C(1B) | 92.19(12) |
| C(6B)-Fe(1B)-C(7B) | 41.92(12) |
| C(1B)-Fe(1B)-C(7B) | 104.66(13) |
| C(6B)-Fe(1B)-C(2B) | 117.29(12) |
| C(1B)-Fe(1B)-C(2B) | 41.78(12) |
| C(7B)-Fe(1B)-C(2B) | 100.66(13) |
| C(6B)-Fe(1B)-C(10B) | 41.82(12) |
| C(1B)-Fe(1B)-C(10B) | 119.33(13) |
| C(7B)-Fe(1B)-C(10B) | 69.16(13) |
| C(2B)-Fe(1B)-C(10B) | 157.34(12) |
| C(6B)-Fe(1B)-C(5B) | 106.20(13) |
| C(1B)-Fe(1B)-C(5B) | 42.36(12) |
| C(7B)-Fe(1B)-C(5B) | 139.90(12) |
| C(2B)-Fe(1B)-C(5B) | 70.07(13) |
| C(10B)-Fe(1B)-C(5B) | 104.11(13) |
| C(6B)-Fe(1B)-C(3B) | 158.39(12) |
| C(1B)-Fe(1B)-C(3B) | 69.94(12) |
| C(7B)-Fe(1B)-C(3B) | 129.33(13) |
| C(2B)-Fe(1B)-C(3B) | 41.12(12) |
| C(10B)-Fe(1B)-C(3B) | 158.79(13) |
| C(5B)-Fe(1B)-C(3B) | 69.07(13) |
| C(6B)-Fe(1B)-C(8B) | 69.83(12) |
| C(1B)-Fe(1B)-C(8B) | 143.20(13) |
| C(7B)-Fe(1B)-C(8B) | 41.01(12) |
| C(2B)-Fe(1B)-C(8B) | 118.23(14) |
| C(10B)-Fe(1B)-C(8B) | 67.93(13) |
| C(5B)-Fe(1B)-C(8B) | 171.65(14) |
| C(3B)-Fe(1B)-C(8B) | 117.39(13) |

| | |
|---|---|
| C(6B)-Fe(1B)-C(4B) | 144.98(13) |
| C(1B)-Fe(1B)-C(4B) | 69.68(12) |
| C(7B)-Fe(1B)-C(4B) | 169.03(13) |
| C(2B)-Fe(1B)-C(4B) | 68.76(13) |
| C(10B)-Fe(1B)-C(4B) | 121.74(13) |
| C(5B)-Fe(1B)-C(4B) | 40.67(12) |
| C(3B)-Fe(1B)-C(4B) | 40.37(12) |
| C(8B)-Fe(1B)-C(4B) | 140.88(12) |
| C(6B)-Fe(1B)-C(9B) | 69.33(12) |
| C(1B)-Fe(1B)-C(9B) | 159.18(13) |
| C(7B)-Fe(1B)-C(9B) | 68.32(13) |
| C(2B)-Fe(1B)-C(9B) | 156.19(14) |
| C(10B)-Fe(1B)-C(9B) | 40.04(12) |
| C(5B)-Fe(1B)-C(9B) | 132.10(14) |
| C(3B)-Fe(1B)-C(9B) | 130.10(12) |
| C(8B)-Fe(1B)-C(9B) | 39.93(13) |
| C(4B)-Fe(1B)-C(9B) | 120.27(12) |
| C(6B)-P(1B)-C(16B) | 104.61(14) |
| C(6B)-P(1B)-C(11B) | 97.32(14) |
| C(16B)-P(1B)-C(11B) | 106.26(14) |
| C(2B)-C(1B)-C(5B) | 107.8(3) |
| C(2B)-C(1B)-C(11B) | 125.6(3) |
| C(5B)-C(1B)-C(11B) | 125.7(3) |
| C(2B)-C(1B)-Fe(1B) | 70.46(17) |
| C(5B)-C(1B)-Fe(1B) | 70.67(17) |
| C(11B)-C(1B)-Fe(1B) | 115.6(2) |
| C(1B)-C(2B)-C(3B) | 108.2(3) |
| C(1B)-C(2B)-C(12B) | 127.5(3) |
| C(3B)-C(2B)-C(12B) | 124.2(3) |
| C(1B)-C(2B)-Fe(1B) | 67.76(17) |
| C(3B)-C(2B)-Fe(1B) | 70.84(18) |
| C(12B)-C(2B)-Fe(1B) | 125.8(2) |
| C(4B)-C(3B)-C(2B) | 107.8(3) |
| C(4B)-C(3B)-C(13B) | 126.8(3) |
| C(2B)-C(3B)-C(13B) | 125.3(3) |
| C(4B)-C(3B)-Fe(1B) | 70.08(18) |

| | |
|---|---|
| C(2B)-C(3B)-Fe(1B) | 68.05(17) |
| C(13B)-C(3B)-Fe(1B) | 129.8(2) |
| C(3B)-C(4B)-C(5B) | 109.1(3) |
| C(3B)-C(4B)-C(14B) | 126.6(3) |
| C(5B)-C(4B)-C(14B) | 124.1(3) |
| C(3B)-C(4B)-Fe(1B) | 69.55(17) |
| C(5B)-C(4B)-Fe(1B) | 68.54(17) |
| C(14B)-C(4B)-Fe(1B) | 131.3(2) |
| C(4B)-C(5B)-C(1B) | 107.0(3) |
| C(4B)-C(5B)-C(15B) | 125.0(3) |
| C(1B)-C(5B)-C(15B) | 128.0(3) |
| C(4B)-C(5B)-Fe(1B) | 70.79(17) |
| C(1B)-C(5B)-Fe(1B) | 66.96(17) |
| C(15B)-C(5B)-Fe(1B) | 128.4(2) |
| C(7B)-C(6B)-C(10B) | 106.5(3) |
| C(7B)-C(6B)-P(1B) | 129.9(2) |
| C(10B)-C(6B)-P(1B) | 121.6(2) |
| C(7B)-C(6B)-Fe(1B) | 69.96(17) |
| C(10B)-C(6B)-Fe(1B) | 70.97(17) |
| P(1B)-C(6B)-Fe(1B) | 111.41(15) |
| C(8B)-C(7B)-C(6B) | 108.4(3) |
| C(8B)-C(7B)-Fe(1B) | 71.43(18) |
| C(6B)-C(7B)-Fe(1B) | 68.12(17) |
| C(9B)-C(8B)-C(7B) | 107.8(3) |
| C(9B)-C(8B)-Fe(1B) | 70.62(19) |
| C(7B)-C(8B)-Fe(1B) | 67.56(17) |
| C(10B)-C(9B)-C(8B) | 108.4(3) |
| C(10B)-C(9B)-Fe(1B) | 68.41(18) |
| C(8B)-C(9B)-Fe(1B) | 69.45(18) |
| C(9B)-C(10B)-C(6B) | 108.7(3) |
| C(9B)-C(10B)-Fe(1B) | 71.55(18) |
| C(6B)-C(10B)-Fe(1B) | 67.21(17) |
| C(1B)-C(11B)-P(1B) | 109.6(2) |
| C(21B)-C(16B)-C(17B) | 118.5(3) |
| C(21B)-C(16B)-P(1B) | 119.2(2) |
| C(17B)-C(16B)-P(1B) | 121.6(2) |

| | |
|---|---|
| C(18B)-C(17B)-C(16B) | 119.4(3) |
| C(18B)-C(17B)-C(22B) | 117.7(3) |
| C(16B)-C(17B)-C(22B) | 122.8(3) |
| C(19B)-C(18B)-C(17B) | 122.7(3) |
| C(18B)-C(19B)-C(20B) | 117.4(3) |
| C(18B)-C(19B)-C(23B) | 121.5(3) |
| C(20B)-C(19B)-C(23B) | 121.0(3) |
| C(19B)-C(20B)-C(21B) | 122.5(3) |
| C(20B)-C(21B)-C(16B) | 119.1(3) |
| C(20B)-C(21B)-C(24B) | 117.5(3) |
| C(16B)-C(21B)-C(24B) | 123.2(3) |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for k9954. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Fe(1A) | 25(1) | 20(1) | 29(1) | -1(1) | -1(1) | 3(1) |
| P(1A) | 28(1) | 18(1) | 33(1) | -1(1) | 0(1) | 2(1) |
| C(1A) | 24(2) | 25(2) | 29(2) | -4(2) | 5(1) | 3(2) |
| C(2A) | 25(2) | 18(2) | 31(2) | -2(2) | 6(1) | 5(2) |
| C(3A) | 26(2) | 18(2) | 34(2) | 1(2) | 5(1) | 7(2) |
| C(4A) | 26(2) | 26(2) | 32(2) | 3(2) | -2(1) | 7(2) |
| C(5A) | 23(2) | 25(2) | 38(2) | -4(2) | 1(2) | 2(2) |
| C(6A) | 29(2) | 16(2) | 32(2) | -2(1) | 1(1) | 6(2) |
| C(7A) | 25(2) | 21(2) | 31(2) | -1(2) | 0(1) | 5(2) |
| C(8A) | 27(2) | 20(2) | 36(2) | -1(2) | 3(2) | 5(2) |
| C(9A) | 37(2) | 24(2) | 26(2) | -2(2) | 2(2) | 6(2) |
| C(10A) | 30(2) | 19(2) | 33(2) | -7(2) | 0(2) | 4(2) |
| C(11A) | 32(2) | 22(2) | 29(2) | 0(2) | 3(1) | 3(2) |
| C(12A) | 33(2) | 19(2) | 33(2) | 1(2) | 0(2) | 1(2) |
| C(13A) | 34(2) | 26(2) | 39(2) | 3(2) | 4(2) | 5(2) |
| C(14A) | 38(2) | 43(3) | 42(2) | -1(2) | -4(2) | 10(2) |
| C(15A) | 26(2) | 33(2) | 53(2) | -5(2) | -1(2) | -1(2) |
| C(16A) | 27(2) | 14(2) | 38(2) | -2(2) | -4(2) | -1(2) |
| C(17A) | 37(2) | 14(2) | 34(2) | -3(2) | -3(2) | -2(2) |
| C(18A) | 48(2) | 22(2) | 34(2) | -1(2) | -4(2) | -1(2) |
| C(19A) | 44(2) | 15(2) | 51(2) | -5(2) | -15(2) | 0(2) |
| C(20A) | 34(2) | 19(2) | 47(2) | -4(2) | -6(2) | 0(2) |
| C(21A) | 28(2) | 14(2) | 41(2) | -1(2) | -3(2) | -1(2) |
| C(22A) | 50(3) | 26(2) | 34(2) | 5(2) | 5(2) | 1(2) |
| C(23A) | 54(3) | 37(3) | 53(2) | -9(2) | -20(2) | 13(2) |
| C(24A) | 33(2) | 21(2) | 45(2) | -2(2) | 4(2) | 7(2) |
| Fe(1B) | 25(1) | 18(1) | 29(1) | 1(1) | -1(1) | -3(1) |
| P(1B) | 26(1) | 24(1) | 30(1) | -1(1) | -1(1) | -2(1) |
| C(1B) | 28(2) | 18(2) | 29(2) | 6(2) | -1(1) | -6(2) |
| C(2B) | 34(2) | 13(2) | 34(2) | 3(2) | -1(2) | -7(2) |
| C(3B) | 28(2) | 17(2) | 31(2) | 1(2) | -4(1) | -6(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(4B) | 25(2) | 19(2) | 33(2) | 2(2) | -4(1) | -7(2) |
| C(5B) | 21(2) | 23(2) | 35(2) | 2(2) | 1(1) | -7(2) |
| C(6B) | 25(2) | 19(2) | 28(2) | 1(2) | -4(1) | -6(2) |
| C(7B) | 19(2) | 25(2) | 36(2) | 0(2) | -4(1) | -8(2) |
| C(8B) | 27(2) | 27(2) | 31(2) | -2(2) | 4(1) | -10(2) |
| C(9B) | 38(2) | 21(2) | 31(2) | 4(2) | -8(2) | -9(2) |
| C(10B) | 31(2) | 14(2) | 35(2) | 2(2) | -2(2) | -3(2) |
| C(11B) | 28(2) | 25(2) | 31(2) | 6(2) | 0(1) | -4(2) |
| C(12B) | 46(2) | 21(2) | 38(2) | -3(2) | -7(2) | 1(2) |
| C(13B) | 39(2) | 28(2) | 36(2) | -1(2) | -6(2) | -5(2) |
| C(14B) | 30(2) | 31(2) | 39(2) | -1(2) | -8(2) | -5(2) |
| C(15B) | 26(2) | 40(2) | 36(2) | 0(2) | 0(2) | -1(2) |
| C(16B) | 27(2) | 20(2) | 28(2) | -4(2) | -1(1) | -1(2) |
| C(17B) | 33(2) | 30(2) | 24(2) | -4(2) | 2(2) | -1(2) |
| C(18B) | 45(2) | 23(2) | 26(2) | -3(2) | -4(2) | 5(2) |
| C(19B) | 32(2) | 21(2) | 41(2) | -10(2) | -11(2) | 6(2) |
| C(20B) | 35(2) | 20(2) | 41(2) | -5(2) | -1(2) | -6(2) |
| C(21B) | 34(2) | 24(2) | 27(2) | -8(2) | -1(2) | 1(2) |
| C(22B) | 52(3) | 40(3) | 32(2) | 7(2) | -2(2) | -11(2) |
| C(23B) | 58(3) | 26(2) | 57(2) | -2(2) | -24(2) | -3(2) |
| C(24B) | 40(2) | 25(2) | 41(2) | 1(2) | -7(2) | -13(2) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for k9954.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(7AA) | -552 | 6196 | -338 | 31 |
| H(8AA) | -619 | 5795 | 1016 | 33 |
| H(9AA) | 1369 | 6256 | 1923 | 35 |
| H(10A) | 2648 | 6942 | 1137 | 32 |
| H(11A) | 1963 | 6285 | -1475 | 33 |
| H(11B) | 3723 | 6497 | -1488 | 33 |
| H(12A) | 1884 | 5108 | -1284 | 42 |
| H(12B) | 806 | 5584 | -1222 | 42 |
| H(12C) | 669 | 5155 | -603 | 42 |
| H(13A) | 3867 | 4679 | 571 | 49 |
| H(13B) | 2042 | 4742 | 331 | 49 |
| H(13C) | 2689 | 4926 | 1157 | 49 |
| H(14A) | 6381 | 5497 | 1195 | 61 |
| H(14B) | 4813 | 5452 | 1677 | 61 |
| H(14C) | 5604 | 5974 | 1550 | 61 |
| H(15A) | 6673 | 6441 | -25 | 56 |
| H(15B) | 5724 | 6643 | 689 | 56 |
| H(15C) | 5248 | 6815 | -167 | 56 |
| H(18A) | -321 | 7543 | -3045 | 41 |
| H(20A) | -2942 | 7743 | -1189 | 40 |
| H(22A) | 2293 | 7346 | -2933 | 55 |
| H(22B) | 2269 | 6817 | -2548 | 55 |
| H(22C) | 3150 | 7258 | -2111 | 55 |
| H(23A) | -3739 | 8120 | -2428 | 73 |
| H(23B) | -3900 | 7615 | -2882 | 73 |
| H(23C) | -2708 | 8024 | -3167 | 73 |
| H(24A) | -53 | 7590 | 176 | 49 |
| H(24B) | -1338 | 7163 | 137 | 49 |
| H(24C) | -1874 | 7717 | 17 | 49 |
| H(7BA) | -5124 | 5793 | -5539 | 32 |

| | | | | |
|---|---|---|---|---|
| H(8BA) | -5428 | 6054 | -6976 | 34 |
| H(9BA) | -7562 | 6726 | -7077 | 36 |
| H(10B) | -8586 | 6887 | -5721 | 32 |
| H(11C) | -7400 | 5331 | -4450 | 34 |
| H(11D) | -9131 | 5451 | -4158 | 34 |
| H(12D) | -7353 | 4518 | -5913 | 53 |
| H(12E) | -6429 | 4890 | -5350 | 53 |
| H(12F) | -6190 | 4915 | -6258 | 53 |
| H(13D) | -9419 | 4822 | -7508 | 51 |
| H(13E) | -7636 | 5009 | -7426 | 51 |
| H(13F) | -8957 | 5347 | -7831 | 51 |
| H(14D) | -12483 | 5709 | -7033 | 50 |
| H(14E) | -11100 | 5845 | -7598 | 50 |
| H(14F) | -11643 | 6230 | -6967 | 50 |
| H(15D) | -12386 | 5954 | -5262 | 51 |
| H(15E) | -11501 | 6412 | -5620 | 51 |
| H(15F) | -10931 | 6200 | -4799 | 51 |
| H(18B) | -4495 | 5686 | -2131 | 38 |
| H(20B) | -2667 | 6778 | -3344 | 39 |
| H(22D) | -7013 | 5428 | -2324 | 62 |
| H(22E) | -7114 | 5240 | -3197 | 62 |
| H(22F) | -8168 | 5692 | -2940 | 62 |
| H(23D) | -1966 | 5969 | -1742 | 71 |
| H(23E) | -1952 | 6550 | -1812 | 71 |
| H(23F) | -949 | 6227 | -2386 | 71 |
| H(24D) | -5981 | 7071 | -4407 | 53 |
| H(24E) | -4585 | 6831 | -4874 | 53 |
| H(24F) | -4190 | 7219 | -4208 | 53 |

© 2001 American Chemical Society, J. Am. Chem. Soc., Resendes ja002750e Supporting Info Page 60

Supp. Material for Compound 9.

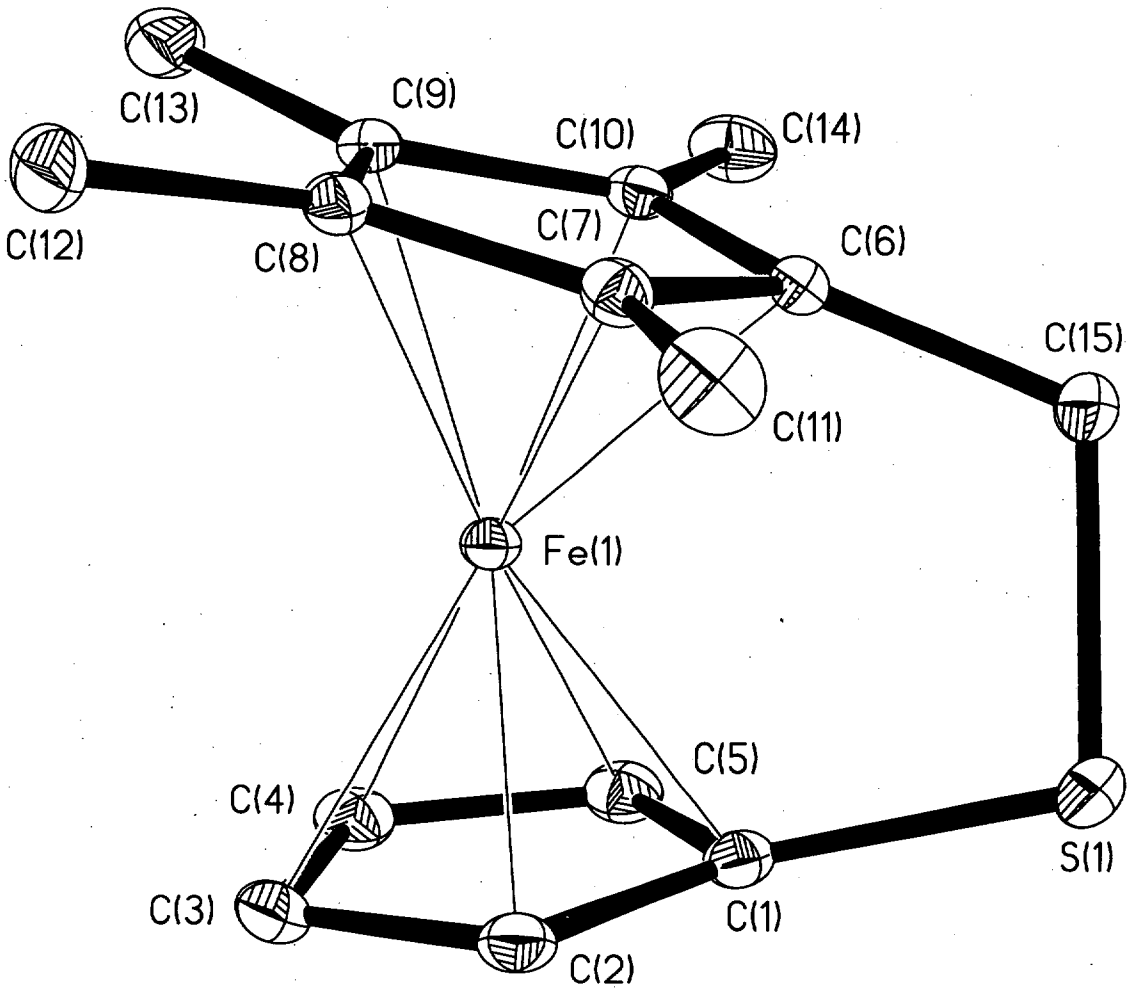


Table 7. Crystal data and structure refinement for S9628a.

| | | |
|---|---|---|
| Identification code | s9628a | |
| Empirical formula | C15 H18 Fe S | |
| Formula weight | 286.20 | |
| Temperature | 173(2) K | |
| Wavelength | 0.71073 ≈ | |
| Crystal system | Monoclinic | |
| Space group | P2(1)/c | |
| Unit cell dimensions | a = 8.0787(6) ≈ | α= 90∞. |
| | b = 24.179(3) ≈ | β= 117.553(7)∞. |
| | c = 7.5462(10) ≈ | γ = 90∞. |
| Volume | 1306.9(2) ≈$^3$ | |
| Z | 4 | |
| Density (calculated) | 1.455 Mg/m$^3$ | |
| Absorption coefficient | 1.287 mm$^{-1}$ | |
| F(000) | 600 | |
| Crystal size | 0.67 x 0.40 x 0.20 mm$^3$ | |
| Theta range for data collection | 2.84 to 31.00∞. | |
| Index ranges | -11<=h<=10, -35<=k<=0, 0<=l<=10 | |
| Reflections collected | 4216 | |
| Independent reflections | 3971 [R(int) = 0.0161] | |
| Completeness to theta = 31.00∞ | 95.3 % | |
| Absorption correction | Integration | |
| Max. and min. transmission | 0.7828 and 0.4792 | |
| Refinement method | Full-matrix least-squares on F$^2$ | |
| Data / restraints / parameters | 3971 / 0 / 227 | |
| Goodness-of-fit on F$^2$ | 1.139 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0365, wR2 = 0.0957 | |
| R indices (all data) | R1 = 0.0413, wR2 = 0.0975 | |
| Extinction coefficient | 0.0008(5) | |
| Largest diff. peak and hole | 0.460 and -0.371 e.≈$^{-3}$ | |

Table 8. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$ x $10^3$) for S9628a. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Fe(1) | 7680(1) | 1271(1) | 2382(1) | 15(1) |
| S(1) | 8285(1) | 68(1) | 1177(1) | 26(1) |
| C(1) | 7922(3) | 468(1) | 2953(3) | 21(1) |
| C(2) | 9383(3) | 754(1) | 4598(3) | 22(1) |
| C(3) | 8538(3) | 1125(1) | 5403(3) | 25(1) |
| C(4) | 6561(3) | 1067(1) | 4286(4) | 25(1) |
| C(5) | 6176(3) | 656(1) | 2793(3) | 24(1) |
| C(6) | 7601(3) | 1153(1) | -267(3) | 17(1) |
| C(7) | 9277(3) | 1445(1) | 1024(3) | 18(1) |
| C(8) | 8749(3) | 1953(1) | 1609(3) | 19(1) |
| C(9) | 6757(3) | 1982(1) | 659(3) | 19(1) |
| C(10) | 6040(3) | 1490(1) | -518(3) | 18(1) |
| C(11) | 11233(3) | 1257(1) | 1609(4) | 30(1) |
| C(12) | 10072(4) | 2387(1) | 2918(4) | 30(1) |
| C(13) | 5610(4) | 2459(1) | 754(4) | 31(1) |
| C(14) | 4014(3) | 1366(1) | -1831(4) | 28(1) |
| C(15) | 7469(4) | 557(1) | -932(3) | 24(1) |

Table 9. Bond lengths [≈] and angles [∞] for S9628a.

| | |
|---|---|
| Fe(1)-C(1) | 1.980(2) |
| Fe(1)-C(6) | 1.9906(19) |
| Fe(1)-C(7) | 2.029(2) |
| Fe(1)-C(2) | 2.030(2) |
| Fe(1)-C(5) | 2.033(2) |
| Fe(1)-C(10) | 2.0351(19) |
| Fe(1)-C(8) | 2.066(2) |
| Fe(1)-C(9) | 2.075(2) |
| Fe(1)-C(4) | 2.079(2) |
| Fe(1)-C(3) | 2.083(2) |
| S(1)-C(1) | 1.783(2) |
| S(1)-C(15) | 1.844(2) |
| C(1)-C(5) | 1.433(3) |
| C(1)-C(2) | 1.435(3) |
| C(2)-C(3) | 1.421(3) |
| C(3)-C(4) | 1.426(3) |
| C(4)-C(5) | 1.426(3) |
| C(6)-C(7) | 1.435(3) |
| C(6)-C(10) | 1.438(3) |
| C(6)-C(15) | 1.513(3) |
| C(7)-C(8) | 1.433(3) |
| C(7)-C(11) | 1.501(3) |
| C(8)-C(9) | 1.429(3) |
| C(8)-C(12) | 1.499(3) |
| C(9)-C(10) | 1.437(3) |
| C(9)-C(13) | 1.501(3) |
| C(10)-C(14) | 1.500(3) |
| | |
| C(1)-Fe(1)-C(6) | 91.85(9) |
| C(1)-Fe(1)-C(7) | 106.98(9) |
| C(6)-Fe(1)-C(7) | 41.83(8) |
| C(1)-Fe(1)-C(2) | 41.92(9) |
| C(6)-Fe(1)-C(2) | 115.72(9) |
| C(7)-Fe(1)-C(2) | 101.37(9) |

| | |
|---|---|
| C(1)-Fe(1)-C(5) | 41.82(9) |
| C(6)-Fe(1)-C(5) | 107.75(9) |
| C(7)-Fe(1)-C(5) | 142.53(9) |
| C(2)-Fe(1)-C(5) | 69.47(9) |
| C(1)-Fe(1)-C(10) | 116.03(9) |
| C(6)-Fe(1)-C(10) | 41.84(8) |
| C(7)-Fe(1)-C(10) | 69.67(8) |
| C(2)-Fe(1)-C(10) | 154.41(9) |
| C(5)-Fe(1)-C(10) | 102.51(9) |
| C(1)-Fe(1)-C(8) | 146.30(9) |
| C(6)-Fe(1)-C(8) | 69.75(8) |
| C(7)-Fe(1)-C(8) | 40.97(8) |
| C(2)-Fe(1)-C(8) | 120.71(9) |
| C(5)-Fe(1)-C(8) | 169.76(9) |
| C(10)-Fe(1)-C(8) | 68.79(8) |
| C(1)-Fe(1)-C(9) | 156.95(9) |
| C(6)-Fe(1)-C(9) | 69.76(8) |
| C(7)-Fe(1)-C(9) | 68.86(8) |
| C(2)-Fe(1)-C(9) | 159.40(9) |
| C(5)-Fe(1)-C(9) | 129.42(9) |
| C(10)-Fe(1)-C(9) | 40.92(8) |
| C(8)-Fe(1)-C(9) | 40.36(8) |
| C(1)-Fe(1)-C(4) | 69.41(10) |
| C(6)-Fe(1)-C(4) | 146.91(9) |
| C(7)-Fe(1)-C(4) | 168.33(9) |
| C(2)-Fe(1)-C(4) | 68.33(10) |
| C(5)-Fe(1)-C(4) | 40.55(10) |
| C(10)-Fe(1)-C(4) | 121.99(9) |
| C(8)-Fe(1)-C(4) | 139.09(9) |
| C(9)-Fe(1)-C(4) | 118.94(9) |
| C(1)-Fe(1)-C(3) | 69.28(9) |
| C(6)-Fe(1)-C(3) | 156.12(9) |
| C(7)-Fe(1)-C(3) | 128.35(9) |
| C(2)-Fe(1)-C(3) | 40.40(9) |
| C(5)-Fe(1)-C(3) | 68.22(9) |
| C(10)-Fe(1)-C(3) | 160.45(9) |

| | |
|---|---|
| C(8)-Fe(1)-C(3) | 118.23(9) |
| C(9)-Fe(1)-C(3) | 131.85(9) |
| C(4)-Fe(1)-C(3) | 40.08(10) |
| C(1)-S(1)-C(15) | 100.55(10) |
| C(5)-C(1)-C(2) | 107.6(2) |
| C(5)-C(1)-S(1) | 127.33(17) |
| C(2)-C(1)-S(1) | 123.85(17) |
| C(5)-C(1)-Fe(1) | 71.07(12) |
| C(2)-C(1)-Fe(1) | 70.90(12) |
| S(1)-C(1)-Fe(1) | 113.73(11) |
| C(3)-C(2)-C(1) | 108.0(2) |
| C(3)-C(2)-Fe(1) | 71.82(13) |
| C(1)-C(2)-Fe(1) | 67.17(12) |
| C(2)-C(3)-C(4) | 108.3(2) |
| C(2)-C(3)-Fe(1) | 67.77(12) |
| C(4)-C(3)-Fe(1) | 69.82(12) |
| C(5)-C(4)-C(3) | 108.1(2) |
| C(5)-C(4)-Fe(1) | 67.96(12) |
| C(3)-C(4)-Fe(1) | 70.10(13) |
| C(4)-C(5)-C(1) | 108.0(2) |
| C(4)-C(5)-Fe(1) | 71.49(13) |
| C(1)-C(5)-Fe(1) | 67.11(12) |
| C(7)-C(6)-C(10) | 107.78(18) |
| C(7)-C(6)-C(15) | 126.41(19) |
| C(10)-C(6)-C(15) | 124.89(19) |
| C(7)-C(6)-Fe(1) | 70.51(11) |
| C(10)-C(6)-Fe(1) | 70.74(11) |
| C(15)-C(6)-Fe(1) | 115.71(14) |
| C(8)-C(7)-C(6) | 107.97(17) |
| C(8)-C(7)-C(11) | 126.3(2) |
| C(6)-C(7)-C(11) | 125.8(2) |
| C(8)-C(7)-Fe(1) | 70.91(11) |
| C(6)-C(7)-Fe(1) | 67.66(11) |
| C(11)-C(7)-Fe(1) | 128.11(16) |
| C(9)-C(8)-C(7) | 108.35(18) |
| C(9)-C(8)-C(12) | 126.1(2) |

| | |
|---|---|
| C(7)-C(8)-C(12) | 125.5(2) |
| C(9)-C(8)-Fe(1) | 70.16(12) |
| C(7)-C(8)-Fe(1) | 68.12(11) |
| C(12)-C(8)-Fe(1) | 129.60(15) |
| C(8)-C(9)-C(10) | 107.88(18) |
| C(8)-C(9)-C(13) | 126.3(2) |
| C(10)-C(9)-C(13) | 125.7(2) |
| C(8)-C(9)-Fe(1) | 69.48(12) |
| C(10)-C(9)-Fe(1) | 68.05(11) |
| C(13)-C(9)-Fe(1) | 131.09(16) |
| C(9)-C(10)-C(6) | 108.00(17) |
| C(9)-C(10)-C(14) | 125.3(2) |
| C(6)-C(10)-C(14) | 126.6(2) |
| C(9)-C(10)-Fe(1) | 71.04(11) |
| C(6)-C(10)-Fe(1) | 67.42(11) |
| C(14)-C(10)-Fe(1) | 128.84(15) |
| C(6)-C(15)-S(1) | 112.51(14) |

---

Symmetry transformations used to generate equivalent atoms:

Table 10. Anisotropic displacement parameters ($\approx^2$x $10^3$) for S9628a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[ h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12} ]$

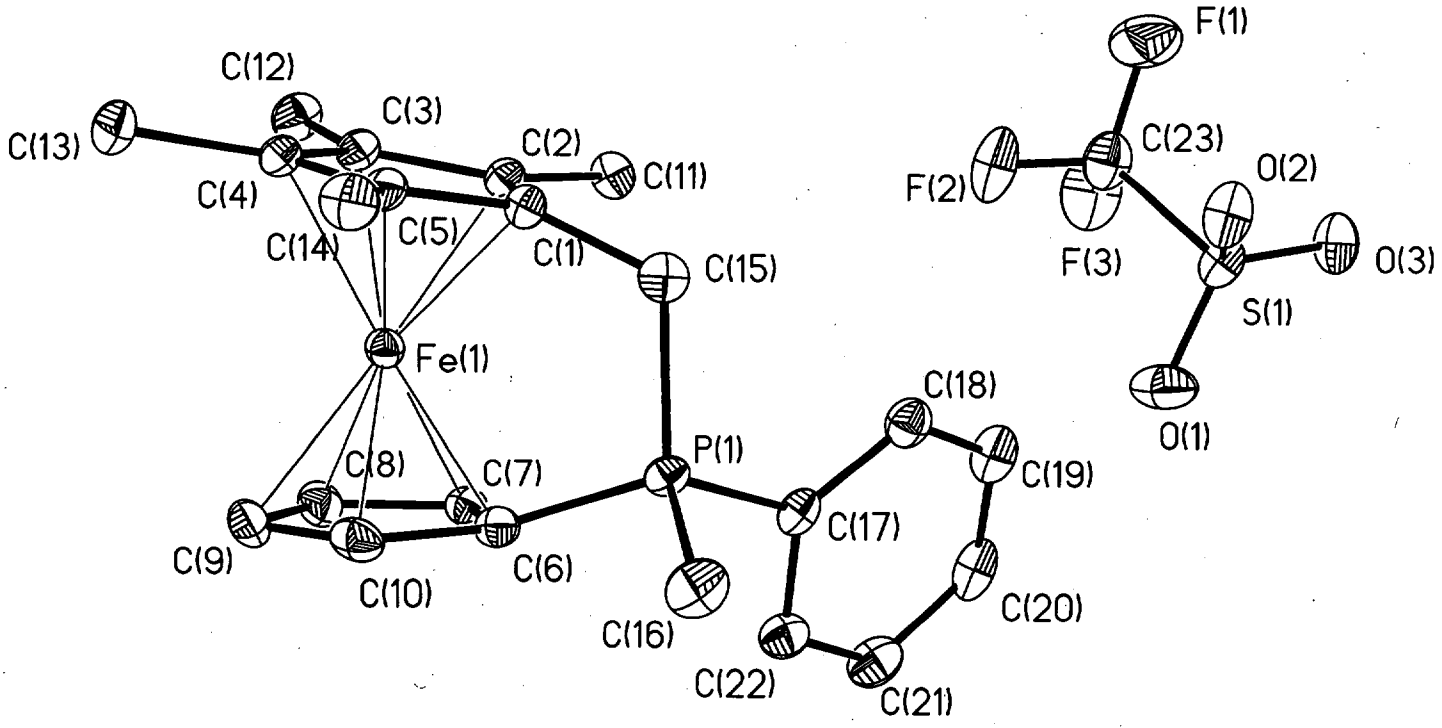
| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Fe(1) | 17(1) | 14(1) | 13(1) | 2(1) | 6(1) | 0(1) |
| S(1) | 37(1) | 15(1) | 24(1) | 1(1) | 12(1) | 3(1) |
| C(1) | 25(1) | 16(1) | 18(1) | 4(1) | 8(1) | 0(1) |
| C(2) | 23(1) | 20(1) | 17(1) | 5(1) | 4(1) | 1(1) |
| C(3) | 33(1) | 24(1) | 16(1) | 3(1) | 10(1) | -2(1) |
| C(4) | 31(1) | 26(1) | 26(1) | 6(1) | 19(1) | 1(1) |
| C(5) | 24(1) | 24(1) | 23(1) | 5(1) | 10(1) | -5(1) |
| C(6) | 22(1) | 16(1) | 13(1) | 0(1) | 8(1) | -1(1) |
| C(7) | 18(1) | 21(1) | 17(1) | 0(1) | 9(1) | -2(1) |
| C(8) | 26(1) | 17(1) | 16(1) | 0(1) | 10(1) | -5(1) |
| C(9) | 26(1) | 16(1) | 16(1) | 4(1) | 11(1) | 3(1) |
| C(10) | 19(1) | 19(1) | 14(1) | 3(1) | 6(1) | 1(1) |
| C(11) | 19(1) | 40(2) | 31(1) | 0(1) | 12(1) | 1(1) |
| C(12) | 39(1) | 26(1) | 24(1) | -6(1) | 14(1) | -15(1) |
| C(13) | 42(1) | 26(1) | 26(1) | 6(1) | 17(1) | 13(1) |
| C(14) | 20(1) | 35(1) | 22(1) | 7(1) | 4(1) | 0(1) |
| C(15) | 34(1) | 17(1) | 18(1) | -2(1) | 10(1) | 0(1) |

Table 11. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (≈$^2$x 10 $^3$) for S9628a.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | 10620(40) | 723(13) | 4910(50) | 31(8) |
| H(3A) | 9210(40) | 1375(12) | 6520(40) | 22(7) |
| H(4A) | 5720(40) | 1261(12) | 4530(50) | 29(8) |
| H(5A) | 4970(40) | 558(11) | 1870(40) | 21(7) |
| H(11A) | 11770(50) | 1370(15) | 840(60) | 45(10) |
| H(11B) | 11380(50) | 886(15) | 1710(50) | 33(8) |
| H(11C) | 11990(60) | 1378(18) | 2700(70) | 59(12) |
| H(12A) | 10550(40) | 2609(13) | 2260(50) | 32(8) |
| H(12B) | 11180(50) | 2243(14) | 3990(50) | 37(9) |
| H(12C) | 9530(50) | 2627(15) | 3530(50) | 42(9) |
| H(13A) | 5260(60) | 2706(17) | -330(60) | 64(12) |
| H(13B) | 6220(40) | 2677(14) | 1910(50) | 34(8) |
| H(13C) | 4450(50) | 2336(16) | 680(60) | 50(10) |
| H(14A) | 3660(50) | 1516(15) | -3130(50) | 43(9) |
| H(14B) | 3160(50) | 1530(16) | -1420(60) | 50(10) |
| H(14C) | 3670(60) | 1031(18) | -1660(60) | 63(12) |
| H(15A) | 8220(40) | 485(13) | -1540(50) | 29(8) |
| H(15B) | 6200(50) | 476(15) | -1820(50) | 43(9) |

© 2001 American Chemical Society, J. Am. Chem. Soc., Resendes ja002750e Supporting Info Page 69


Supp. Material for Compound 13



© 2001 American Chemical Society, J. Am. Chem. Soc., Resendes ja002750e Supporting Info Page 70

$L\,CH_2$-PCy Me $_3$ Cl + I monomer.

S70

Table 1. Crystal data and structure refinement for k0040.

| | | |
|---|---|---|
| Identification code | k0040 | |
| Empirical formula | C23 H26 F3 Fe O3 P S | |
| Formula weight | 526.32 | |
| Temperature | 150(1) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | C2/c | |
| Unit cell dimensions | a = 25.8739(13) Å | α= 90°. |
| | b = 6.7719(3) Å | β= 109.336(2)°. |
| | c = 27.7679(16) Å | γ = 90°. |
| Volume | 4590.9(4) Å$^3$ | |
| Z | 8 | |
| Density (calculated) | 1.523 Mg/m$^3$ | |
| Absorption coefficient | 0.865 mm$^{-1}$ | |
| F(000) | 2176 | |
| Crystal size | 0.15 x 0.05 x 0.05 mm$^3$ | |
| Theta range for data collection | 2.63 to 27.53°. | |
| Index ranges | 0<=h<=33, 0<=k<=8, -36<=l<=33 | |
| Reflections collected | 24533 | |
| Independent reflections | 5167 [R(int) = 0.048] | |
| Completeness to theta = 27.53° | 97.6 % | |
| Absorption correction | multi-scan (Denzo-SMN) | |
| Max. and min. transmission | 0.9580 and 0.8812 | |
| Refinement method | Full-matrix least-squares on F$^2$ | |
| Data / restraints / parameters | 5167 / 2 / 304 | |
| Goodness-of-fit on F$^2$ | 1.028 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0607, wR2 = 0.1188 | |
| R indices (all data) | R1 = 0.0997, wR2 = 0.1330 | |
| Largest diff. peak and hole | 0.401 and -0.376 e.Å$^{-3}$ | |

$\alpha = 11.37(7)^\circ$

$\beta(CH_2) = 10.5(4)^\circ$

$\beta(P) = 18.6(3)^\circ$

$\delta = -3.1(6)^\circ$

Cp - Fe - Cp $\Rightarrow$ 172.2(2)°

Fe(1) ··· P(1) distance 3.035(1) Å.

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for k0040. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Fe(1) | 743(1) | 9703(1) | 1301(1) | 23(1) |
| P(1) | 1828(1) | 8896(2) | 1139(1) | 25(1) |
| Fe(1*) | 730(4) | 4981(15) | 1311(4) | 34(3) |
| P(1*) | 1804(7) | 6050(30) | 1163(8) | 43(6) |
| C(1) | 1202(1) | 12050(5) | 1268(1) | 25(1) |
| C(2) | 692(1) | 12143(5) | 855(1) | 25(1) |
| C(3) | 262(1) | 12172(5) | 1074(1) | 27(1) |
| C(4) | 509(2) | 12144(5) | 1617(1) | 28(1) |
| C(5) | 1089(2) | 12101(5) | 1738(1) | 28(1) |
| C(6) | 1257(2) | 7631(5) | 1226(1) | 27(1) |
| C(7) | 731(1) | 7411(5) | 834(1) | 26(1) |
| C(8) | 337(2) | 7081(5) | 1076(2) | 34(1) |
| C(9) | 606(2) | 7080(6) | 1610(2) | 36(1) |
| C(10) | 1171(2) | 7402(5) | 1710(1) | 33(1) |
| C(11) | 615(2) | 12251(6) | 295(1) | 31(1) |
| C(12) | -339(2) | 12282(6) | 787(2) | 38(1) |
| C(13) | 209(2) | 12205(6) | 2000(2) | 43(1) |
| C(14) | 1506(2) | 12152(6) | 2266(1) | 38(1) |
| C(15) | 1760(2) | 11552(6) | 1224(1) | 31(1) |
| C(16) | 2437(2) | 7992(6) | 1609(2) | 42(1) |
| C(17) | 1819(2) | 8358(6) | 500(1) | 30(1) |
| C(18) | 1936(2) | 9763(6) | 192(2) | 35(1) |
| C(19) | 1908(2) | 9274(7) | -301(2) | 42(1) |
| C(20) | 1779(2) | 7401(7) | -478(2) | 41(1) |
| C(21) | 1683(2) | 5938(7) | -168(2) | 43(1) |
| C(22) | 1699(2) | 6421(6) | 324(2) | 37(1) |
| F(1) | 1087(1) | 15267(5) | -1769(1) | 85(1) |
| F(2) | 871(1) | 12999(5) | -1329(1) | 75(1) |
| F(3) | 694(1) | 12606(5) | -2130(1) | 80(1) |
| C(23) | 1059(2) | 13303(8) | -1715(2) | 53(1) |
| O(1) | 1616(2) | 10106(4) | -1544(1) | 63(1) |

| | | | | |
|---|---|---|---|---|
| O(2) | 2052(1) | 13097(5) | -1121(1) | 48(1) |
| O(3) | 1878(1) | 12688(5) | -2028(1) | 48(1) |
| S(1) | 1728(1) | 12184(2) | -1587(1) | 37(1) |

Table 3. Bond lengths [Å] and angles [°] for k0040.

| | |
|---|---|
| Fe(1)...P(1) | 3.035(1) |
| Fe(1)-C(6) | 1.990(4) |
| Fe(1)-C(1) | 2.003(4) |
| Fe(1)-C(7) | 2.015(3) |
| Fe(1)-C(10) | 2.028(4) |
| Fe(1)-C(2) | 2.041(4) |
| Fe(1)-C(5) | 2.048(4) |
| Fe(1)-C(8) | 2.052(4) |
| Fe(1)-C(9) | 2.054(4) |
| Fe(1)-C(3) | 2.055(4) |
| Fe(1)-C(4) | 2.055(4) |
| P(1)-C(16) | 1.788(4) |
| P(1)-C(6) | 1.792(4) |
| P(1)-C(17) | 1.804(4) |
| P(1)-C(15) | 1.830(4) |
| C(1)-C(5) | 1.427(5) |
| C(1)-C(2) | 1.433(5) |
| C(1)-C(15) | 1.528(5) |
| C(2)-C(3) | 1.434(5) |
| C(2)-C(11) | 1.505(5) |
| C(3)-C(4) | 1.430(5) |
| C(3)-C(12) | 1.496(5) |
| C(4)-C(5) | 1.427(5) |
| C(4)-C(13) | 1.510(5) |
| C(5)-C(14) | 1.506(5) |
| C(6)-C(7) | 1.440(5) |
| C(6)-C(10) | 1.443(5) |
| C(7)-C(8) | 1.412(5) |
| C(8)-C(9) | 1.414(5) |
| C(9)-C(10) | 1.411(5) |
| C(17)-C(18) | 1.379(5) |
| C(17)-C(22) | 1.398(5) |
| C(18)-C(19) | 1.388(5) |
| C(19)-C(20) | 1.361(6) |

| | |
|---|---|
| C(20)-C(21) | 1.387(6) |
| C(21)-C(22) | 1.394(5) |
| F(1)-C(23) | 1.343(6) |
| F(2)-C(23) | 1.333(5) |
| F(3)-C(23) | 1.313(5) |
| C(23)-S(1) | 1.812(5) |
| O(1)-S(1) | 1.450(3) |
| O(2)-S(1) | 1.428(3) |
| O(3)-S(1) | 1.443(3) |

| | |
|---|---|
| C(6)-Fe(1)-C(1) | 97.41(15) |
| C(6)-Fe(1)-C(7) | 42.12(14) |
| C(1)-Fe(1)-C(7) | 117.75(14) |
| C(6)-Fe(1)-C(10) | 42.06(14) |
| C(1)-Fe(1)-C(10) | 114.41(15) |
| C(7)-Fe(1)-C(10) | 70.00(15) |
| C(6)-Fe(1)-C(2) | 114.75(14) |
| C(1)-Fe(1)-C(2) | 41.51(13) |
| C(7)-Fe(1)-C(2) | 104.47(14) |
| C(10)-Fe(1)-C(2) | 151.07(15) |
| C(6)-Fe(1)-C(5) | 116.42(15) |
| C(1)-Fe(1)-C(5) | 41.23(14) |
| C(7)-Fe(1)-C(5) | 154.47(15) |
| C(10)-Fe(1)-C(5) | 103.08(15) |
| C(2)-Fe(1)-C(5) | 69.22(14) |
| C(6)-Fe(1)-C(8) | 69.52(15) |
| C(1)-Fe(1)-C(8) | 157.54(15) |
| C(7)-Fe(1)-C(8) | 40.62(14) |
| C(10)-Fe(1)-C(8) | 68.58(16) |
| C(2)-Fe(1)-C(8) | 126.33(15) |
| C(5)-Fe(1)-C(8) | 161.04(15) |
| C(6)-Fe(1)-C(9) | 69.36(16) |
| C(1)-Fe(1)-C(9) | 153.05(16) |
| C(7)-Fe(1)-C(9) | 68.58(15) |
| C(10)-Fe(1)-C(9) | 40.42(16) |
| C(2)-Fe(1)-C(9) | 165.37(15) |

| | |
|---|---|
| C(5)-Fe(1)-C(9) | 122.66(15) |
| C(8)-Fe(1)-C(9) | 40.29(15) |
| C(6)-Fe(1)-C(3) | 154.07(15) |
| C(1)-Fe(1)-C(3) | 69.43(14) |
| C(7)-Fe(1)-C(3) | 123.43(14) |
| C(10)-Fe(1)-C(3) | 163.69(16) |
| C(2)-Fe(1)-C(3) | 40.98(14) |
| C(5)-Fe(1)-C(3) | 68.80(14) |
| C(8)-Fe(1)-C(3) | 114.44(15) |
| C(9)-Fe(1)-C(3) | 131.36(16) |
| C(6)-Fe(1)-C(4) | 155.97(15) |
| C(1)-Fe(1)-C(4) | 69.14(14) |
| C(7)-Fe(1)-C(4) | 161.86(14) |
| C(10)-Fe(1)-C(4) | 124.17(15) |
| C(2)-Fe(1)-C(4) | 68.84(14) |
| C(5)-Fe(1)-C(4) | 40.70(14) |
| C(8)-Fe(1)-C(4) | 129.21(15) |
| C(9)-Fe(1)-C(4) | 113.61(15) |
| C(3)-Fe(1)-C(4) | 40.73(14) |
| C(16)-P(1)-C(6) | 107.77(19) |
| C(16)-P(1)-C(17) | 111.70(18) |
| C(6)-P(1)-C(17) | 107.02(17) |
| C(16)-P(1)-C(15) | 109.99(19) |
| C(6)-P(1)-C(15) | 109.51(17) |
| C(17)-P(1)-C(15) | 110.73(18) |
| C(5)-C(1)-C(2) | 108.6(3) |
| C(5)-C(1)-C(15) | 124.3(3) |
| C(2)-C(1)-C(15) | 126.0(3) |
| C(5)-C(1)-Fe(1) | 71.1(2) |
| C(2)-C(1)-Fe(1) | 70.7(2) |
| C(15)-C(1)-Fe(1) | 114.7(2) |
| C(1)-C(2)-C(3) | 107.4(3) |
| C(1)-C(2)-C(11) | 127.0(3) |
| C(3)-C(2)-C(11) | 125.5(3) |
| C(1)-C(2)-Fe(1) | 67.8(2) |
| C(3)-C(2)-Fe(1) | 70.0(2) |

| | |
|---|---|
| C(11)-C(2)-Fe(1) | 128.7(3) |
| C(4)-C(3)-C(2) | 107.9(3) |
| C(4)-C(3)-C(12) | 125.8(3) |
| C(2)-C(3)-C(12) | 126.3(3) |
| C(4)-C(3)-Fe(1) | 69.6(2) |
| C(2)-C(3)-Fe(1) | 69.0(2) |
| C(12)-C(3)-Fe(1) | 128.4(3) |
| C(5)-C(4)-C(3) | 108.5(3) |
| C(5)-C(4)-C(13) | 125.5(3) |
| C(3)-C(4)-C(13) | 126.1(3) |
| C(5)-C(4)-Fe(1) | 69.4(2) |
| C(3)-C(4)-Fe(1) | 69.6(2) |
| C(13)-C(4)-Fe(1) | 128.0(3) |
| C(4)-C(5)-C(1) | 107.6(3) |
| C(4)-C(5)-C(14) | 126.0(3) |
| C(1)-C(5)-C(14) | 126.4(3) |
| C(4)-C(5)-Fe(1) | 69.9(2) |
| C(1)-C(5)-Fe(1) | 67.7(2) |
| C(14)-C(5)-Fe(1) | 128.8(3) |
| C(7)-C(6)-C(10) | 107.2(3) |
| C(7)-C(6)-P(1) | 124.2(3) |
| C(10)-C(6)-P(1) | 124.4(3) |
| C(7)-C(6)-Fe(1) | 69.9(2) |
| C(10)-C(6)-Fe(1) | 70.4(2) |
| P(1)-C(6)-Fe(1) | 106.62(17) |
| C(8)-C(7)-C(6) | 107.9(3) |
| C(8)-C(7)-Fe(1) | 71.1(2) |
| C(6)-C(7)-Fe(1) | 68.0(2) |
| C(7)-C(8)-C(9) | 108.5(3) |
| C(7)-C(8)-Fe(1) | 68.3(2) |
| C(9)-C(8)-Fe(1) | 69.9(2) |
| C(10)-C(9)-C(8) | 109.0(3) |
| C(10)-C(9)-Fe(1) | 68.8(2) |
| C(8)-C(9)-Fe(1) | 69.8(2) |
| C(9)-C(10)-C(6) | 107.6(3) |
| C(9)-C(10)-Fe(1) | 70.8(2) |

| | |
|---|---|
| C(6)-C(10)-Fe(1) | 67.6(2) |
| C(1)-C(15)-P(1) | 111.2(3) |
| C(18)-C(17)-C(22) | 120.0(4) |
| C(18)-C(17)-P(1) | 122.5(3) |
| C(22)-C(17)-P(1) | 117.5(3) |
| C(17)-C(18)-C(19) | 119.8(4) |
| C(20)-C(19)-C(18) | 120.3(4) |
| C(19)-C(20)-C(21) | 121.0(4) |
| C(20)-C(21)-C(22) | 119.2(4) |
| C(21)-C(22)-C(17) | 119.5(4) |
| F(3)-C(23)-F(2) | 107.6(4) |
| F(3)-C(23)-F(1) | 107.9(4) |
| F(2)-C(23)-F(1) | 106.9(4) |
| F(3)-C(23)-S(1) | 112.6(4) |
| F(2)-C(23)-S(1) | 110.9(3) |
| F(1)-C(23)-S(1) | 110.7(3) |
| O(2)-S(1)-O(3) | 115.12(18) |
| O(2)-S(1)-O(1) | 114.8(2) |
| O(3)-S(1)-O(1) | 114.61(19) |
| O(2)-S(1)-C(23) | 103.4(2) |
| O(3)-S(1)-C(23) | 104.0(2) |
| O(1)-S(1)-C(23) | 102.6(2) |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for k0040. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Fe(1) | 27(1) | 22(1) | 21(1) | 1(1) | 8(1) | 0(1) |
| P(1) | 22(1) | 27(1) | 22(1) | 1(1) | 3(1) | 5(1) |
| C(1) | 24(2) | 27(2) | 22(2) | -1(2) | 7(2) | 0(1) |
| C(2) | 24(2) | 26(2) | 23(2) | -1(2) | 7(2) | 2(1) |
| C(3) | 25(2) | 28(2) | 28(2) | -3(2) | 7(2) | 1(2) |
| C(4) | 35(2) | 25(2) | 26(2) | -4(2) | 14(2) | -1(2) |
| C(5) | 37(2) | 26(2) | 20(2) | -3(2) | 10(2) | 2(2) |
| C(6) | 33(2) | 25(2) | 22(2) | 0(2) | 8(2) | 3(2) |
| C(7) | 31(2) | 24(2) | 22(2) | -2(2) | 8(2) | 0(2) |
| C(8) | 36(2) | 29(2) | 37(2) | -2(2) | 14(2) | -7(2) |
| C(9) | 50(3) | 30(2) | 37(2) | 3(2) | 25(2) | -4(2) |
| C(10) | 45(2) | 28(2) | 22(2) | 5(2) | 6(2) | 4(2) |
| C(11) | 32(2) | 37(2) | 21(2) | 1(2) | 4(2) | -3(2) |
| C(12) | 29(2) | 39(2) | 44(3) | -5(2) | 9(2) | 0(2) |
| C(13) | 55(3) | 42(3) | 42(3) | -5(2) | 30(2) | 0(2) |
| C(14) | 45(2) | 40(2) | 22(2) | -2(2) | 4(2) | -1(2) |
| C(15) | 27(2) | 33(2) | 29(2) | -2(2) | 3(2) | -1(2) |
| C(16) | 32(2) | 50(3) | 34(2) | 1(2) | -1(2) | 9(2) |
| C(17) | 28(2) | 36(2) | 27(2) | -5(2) | 10(2) | 4(2) |
| C(18) | 30(2) | 41(2) | 34(2) | 2(2) | 10(2) | 5(2) |
| C(19) | 33(2) | 61(3) | 29(2) | -2(2) | 9(2) | 4(2) |
| C(20) | 26(2) | 70(3) | 26(2) | -8(2) | 6(2) | 4(2) |
| C(21) | 38(2) | 43(3) | 41(3) | -11(2) | 7(2) | 3(2) |
| C(22) | 34(2) | 36(2) | 39(2) | -1(2) | 9(2) | 3(2) |
| F(1) | 85(2) | 60(2) | 104(3) | 20(2) | 23(2) | 31(2) |
| F(2) | 48(2) | 119(3) | 68(2) | -5(2) | 31(2) | 6(2) |
| F(3) | 39(2) | 127(3) | 54(2) | -4(2) | -9(1) | -5(2) |
| C(23) | 36(3) | 74(4) | 45(3) | 2(3) | 8(2) | 4(2) |
| O(1) | 101(3) | 39(2) | 48(2) | 0(2) | 25(2) | 12(2) |
| O(2) | 34(2) | 78(2) | 27(2) | -11(2) | 5(1) | -4(2) |
| O(3) | 49(2) | 73(2) | 25(2) | -1(2) | 16(1) | -4(2) |

© 2001 American Chemical Society, J. Am. Chem. Soc., Resendes ja002750e Supporting Info Page 79 

| | | | | | | |
|---|---|---|---|---|---|---|
| S(1) | 34(1) | 50(1) | 25(1) | -4(1) | 6(1) | 7(1) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for k0040.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(7A) | 658 | 7489 | 458 | 31 |
| H(8A) | -66 | 6928 | 900 | 40 |
| H(9A) | 423 | 6935 | 1874 | 44 |
| H(10A) | 1458 | 7480 | 2055 | 40 |
| H(11A) | 571 | 13633 | 184 | 47 |
| H(11B) | 288 | 11501 | 102 | 47 |
| H(11C) | 937 | 11690 | 233 | 47 |
| H(12A) | -448 | 13667 | 717 | 57 |
| H(12B) | -543 | 11686 | 991 | 57 |
| H(12C) | -421 | 11566 | 463 | 57 |
| H(13A) | 177 | 13577 | 2098 | 64 |
| H(13B) | 414 | 11440 | 2303 | 64 |
| H(13C) | -157 | 11636 | 1848 | 64 |
| H(14A) | 1596 | 13526 | 2370 | 56 |
| H(14B) | 1839 | 11460 | 2265 | 56 |
| H(14C) | 1356 | 11502 | 2506 | 56 |
| H(15A) | 2053 | 11996 | 1536 | 38 |
| H(15B) | 1805 | 12267 | 929 | 38 |
| H(16A) | 2479 | 6583 | 1551 | 62 |
| H(16B) | 2410 | 8179 | 1950 | 62 |
| H(16C) | 2754 | 8717 | 1584 | 62 |
| H(18A) | 2036 | 11062 | 318 | 43 |
| H(19A) | 1979 | 10251 | -517 | 50 |
| H(20A) | 1755 | 7090 | -818 | 50 |
| H(21A) | 1607 | 4623 | -290 | 51 |
| H(22A) | 1628 | 5440 | 539 | 44 |