Supporting Information

Contents

Experimental details

All reactions were routinely performed under an inert atmosphere of argon or nitrogen by using Schlenk and glovebox techniques and dry deoxygenated solvents. Solvents were dried using a MBRAUN MB SPS-800 system. Tetrahydrofuran and benzene were also distilled on Na/benzophenone. Nuclear magnetic resonance spectra were recorded on a BrukerAC-300 SY spectrometer operating at 300.0 MHz for ^{1}H, 75.5 MHz for ^{13}C, and 121.5 MHz for ^{31}P. Solvent peaks are used as an internal reference relative to Me_4Si for ^{1}H and ^{13}C chemical shifts (ppm); ^{31}P chemical shifts are relative to a 85% H_3PO_4 external reference. Coupling constants are given in hertz. The following abbreviations are used: s, singlet; bs, broad singlet. $[PdCl_2(PPh)_3]_2$ was obtained by reaction of triphenylphosphine on $[(COD)PdCl_2]$[1], $[RuCl_2(PPh_3)_4]$,[2] $[FeCl_2(THF)_{1.5}]$[3] and complexes **1**[4], and **6**[5] were prepared according to literature procedures. $CoCl_2$ was bought as the hydrate and dried by heating under vacuum. All other reagents and chemicals were obtained commercially and used as received

Synthesis of complex 4: Route A To a solution of **1** (100 mg, 0.073 mmol) in THF (5 mL) was added $CoCl_2$ (19 mg, 0.15 mmol). The solution was heated at 65°C for 24h and became dark green. THF was evaporated under vacuum and toluene was added. Impurities were removed by filtration and the surnactant was dried under vacuum. Complex **4** was isolated with 80% yield. Route B To a solution of complex **6** (155 mg, 0.2 mmol) in THF (5 mL) was added $CoCl_2$ (25.9 mg, 0.2 mmol). The solution turned immediately green and green crystals precipitated. These crystals were identified as complex **4** by X-Ray diffraction analysis.

Synthesis of complex 2: Route A $RuCl_2(PPh_3)_4$ (71.1 mg, 0.058 mmol) was added to a solution of complex **1** (40 mg, 0.029 mmol) in THF (0.6 mL) in an NMR tube. The solution immediately turned brown. After 15 minutes, completion of the reaction was checked by ^{31}P NMR. Route B $RuCl_2(PPh_3)_4$ (30 mg, 0.025 mmol) was added to a solution of complex **6** (17 mg, 0.025 mmol) in THF (0.6 mL) in an NMR tube. The solution immediately turned brown. After 15 minutes, completion of the reaction was checked by ^{31}P NMR.

Synthesis of complex 7: To a solution of **6** (388.6 mg, 0.5 mmol) in THF (10 mL) was added $FeCl_2(THF)_{1.5}$ (117.4 mg, 0.5 mmol). The solution turned immediately to dark green and a dark precipitate of complex appeared. After filtration the solid was dried under vacuum, then washed twice with 5mL of THF that was condensed (from a sodium/benzophenone flask), in which complex **7** is only sparingly soluble. This procedure allows the extraction of $ScCl_3.THF_3$ from the solid. The solid was then dried under vacuum and the title complex **7** was isolated in a 30 % yield. ^{1}H NMR (C_6D_6, 25°C) δ_H 10.08 (bs, 8H, H_{arom}), 8.51 (bs, 8H, H_{arom}), 7.02 (bs, 8H, H_{arom}), 6.28 (bs, 4H, H_{arom}), 4.5 (bs, 8H, H_{arom}), 4.03 (bs, 4H, H_{arom}). ^{13}C NMR (C_6D_6, 25°C) δ_C 203.0 (bs, C_{ipso}), 179.3 (bs; C_{ipso}), 153.4 (bs,

CH_{arom}), 141.5 (bs, CH_{arom}), 137.4 (bs, CH_{arom}), 132.4 (bs, CH_{arom}). Elemental analysis calcd (%) for: C 59.77, H 4.01; found: C 58.93, H 3.94. mp: 252°C with decomposition.

X-Ray crystal structure analysis:

General: Data were collected at 150.0-(1) K on a Nonius Kappa CCD diffractometer using a Mo Kα (λ = 0.71070 Å) X-ray source and a graphite monochromator. All data were measured using phi and omega scans. Experimental details are described in Tables S1-1 – S2-5. The crystal structures were solved using SIR 97[6] and Shelxl-97[7]. ORTEP drawings were made using ORTEP III for Windows[8]. CCDC 848404-848405 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge at http://www.ccdc.cam.ac.uk/conts/retrieving.html or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk

Crystallographic data for 5:

Figure S1. Molecular structure of 5

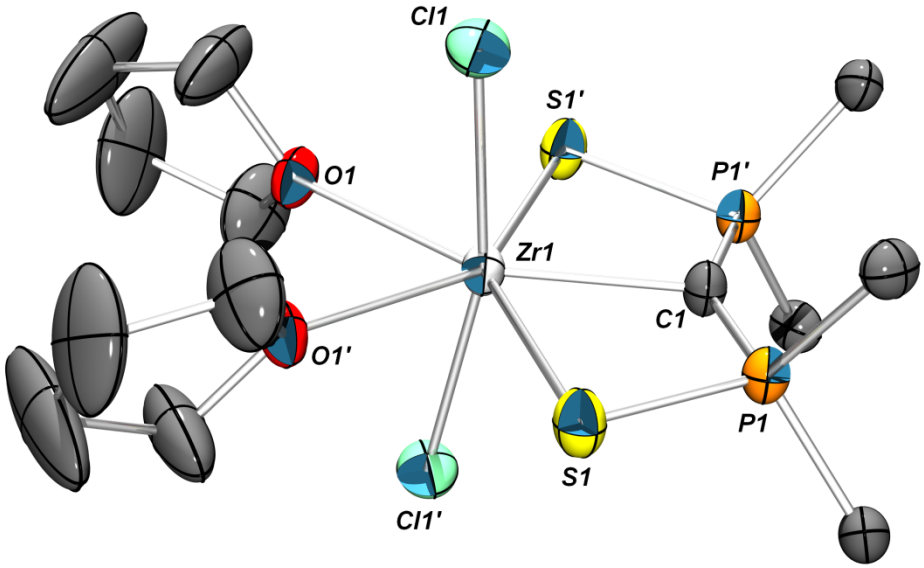

Table S1-1. Crystal data for 5

Compound	5
Molecular formula	$C_{33}H_{32}Cl_2O_2P_2S_2Zr$, C_4H_8O
Molecular weight	820.87
Crystal habit	Pale Yellow Block

Crystal dimensions (mm)	0.22x0.18x0.16
Crystal system	trigonal
Space group	P3121
a(Å)	12.072(1)
b(Å)	12.072(1)
c(Å)	22.609(1)
α(°)	90.00
β(°)	90.00
γ(°)	120.00
V(Å^3)	2853.4(4)
Z	3
d(g-cm^{-3})	1.433
F(000)	1266
μ(cm^{-1})	0.658
Absorption corrections	multi-scan ; 0.8688 min, 0.9020 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	27.47
HKL ranges	-15 15 ; -15 15 ; -29 21
Reflections measured	13053
Unique data	4300
Rint	0.0279
Reflections used	4193
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	constr
Parameters refined	191
Reflections / parameter	21
wR2	0.0939
R1	0.0326
Flack's parameter	0.02(5)
Weights a, b	0.0433 ; 2.4598
GoF	1.128
difference peak / hole (e Å^{-3})	0.634(0.066) / -0.406(0.066)

Table S1-2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 5

atom	x	y	z	U(eq)
Zr(1)	1087(1)	0	3333	24(1)
P(1)	3739(1)	919(1)	3907(1)	26(1)
S(1)	2474(1)	1346(1)	4273(1)	33(1)
Cl(1)	-164(1)	-1983(1)	3914(1)	39(1)
O(1)	-845(2)	-709(2)	2807(1)	34(1)
C(1)	2897(3)	0	3333	27(1)
C(2)	5187(3)	2376(3)	3693(1)	30(1)
C(3)	5139(4)	3470(4)	3570(2)	51(1)
C(4)	6201(5)	4549(4)	3348(2)	65(1)
C(5)	7324(4)	4535(4)	3246(2)	53(1)
C(6)	7368(4)	3449(4)	3358(2)	58(1)
C(7)	6311(3)	2367(4)	3584(2)	49(1)
C(8)	4271(3)	175(3)	4447(1)	30(1)
C(9)	5160(4)	892(4)	4881(2)	43(1)
C(10)	5571(4)	293(4)	5281(2)	51(1)
C(11)	5082(4)	-997(4)	5261(2)	46(1)
C(12)	4178(4)	-1718(4)	4845(2)	48(1)
C(13)	3762(3)	-1144(3)	4432(2)	38(1)
C(14)	-1820(4)	-2049(4)	2689(3)	72(2)
C(15)	-2910(5)	-1985(7)	2449(4)	103(2)
C(16)	-2588(5)	-709(7)	2343(5)	145(4)
C(17)	-1180(5)	115(5)	2478(3)	84(2)

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

Table S1-3. Bond lengths (Å) and angles (deg) for 5

Zr(1)-C(1)	2.185(4)	Zr(1)-O(1)#4	2.364(2)
Zr(1)-O(1)	2.364(2)	Zr(1)-Cl(1)	2.4744(8)
Zr(1)-Cl(1)#4	2.4745(8	Zr(1)-S(1)#4	2.6905(8)
Zr(1)-S(1)	2.6905(8	Zr(1)-P(1)	3.1007(8)
Zr(1)-P(1)#4	3.1008(8	P(1)-C(1)	1.679(1)
P(1)-C(8)	1.812(3)	P(1)-C(2)	1.819(3)
P(1)-S(1)	2.017(1)	O(1)-C(17)	1.452(5)
O(1)-C(14)	1.473(5)	C(1)-P(1)#4	1.679(1)
C(2)-C(3)	1.379(5)	C(2)-C(7)	1.385(5)
C(3)-C(4)	1.387(6)	C(3)-H(3)	0.9500
C(4)-C(5)	1.383(7)	C(4)-H(4)	0.9500
C(5)-C(6)	1.363(6)	C(5)-H(5)	0.9500
C(6)-C(7)	1.388(5)	C(6)-H(6)	0.9500
C(7)-H(7)	0.9500	C(8)-C(9)	1.391(4)
C(8)-C(13)	1.392(4)	C(9)-C(10)	1.396(5)
C(9)-H(9)	0.9500	C(10)-C(11)	1.363(6)
C(10)-H(10)	0.9500	C(11)-C(12)	1.374(6)
C(11)-H(11)	0.9500	C(12)-C(13)	1.395(5)
C(12)-H(12)	0.9500	C(13)-H(13)	0.9500
C(14)-C(15)	1.461(7)	C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900	C(15)-C(16)	1.41(1)
C(15)-H(15)	0.9500	C(16)-C(17)	1.511(6)
C(16)-H(16)	0.9500	C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900		

C(1)-Zr(1)-O(1)#4	143.64(6)	C(1)-Zr(1)-O(1)	143.64(6)
O(1)#4-Zr(1)-O(1)	72.7(1)	C(1)-Zr(1)-Cl(1)	97.24(2)
O(1)#4-Zr(1)-Cl(1)	83.92(5)	O(1)-Zr(1)-Cl(1)	84.43(6)
C(1)-Zr(1)-Cl(1)#4	97.25(2)	O(1)#4-Zr(1)-Cl(1)#4	84.43(6)
O(1)-Zr(1)-Cl(1)#4	83.92(5)	Cl(1)-Zr(1)-Cl(1)#4	165.51(4)
C(1)-Zr(1)-S(1)#4	71.30(2)	O(1)#4-Zr(1)-S(1)#4	145.04(6)
O(1)-Zr(1)-S(1)#4	72.35(6)	Cl(1)-Zr(1)-S(1)#4	91.24(3)
Cl(1)#4-Zr(1)-S(1)#4	93.39(3)	C(1)-Zr(1)-S(1)	71.30(2)

O(1)#4-Zr(1)-S(1)	72.35(6)	O(1)-Zr(1)-S(1)	145.04(6)
Cl(1)-Zr(1)-S(1)	93.39(3)	Cl(1)#4-Zr(1)-S(1)	91.24(3)
S(1)#4-Zr(1)-S(1)	142.61(3)	C(1)-Zr(1)-P(1)	31.37(1)
O(1)#4-Zr(1)-P(1)	112.33(6)	O(1)-Zr(1)-P(1)	174.40(6)
Cl(1)-Zr(1)-P(1)	98.35(3)	Cl(1)#4-Zr(1)-P(1)	94.03(3)
S(1)#4-Zr(1)-P(1)	102.64(2)	S(1)-Zr(1)-P(1)	39.99(2)
C(1)-Zr(1)-P(1)#4	31.37(1)	O(1)#4-Zr(1)-P(1)#4	174.39(6)
O(1)-Zr(1)-P(1)#4	112.33(6)	Cl(1)-Zr(1)-P(1)#4	94.02(2)
Cl(1)#4-Zr(1)-P(1)#4	98.35(3)	S(1)#4-Zr(1)-P(1)#4	39.99(2)
S(1)-Zr(1)-P(1)#4	102.64(2)	P(1)-Zr(1)-P(1)#4	62.74(3)
C(1)-P(1)-C(8)	116.1(1)	C(1)-P(1)-C(2)	113.9(1)
C(8)-P(1)-C(2)	104.5(1)	C(1)-P(1)-S(1)	101.5(1)
C(8)-P(1)-S(1)	110.6(1)	C(2)-P(1)-S(1)	110.3(1)
C(1)-P(1)-Zr(1)	42.7(1)	C(8)-P(1)-Zr(1)	131.5(1)
C(2)-P(1)-Zr(1)	123.8(1)	S(1)-P(1)-Zr(1)	58.99(3)
P(1)-S(1)-Zr(1)	81.02(3)	C(17)-O(1)-C(14)	108.4(3)
C(17)-O(1)-Zr(1)	124.9(2)	C(14)-O(1)-Zr(1)	126.2(2)
P(1)#4-C(1)-P(1)	148.1(3)	P(1)#4-C(1)-Zr(1)	106.0(1)
P(1)-C(1)-Zr(1)	106.0(1)	C(3)-C(2)-C(7)	118.8(3)
C(3)-C(2)-P(1)	120.0(3)	C(7)-C(2)-P(1)	120.8(3)
C(2)-C(3)-C(4)	120.7(4)	C(2)-C(3)-H(3)	119.6
C(4)-C(3)-H(3)	119.6	C(5)-C(4)-C(3)	120.0(4)
C(5)-C(4)-H(4)	120.0	C(3)-C(4)-H(4)	120.0
C(6)-C(5)-C(4)	119.4(4)	C(6)-C(5)-H(5)	120.3
C(4)-C(5)-H(5)	120.3	C(5)-C(6)-C(7)	120.9(4)
C(5)-C(6)-H(6)	119.6	C(7)-C(6)-H(6)	119.6
C(2)-C(7)-C(6)	120.2(4)	C(2)-C(7)-H(7)	119.9
C(6)-C(7)-H(7)	119.9	C(9)-C(8)-C(13)	119.4(3)
C(9)-C(8)-P(1)	121.4(3)	C(13)-C(8)-P(1)	119.3(2)
C(8)-C(9)-C(10)	119.9(4)	C(8)-C(9)-H(9)	120.1
C(10)-C(9)-H(9)	120.1	C(11)-C(10)-C(9)	120.5(4)
C(11)-C(10)-H(10)	119.7	C(9)-C(10)-H(10)	119.7
C(10)-C(11)-C(12)	119.9(3)	C(10)-C(11)-H(11)	120.0
C(12)-C(11)-H(11)	120.0	C(11)-C(12)-C(13)	120.9(4)
C(11)-C(12)-H(12)	119.6	C(13)-C(12)-H(12)	119.6
C(8)-C(13)-C(12)	119.3(3)	C(8)-C(13)-H(13)	120.3
C(12)-C(13)-H(13)	120.3	C(15)-C(14)-O(1)	104.8(4)
C(15)-C(14)-H(14A)	110.8	O(1)-C(14)-H(14A)	110.8
C(15)-C(14)-H(14B)	110.8	O(1)-C(14)-H(14B)	110.8
H(14A)-C(14)-H(14B)	108.9	C(16)-C(15)-C(14)	111.0(4)
C(16)-C(15)-H(15)	124.5	C(14)-C(15)-H(15)	124.5
C(15)-C(16)-C(17)	106.8(5)	C(15)-C(16)-H(16)	126.6
C(17)-C(16)-H(16)	126.6	O(1)-C(17)-C(16)	105.1(4)
O(1)-C(17)-H(17A)	110.7	C(16)-C(17)-H(17A)	110.7
O(1)-C(17)-H(17B)	110.7	C(16)-C(17)-H(17B)	110.7
H(17A)-C(17)-H(17B)	108.8		

Estimated standard deviations are given in the parenthesis.
Symmetry operators ::

1: x, y, z	2: -y, x-y, z+1/3	3: -x+y, -x, z+2/3
4: x-y, -y, -z+2/3	5: -x, -x+y, -z+1/3	6: y, x, -z

Table S1-4. Anisotropic displacement parameters (A^2 x 10^3) for 5

atom	U11	U22	U33	U23	U13	U12
Zr(1)	19(1)	20(1)	32(1)	2(1)	1(1)	10(1)
P(1)	23(1)	27(1)	29(1)	-3(1)	-2(1)	13(1)
S(1)	30(1)	38(1)	36(1)	-9(1)	-1(1)	20(1)
Cl(1)	40(1)	27(1)	50(1)	13(1)	9(1)	17(1)
O(1)	22(1)	30(1)	47(1)	2(1)	-6(1)	12(1)
C(1)	22(1)	30(2)	30(2)	-3(2)	-1(1)	15(1)
C(2)	28(1)	27(1)	31(1)	-2(1)	-4(1)	10(1)
C(3)	46(2)	36(2)	69(2)	7(2)	11(2)	19(2)
C(4)	67(3)	37(2)	83(3)	15(2)	18(3)	20(2)
C(5)	40(2)	42(2)	51(2)	9(2)	5(2)	1(2)
C(6)	31(2)	66(3)	68(3)	16(2)	5(2)	16(2)

C(7)	31(2)	47(2)	66(2)	14(2)	2(2)	18(2)
C(8)	25(1)	35(2)	30(1)	1(1)	1(1)	15(1)
C(9)	42(2)	41(2)	40(2)	-2(1)	-12(1)	16(2)
C(10)	41(2)	67(3)	43(2)	0(2)	-14(2)	26(2)
C(11)	40(2)	68(3)	39(2)	16(2)	5(1)	34(2)
C(12)	54(2)	43(2)	51(2)	10(2)	1(2)	26(2)
C(13)	39(2)	35(2)	38(2)	2(1)	-1(1)	17(1)
C(14)	40(2)	47(2)	114(4)	-5(3)	-23(2)	9(2)
C(15)	36(2)	78(4)	177(7)	-41(4)	-43(3)	16(3)
C(16)	41(3)	99(5)	250(10)	83(6)	-55(4)	2(3)
C(17)	40(2)	71(3)	124(5)	43(3)	-21(3)	16(2)

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

Table S1-5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 5

atom	x	y	z	U(eq)
H(3)	4370	3486	3639	61
H(4)	6158	5298	3265	78
H(5)	8057	5274	3098	64
H(6)	8133	3431	3281	70
H(7)	6359	1620	3662	58
H(9)	5486	1789	4904	52
H(10)	6197	789	5570	61
H(11)	5367	-1398	5536	55
H(12)	3831	-2618	4837	58
H(13)	3138	-1649	4145	46
H(14A)	-1500.9999	-2440	2400	87
H(14B)	-2060	-2559	3058	87
H(15)	-3727	-2708	2374	123
H(16)	-3149	-422	2211	174
H(17A)	-675.9999	417	2109	101
H(17B)	-1021	866	2718	101

Crystallographic data for 7:

Figure S2. Molecular structure of 7

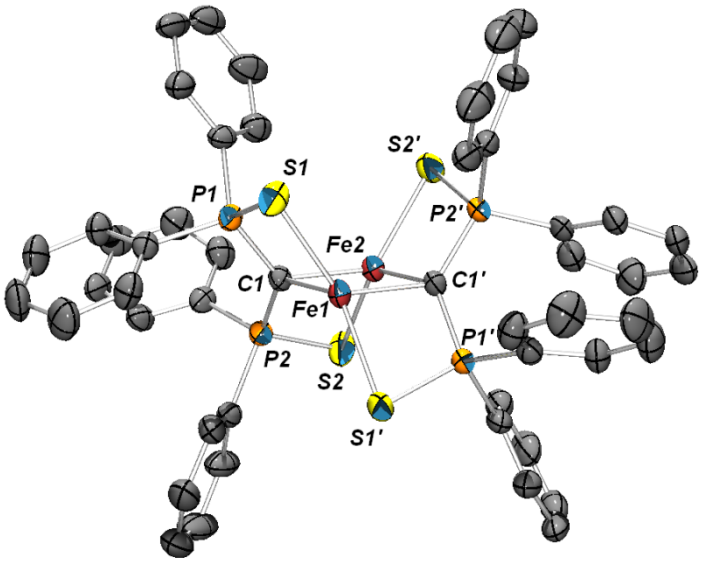

Table S2-1. Crystal data for 7

Compound	7
Molecular formula	$C_{50}H_{40}Fe_2P_4S_4$, $2(C_4H_8O)$
Molecular weight	1148.85
Crystal habit	red plate
Crystal dimensions(mm)	0.20x0.08x0.02
Crystal system	tetragonal
Space group	P-421c
a(Å)	16.980(1)
b(Å)	16.980(1)
c(Å)	19.740(1)
α(°)	90.00
β(°)	90.00
γ(°)	90.00
V(Å^3)	5691.4(6)
Z	4
d(g-cm^{-3})	1.341
F(000)	2384
μ(cm^{-1})	0.809
Absorption corrections	multi-scan ; 0.8549 min, 0.9840 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	27.48

HKL ranges	-21 22 ; -18 22 ; -25 16
Reflections measured	35123
Unique data	6506
Rint	0.0486
Reflections used	5826
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	constr
Parameters refined	272
Reflections / parameter	21
wR2	0.1144
R1	0.0466
Flack's parameter	0.55(3)
Weights a, b	0.0527 ; 4.5870
GoF	1.093
difference peak / hole (e $Å^{-3}$)	0.302(0.060) / -0.266(0.060)

Table S2-2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 7

atom	x	y	z	U(eq)
Fe(1)	5000	5000	3636(1)	28(1)
Fe(2)	5000	5000	2335(1)	29(1)
S(1)	3760(1)	5387(1)	4089(1)	42(1)
S(2)	5339(1)	3794(1)	1824(1)	45(1)
P(1)	3439(1)	4564(1)	3398(1)	29(1)
P(2)	4530(1)	3474(1)	2535(1)	30(1)
C(1)	4304(2)	4322(2)	2979(2)	27(1)
C(2)	2966(2)	3741(2)	3823(2)	31(1)
C(3)	3249(2)	3494(3)	4447(2)	44(1)
C(4)	2945(3)	2825(3)	4745(2)	57(1)
C(5)	2346(3)	2399(3)	4421(3)	57(1)
C(6)	2059(3)	2645(3)	3805(3)	52(1)
C(7)	2371(2)	3312(2)	3505(2)	40(1)
C(8)	2660(2)	4954(2)	2853(2)	36(1)
C(9)	1924(2)	5124(2)	3125(3)	46(1)
C(10)	1321(2)	5404(2)	2708(3)	58(1)
C(11)	1464(3)	5515(2)	2034(3)	57(1)
C(12)	2184(3)	5368(3)	1770(3)	59(1)
C(13)	2791(2)	5076(2)	2175(2)	43(1)
C(14)	3682(2)	3032(2)	2122(2)	33(1)
C(15)	3285(2)	2403(2)	2412(2)	39(1)
C(16)	2598(2)	2120(2)	2115(2)	45(1)
C(17)	2302(3)	2466(2)	1539(3)	50(1)
C(18)	2689(3)	3088(3)	1247(2)	52(1)
C(19)	3390(3)	3364(2)	1527(2)	45(1)
C(20)	4947(2)	2690(2)	3043(2)	37(1)
C(21)	4962(2)	2736(2)	3733(2)	48(1)
C(22)	5268(3)	2115(3)	4134(3)	64(1)
C(23)	5566(3)	1458(3)	3809(4)	82(2)
C(24)	5571(3)	1424(3)	3097(5)	82(2)
C(25)	5256(2)	2028(2)	2718(3)	58(1)

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

Table S2-3. Bond lengths (Å) and angles (deg) for 7

Fe(1)-C(1)#3	2.099(3)	Fe(1)-C(1)	2.099(3)
Fe(1)-S(1)	2.380(1)	Fe(1)-S(1)#3	2.380(1)
Fe(1)-Fe(2)	2.5683(8	Fe(1)-P(1)#3	2.792(1)
Fe(1)-P(1)	2.792(1)	Fe(2)-C(1)#3	2.082(3)
Fe(2)-C(1)	2.082(3)	Fe(2)-S(2)	2.355(1)
Fe(2)-S(2)#3	2.355(1)	Fe(2)-P(2)	2.7400(8)
Fe(2)-P(2)#3	2.7400(8	S(1)-P(1)	2.028(1)
S(2)-P(2)	2.037(1)	P(1)-C(1)	1.736(4)
P(1)-C(2)	1.816(4)	P(1)-C(8)	1.829(4)
P(2)-C(1)	1.728(3)	P(2)-C(20)	1.811(4)
P(2)-C(14)	1.817(4)	C(2)-C(3)	1.387(5)
C(2)-C(7)	1.395(5)	C(3)-C(4)	1.379(6)
C(3)-H(3)	0.9500	C(4)-C(5)	1.404(7)
C(4)-H(4)	0.9500	C(5)-C(6)	1.374(7)
C(5)-H(5)	0.9500	C(6)-C(7)	1.383(6)
C(6)-H(6)	0.9500	C(7)-H(7)	0.9500
C(8)-C(13)	1.373(6)	C(8)-C(9)	1.391(5)
C(9)-C(10)	1.398(6)	C(9)-H(9)	0.9500
C(10)-C(11)	1.366(7)	C(10)-H(10)	0.9500
C(11)-C(12)	1.352(7)	C(11)-H(11)	0.9500
C(12)-C(13)	1.394(6)	C(12)-H(12)	0.9500
C(13)-H(13)	0.9500	C(14)-C(15)	1.385(5)
C(14)-C(19)	1.394(6)	C(15)-C(16)	1.390(5)
C(15)-H(15)	0.9500	C(16)-C(17)	1.374(7)
C(16)-H(16)	0.9500	C(17)-C(18)	1.370(7)
C(17)-H(17)	0.9500	C(18)-C(19)	1.394(6)
C(18)-H(18)	0.9500	C(19)-H(19)	0.9500
C(20)-C(21)	1.366(6)	C(20)-C(25)	1.396(6)
C(21)-C(22)	1.416(6)	C(21)-H(21)	0.9500
C(22)-C(23)	1.384(8)	C(22)-H(22)	0.9500
C(23)-C(24)	1.41(1)	C(23)-H(23)	0.9500
C(24)-C(25)	1.378(7)	C(24)-H(24)	0.9500
C(25)-H(25)	0.9500		

C(1)#3-Fe(1)-C(1)	103.6(2)	C(1)#3-Fe(1)-S(1)	125.4(1)
C(1)-Fe(1)-S(1)	83.4(1)	C(1)#3-Fe(1)-S(1)#3	83.4(1)
C(1)-Fe(1)-S(1)#3	125.4(1)	S(1)-Fe(1)-S(1)#3	135.85(6)
C(1)#3-Fe(1)-Fe(2)	51.8(1)	C(1)-Fe(1)-Fe(2)	51.8(1)
S(1)-Fe(1)-Fe(2)	112.08(3)	S(1)#3-Fe(1)-Fe(2)	112.08(3)
C(1)#3-Fe(1)-P(1)#3	38.4(1)	C(1)-Fe(1)-P(1)#3	125.2(1)
S(1)-Fe(1)-P(1)#3	146.06(3)	S(1)#3-Fe(1)-P(1)#3	45.30(3)
Fe(2)-Fe(1)-P(1)#3	80.33(2)	C(1)#3-Fe(1)-P(1)	125.2(1)
C(1)-Fe(1)-P(1)	38.4(1)	S(1)-Fe(1)-P(1)	45.30(3)
S(1)#3-Fe(1)-P(1)	146.06(3)	Fe(2)-Fe(1)-P(1)	80.33(2)
P(1)#3-Fe(1)-P(1)	160.65(5)	C(1)#3-Fe(2)-C(1)	104.8(2)
C(1)#3-Fe(2)-S(2)	127.1(1)	C(1)-Fe(2)-S(2)	85.3(1)
C(1)#3-Fe(2)-S(2)#3	85.3(1)	C(1)-Fe(2)-S(2)#3	127.1(1)
S(2)-Fe(2)-S(2)#3	129.31(6)	C(1)#3-Fe(2)-Fe(1)	52.4(1)
C(1)-Fe(2)-Fe(1)	52.4(1)	S(2)-Fe(2)-Fe(1)	115.35(3)
S(2)#3-Fe(2)-Fe(1)	115.35(3)	C(1)#3-Fe(2)-P(2)	126.9(1)
C(1)-Fe(2)-P(2)	39.1(1)	S(2)-Fe(2)-P(2)	46.39(3)
S(2)#3-Fe(2)-P(2)	144.44(3)	Fe(1)-Fe(2)-P(2)	81.69(2)
C(1)#3-Fe(2)-P(2)#3	39.1(1)	C(1)-Fe(2)-P(2)#3	126.9(1)
S(2)-Fe(2)-P(2)#3	144.45(3)	S(2)#3-Fe(2)-P(2)#3	46.39(3)
Fe(1)-Fe(2)-P(2)#3	81.69(2)	P(2)-Fe(2)-P(2)#3	163.38(5)
P(1)-S(1)-Fe(1)	78.16(4)	P(2)-S(2)-Fe(2)	76.82(4)
C(1)-P(1)-C(2)	114.4(2)	C(1)-P(1)-C(8)	114.6(2)
C(2)-P(1)-C(8)	103.3(2)	C(1)-P(1)-S(1)	104.8(1)
C(2)-P(1)-S(1)	109.8(1)	C(8)-P(1)-S(1)	109.9(1)
C(1)-P(1)-Fe(1)	48.6(1)	C(2)-P(1)-Fe(1)	123.1(1)
C(8)-P(1)-Fe(1)	133.6(1)	S(1)-P(1)-Fe(1)	56.54(3)
C(1)-P(2)-C(20)	114.8(2)	C(1)-P(2)-C(14)	113.3(2)
C(20)-P(2)-C(14)	104.7(2)	C(1)-P(2)-S(2)	106.1(1)
C(20)-P(2)-S(2)	108.3(1)	C(14)-P(2)-S(2)	109.6(1)
C(1)-P(2)-Fe(2)	49.4(1)	C(20)-P(2)-Fe(2)	131.4(1)
C(14)-P(2)-Fe(2)	123.8(1)	S(2)-P(2)-Fe(2)	56.79(4)

P(2)-C(1)-P(1)	128.8(2)	P(2)-C(1)-Fe(2)	91.5(2)
P(1)-C(1)-Fe(2)	129.9(2)	P(2)-C(1)-Fe(1)	130.2(2)
P(1)-C(1)-Fe(1)	93.0(2)	Fe(2)-C(1)-Fe(1)	75.8(1)
C(3)-C(2)-C(7)	119.5(4)	C(3)-C(2)-P(1)	119.4(3)
C(7)-C(2)-P(1)	120.9(3)	C(4)-C(3)-C(2)	119.9(4)
C(4)-C(3)-H(3)	120.1	C(2)-C(3)-H(3)	120.1
C(3)-C(4)-C(5)	120.1(4)	C(3)-C(4)-H(4)	119.9
C(5)-C(4)-H(4)	119.9	C(6)-C(5)-C(4)	120.2(4)
C(6)-C(5)-H(5)	119.9	C(4)-C(5)-H(5)	119.9
C(5)-C(6)-C(7)	119.4(4)	C(5)-C(6)-H(6)	120.3
C(7)-C(6)-H(6)	120.3	C(6)-C(7)-C(2)	120.9(4)
C(6)-C(7)-H(7)	119.6	C(2)-C(7)-H(7)	119.6
C(13)-C(8)-C(9)	119.4(4)	C(13)-C(8)-P(1)	120.8(3)
C(9)-C(8)-P(1)	119.8(3)	C(8)-C(9)-C(10)	120.1(5)
C(8)-C(9)-H(9)	120.0	C(10)-C(9)-H(9)	120.0
C(11)-C(10)-C(9)	119.4(4)	C(11)-C(10)-H(10)	120.3
C(9)-C(10)-H(10)	120.3	C(12)-C(11)-C(10)	120.7(4)
C(12)-C(11)-H(11)	119.6	C(10)-C(11)-H(11)	119.6
C(11)-C(12)-C(13)	120.9(5)	C(11)-C(12)-H(12)	119.6
C(13)-C(12)-H(12)	119.6	C(8)-C(13)-C(12)	119.5(4)
C(8)-C(13)-H(13)	120.2	C(12)-C(13)-H(13)	120.2
C(15)-C(14)-C(19)	119.1(4)	C(15)-C(14)-P(2)	121.3(3)
C(19)-C(14)-P(2)	119.5(3)	C(14)-C(15)-C(16)	120.1(4)
C(14)-C(15)-H(15)	120.0	C(16)-C(15)-H(15)	120.0
C(17)-C(16)-C(15)	120.5(4)	C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8	C(18)-C(17)-C(16)	120.1(4)
C(18)-C(17)-H(17)	119.9	C(16)-C(17)-H(17)	119.9
C(17)-C(18)-C(19)	120.1(4)	C(17)-C(18)-H(18)	119.9
C(19)-C(18)-H(18)	119.9	C(14)-C(19)-C(18)	120.1(4)
C(14)-C(19)-H(19)	120.0	C(18)-C(19)-H(19)	120.0
C(21)-C(20)-C(25)	119.8(4)	C(21)-C(20)-P(2)	121.2(3)
C(25)-C(20)-P(2)	119.0(3)	C(20)-C(21)-C(22)	121.5(4)
C(20)-C(21)-H(21)	119.3	C(22)-C(21)-H(21)	119.3
C(23)-C(22)-C(21)	118.3(6)	C(23)-C(22)-H(22)	120.8
C(21)-C(22)-H(22)	120.8	C(22)-C(23)-C(24)	120.0(5)
C(22)-C(23)-H(23)	120.0	C(24)-C(23)-H(23)	120.0
C(25)-C(24)-C(23)	120.6(5)	C(25)-C(24)-H(24)	119.7
C(23)-C(24)-H(24)	119.7	C(24)-C(25)-C(20)	119.7(6)
C(24)-C(25)-H(25)	120.1	C(20)-C(25)-H(25)	120.1

Estimated standard deviations are given in the parenthesis.

Symmetry operators ::

1: x, y, z 2: y, -x, -z 3: -x, -y, z

4: -y, x, -z 5: x+1/2, -y+1/2, -z+1/ 6: -y+1/2, -x+1/2, z+1/

7: -x+1/2, y+1/2, -z+1/ 8: y+1/2, x+1/2, z+1/2

Table S2-4. Anisotropic displacement parameters (A^2 x 10^3) for 7

atom	U11	U22	U33	U23	U13	U12
Fe(1)	28(1)	25(1)	32(1)	0	0	-5(1)
Fe(2)	28(1)	25(1)	33(1)	0	0	-1(1)
S(1)	35(1)	39(1)	52(1)	-21(1)	6(1)	-4(1)
S(2)	42(1)	36(1)	56(1)	-12(1)	19(1)	-4(1)
P(1)	26(1)	25(1)	38(1)	-6(1)	2(1)	-2(1)
P(2)	28(1)	21(1)	41(1)	-5(1)	2(1)	0(1)
C(1)	28(2)	23(2)	30(2)	-2(1)	1(1)	-1(1)
C(2)	32(2)	29(2)	34(2)	-5(1)	4(1)	-1(1)
C(3)	39(2)	53(2)	39(2)	0(2)	4(2)	-7(2)
C(4)	59(3)	68(3)	45(2)	14(2)	7(2)	-8(2)
C(5)	58(3)	48(2)	64(3)	12(2)	16(2)	-16(2)
C(6)	48(2)	48(3)	61(3)	0(2)	3(2)	-18(2)
C(7)	37(2)	35(2)	48(2)	-2(2)	-2(2)	-8(2)
C(8)	30(2)	24(2)	55(2)	-6(2)	-6(2)	5(1)
C(9)	34(2)	33(2)	72(3)	-3(2)	2(2)	3(2)
C(10)	30(2)	33(2)	112(4)	-8(2)	-14(2)	5(2)
C(11)	47(2)	35(2)	89(4)	-6(2)	-26(2)	3(2)
C(12)	55(3)	47(2)	75(3)	-6(2)	-32(2)	6(2)
C(13)	41(2)	38(2)	51(2)	-3(2)	-10(2)	2(2)
C(14)	31(2)	27(2)	41(2)	-12(1)	0(2)	1(1)
C(15)	37(2)	26(2)	52(2)	-3(2)	-9(2)	-1(1)
C(16)	34(2)	27(2)	75(3)	-7(2)	-3(2)	-4(2)
C(17)	44(2)	42(2)	63(3)	-22(2)	-15(2)	2(2)
C(18)	54(3)	53(3)	49(3)	-3(2)	-14(2)	-3(2)
C(19)	50(2)	38(2)	47(2)	-5(2)	0(2)	-4(2)
C(20)	27(2)	25(2)	59(2)	1(2)	-5(2)	0(1)
C(21)	35(2)	33(2)	76(3)	10(2)	3(2)	0(2)
C(22)	45(3)	58(3)	90(4)	34(3)	-10(2)	-3(2)
C(23)	47(3)	41(3)	156(7)	34(3)	-18(3)	1(2)
C(24)	51(3)	29(2)	165(7)	-9(3)	-28(4)	11(2)
C(25)	41(2)	33(2)	100(4)	-8(2)	-13(2)	9(2)

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

Table S2-5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 7

atom	x	y	z	U(eq)
H(3)	3652	3784	4668	53
H(4)	3142	2652	5170	69
H(5)	2137	1938	4627	68
H(6)	1650	2359	3587	63
H(7)	2178	3480	3078	48
H(9)	1831	5049	3596	55
H(10)	816	5516	2892	70
H(11)	1053	5697	1747	68
H(12)	2278	5466	1303	71
H(13)	3291	4962	1982	52
H(15)	3482	2166	2813	46
H(16)	2331	1685	2312	54
H(17)	1830	2273	1342	60
H(18)	2478	3332	854	62
H(19)	3670	3779	1312	54
H(21)	4763	3194	3950	58
H(22)	5268	2149	4615	77
H(23)	5766	1030	4066	98
H(24)	5793	980	2875	98
H(25)	5250	1995	2237	69

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