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Table S20. (Cont'd.)

atom	x/a	y/b	z/c	U(iso)
C(27)	320(13)	4142(6)	6758(7)	62(6)
P(4)	3364(3)	2895(2)	8626(2)	40(1)
C(28)	4042(17)	3378(7)	8640(9)	88(9)
C(29)	4892(20)	3359(11)	8916(13)	212(23)
C(30)	4114(15)	3597(8)	8085(9)	98(9)
C(31)	2750(15)	2896(6)	9284(6)	63(7)
C(32)	2066(16)	3223(7)	9273(8)	92(9)
C(33)	3332(17)	2901(6)	9764(7)	96(10)
C(34)	4061(12)	2417(7)	8660(9)	71(7)
C(35)	3560(14)	2016(6)	8821(7)	61(7)
C(36)	4473(17)	2353(10)	8133(9)	139(14)
N(1)	-712(20)	2433(10)	5078(13)	170(12)
C(37)	-79(14)	1959(6)	5806(7)	64(6)
C(38)	-509(17)	2204(8)	5385(9)	83(8)

Table S21. Interatomic Distances (Å) for
[Fe₁₆S₁₆(PⁱPr₃)₈]·2MeCN.

Fe(1)-S(5)	2.311(4)	S(2)-Fe(2')	2.287(5)
Fe(1)-S(3)	2.325(5)	S(6)-Fe(6')	2.303(5)
Fe(1)-S(2)	2.342(5)	P(1)-C(7)	1.83(2)
Fe(1)-S(1)	2.389(4)	P(1)-C(4)	1.86(2)
Fe(1)-Fe(2)	2.519(3)	P(1)-C(1)	1.89(2)
Fe(1)-Fe(3)	2.680(3)	C(1)-C(2)	1.50(2)
Fe(1)-Fe(4)	2.705(3)	C(1)-C(3)	1.55(2)
Fe(1)-Fe(5)	2.767(3)	C(4)-C(5)	1.48(2)
Fe(2)-S(2')	2.287(5)	C(4)-C(6)	1.53(3)
Fe(2)-S(4)	2.318(5)	C(7)-C(9)	1.53(3)
Fe(2)-S(1)	2.351(4)	C(7)-C(8)	1.57(3)
Fe(2)-S(2)	2.395(4)	P(2)-C(10)	1.82(2)
Fe(2)-Fe(3)	2.672(3)	P(2)-C(13)	1.86(2)
Fe(2)-Fe(4)	2.703(3)	P(2)-C(16)	1.87(2)
Fe(2)-Fe(2')	2.800(4)	C(10)-C(12)	1.49(2)
Fe(3)-S(4)	2.267(4)	C(10)-C(11)	1.59(2)
Fe(3)-S(3)	2.274(5)	C(13)-C(14)	1.50(3)
Fe(3)-S(2)	2.359(5)	C(13)-C(15)	1.54(2)
Fe(3)-P(1)	2.397(5)	C(16)-C(18)	1.48(2)
Fe(3)-Fe(4)	2.669(3)	C(16)-C(17)	1.53(2)
Fe(4)-S(3)	2.279(5)	P(3)-C(19)	1.85(2)
Fe(4)-S(4)	2.284(5)	P(3)-C(25)	1.87(2)
Fe(4)-S(1)	2.345(5)	P(3)-C(22)	1.87(2)
Fe(4)-P(2)	2.399(5)	C(19)-C(20)	1.52(2)
Fe(5)-S(1)	2.315(4)	C(19)-C(21)	1.52(2)
Fe(5)-S(7)	2.325(5)	C(22)-C(24)	1.49(3)
Fe(5)-S(6)	2.341(5)	C(22)-C(23)	1.52(3)
Fe(5)-S(5)	2.393(4)	C(25)-C(27)	1.47(2)
Fe(5)-Fe(6)	2.525(3)	C(25)-C(26)	1.52(2)
Fe(5)-Fe(8)	2.686(3)	P(4)-C(28)	1.85(2)
Fe(5)-Fe(7)	2.687(3)	P(4)-C(34)	1.85(2)
Fe(6)-S(6')	2.303(5)	P(4)-C(31)	1.92(2)
Fe(6)-S(8)	2.315(5)	C(28)-C(29)	1.52(3)
Fe(6)-S(5)	2.343(4)	C(28)-C(30)	1.55(3)
Fe(6)-S(6)	2.382(4)	C(31)-C(32)	1.49(3)
Fe(6)-Fe(8)	2.659(4)	C(31)-C(33)	1.52(3)
Fe(6)-Fe(7)	2.705(3)	C(34)-C(36)	1.49(3)
Fe(6)-Fe(6')	2.753(5)	C(34)-C(35)	1.53(3)
Fe(7)-S(7)	2.262(5)	N(1)-C(38)	1.09(3)
Fe(7)-S(8)	2.268(4)	C(37)-C(38)	1.47(3)
Fe(7)-S(6)	2.368(5)		
Fe(7)-P(3)	2.375(5)		
Fe(7)-Fe(8)	2.657(3)		
Fe(8)-S(7)	2.277(4)		
Fe(8)-S(8)	2.286(5)		
Fe(8)-S(5)	2.360(5)		
Fe(8)-P(4)	2.384(5)		

Table S22. Bond Angles (deg) for $[\text{Fe}_{16}\text{S}_{16}(\text{P}^i\text{Pr}_3)_8] \cdot 2\text{MeCN}$.

S(5)-Fe(1)-S(3)	120.1(2)	Fe(3)-Fe(2)-Fe(4)	59.54(9)
S(5)-Fe(1)-S(2)	107.3(2)	S(2')-Fe(2)-Fe(2')	55.06(12)
S(3)-Fe(1)-S(2)	104.6(2)	S(4)-Fe(2)-Fe(2')	125.13(11)
S(5)-Fe(1)-S(1)	107.0(2)	S(1)-Fe(2)-Fe(2')	130.39(11)
S(3)-Fe(1)-S(1)	104.0(2)	S(2)-Fe(2)-Fe(2')	51.53(12)
S(2)-Fe(1)-S(1)	114.1(2)	Fe(1)-Fe(2)-Fe(2')	99.08(10)
S(5)-Fe(1)-Fe(2)	136.0(2)	Fe(3)-Fe(2)-Fe(2')	99.36(10)
S(3)-Fe(1)-Fe(2)	103.84(13)	Fe(4)-Fe(2)-Fe(2')	156.10(13)
S(2)-Fe(1)-Fe(2)	58.90(12)	S(4)-Fe(3)-S(3)	106.7(2)
S(1)-Fe(1)-Fe(2)	57.16(12)	S(4)-Fe(3)-S(2)	107.8(2)
S(5)-Fe(1)-Fe(3)	148.99(13)	S(3)-Fe(3)-S(2)	105.6(2)
S(3)-Fe(1)-Fe(3)	53.46(12)	S(4)-Fe(3)-P(1)	119.6(2)
S(2)-Fe(1)-Fe(3)	55.55(12)	S(3)-Fe(3)-P(1)	115.8(2)
S(1)-Fe(1)-Fe(3)	103.80(12)	S(2)-Fe(3)-P(1)	99.8(2)
Fe(2)-Fe(1)-Fe(3)	61.75(8)	S(4)-Fe(3)-Fe(4)	54.40(12)
S(5)-Fe(1)-Fe(4)	146.41(14)	S(3)-Fe(3)-Fe(4)	54.21(12)
S(3)-Fe(1)-Fe(4)	53.24(12)	S(2)-Fe(3)-Fe(4)	106.69(13)
S(2)-Fe(1)-Fe(4)	106.05(13)	P(1)-Fe(3)-Fe(4)	153.3(2)
S(1)-Fe(1)-Fe(4)	54.40(12)	S(4)-Fe(3)-Fe(2)	55.26(12)
Fe(2)-Fe(1)-Fe(4)	62.20(9)	S(3)-Fe(3)-Fe(2)	100.65(13)
Fe(3)-Fe(1)-Fe(4)	59.41(8)	S(2)-Fe(3)-Fe(2)	56.44(11)
S(5)-Fe(1)-Fe(5)	55.35(11)	P(1)-Fe(3)-Fe(2)	141.5(2)
S(3)-Fe(1)-Fe(5)	119.6(2)	Fe(4)-Fe(3)-Fe(2)	60.82(9)
S(2)-Fe(1)-Fe(5)	135.6(2)	S(4)-Fe(3)-Fe(1)	100.70(13)
S(1)-Fe(1)-Fe(5)	52.74(10)	S(3)-Fe(3)-Fe(1)	55.24(13)
Fe(2)-Fe(1)-Fe(5)	102.96(10)	S(2)-Fe(3)-Fe(1)	54.94(12)
Fe(3)-Fe(1)-Fe(5)	155.46(10)	P(1)-Fe(3)-Fe(1)	138.38(14)
Fe(4)-Fe(1)-Fe(5)	96.95(9)	Fe(4)-Fe(3)-Fe(1)	60.76(8)
S(2')-Fe(2)-S(4)	120.6(2)	Fe(2)-Fe(3)-Fe(1)	56.15(8)
S(2')-Fe(2)-S(1)	107.6(2)	S(3)-Fe(4)-S(4)	105.9(2)
S(4)-Fe(2)-S(1)	104.0(2)	S(3)-Fe(4)-S(1)	106.9(2)
S(2')-Fe(2)-S(2)	106.33(14)	S(4)-Fe(4)-S(1)	105.2(2)
S(4)-Fe(2)-S(2)	105.0(2)	S(3)-Fe(4)-P(2)	120.2(2)
S(1)-Fe(2)-S(2)	113.6(2)	S(4)-Fe(4)-P(2)	107.5(2)
S(2')-Fe(2)-Fe(1)	135.2(2)	S(1)-Fe(4)-P(2)	110.0(2)
S(4)-Fe(2)-Fe(1)	104.2(2)	S(3)-Fe(4)-Fe(3)	54.02(13)
S(1)-Fe(2)-Fe(1)	58.64(11)	S(4)-Fe(4)-Fe(3)	53.80(12)
S(2)-Fe(2)-Fe(1)	56.87(12)	S(1)-Fe(4)-Fe(3)	105.40(13)
S(2')-Fe(2)-Fe(3)	146.95(14)	P(2)-Fe(4)-Fe(3)	143.6(2)
S(4)-Fe(2)-Fe(3)	53.47(12)	S(3)-Fe(4)-Fe(2)	99.57(14)
S(1)-Fe(2)-Fe(3)	105.15(14)	S(4)-Fe(4)-Fe(2)	54.61(13)
S(2)-Fe(2)-Fe(3)	55.19(12)	S(1)-Fe(4)-Fe(2)	54.95(12)
Fe(1)-Fe(2)-Fe(3)	62.10(8)	P(2)-Fe(4)-Fe(2)	140.1(2)
S(2')-Fe(2)-Fe(4)	148.77(12)	Fe(3)-Fe(4)-Fe(2)	59.64(8)
S(4)-Fe(2)-Fe(4)	53.45(13)	S(3)-Fe(4)-Fe(1)	54.80(12)
S(1)-Fe(2)-Fe(4)	54.76(12)	S(4)-Fe(4)-Fe(1)	99.52(14)
S(2)-Fe(2)-Fe(4)	104.61(14)	S(1)-Fe(4)-Fe(1)	55.91(11)
Fe(1)-Fe(2)-Fe(4)	62.28(9)	P(2)-Fe(4)-Fe(1)	152.4(2)

Table S22. (Cont'd.)

Fe(3)-Fe(4)-Fe(1)	59.84(8)	S(6)-Fe(6)-Fe(7)	55.05(12)
Fe(2)-Fe(4)-Fe(1)	55.52(8)	Fe(5)-Fe(6)-Fe(7)	61.72(8)
S(1)-Fe(5)-S(7)	120.5(2)	Fe(8)-Fe(6)-Fe(7)	59.39(9)
S(1)-Fe(5)-S(6)	107.1(2)	S(6')-Fe(6)-Fe(6')	55.35(12)
S(7)-Fe(5)-S(6)	104.9(2)	S(8)-Fe(6)-Fe(6')	123.45(12)
S(1)-Fe(5)-S(5)	106.8(2)	S(5)-Fe(6)-Fe(6')	130.06(12)
S(7)-Fe(5)-S(5)	104.6(2)	S(6)-Fe(6)-Fe(6')	52.68(12)
S(6)-Fe(5)-S(5)	113.1(2)	Fe(5)-Fe(6)-Fe(6')	100.42(10)
S(1)-Fe(5)-Fe(6)	135.8(2)	Fe(8)-Fe(6)-Fe(6')	157.24(13)
S(7)-Fe(5)-Fe(6)	103.66(14)	Fe(7)-Fe(6)-Fe(6')	100.11(11)
S(6)-Fe(5)-Fe(6)	58.48(12)	S(7)-Fe(7)-S(8)	107.1(2)
S(5)-Fe(5)-Fe(6)	56.83(12)	S(7)-Fe(7)-S(6)	106.0(2)
S(1)-Fe(5)-Fe(8)	147.6(2)	S(8)-Fe(7)-S(6)	105.9(2)
S(7)-Fe(5)-Fe(8)	53.47(12)	S(7)-Fe(7)-P(3)	116.0(2)
S(6)-Fe(5)-Fe(8)	104.99(13)	S(8)-Fe(7)-P(3)	119.2(2)
S(5)-Fe(5)-Fe(8)	55.02(12)	S(6)-Fe(7)-P(3)	101.2(2)
Fe(6)-Fe(5)-Fe(8)	61.27(9)	S(7)-Fe(7)-Fe(8)	54.43(12)
S(1)-Fe(5)-Fe(7)	148.22(13)	S(8)-Fe(7)-Fe(8)	54.63(13)
S(7)-Fe(5)-Fe(7)	53.07(13)	S(6)-Fe(7)-Fe(8)	105.10(13)
S(6)-Fe(5)-Fe(7)	55.69(12)	P(3)-Fe(7)-Fe(8)	153.6(2)
S(5)-Fe(5)-Fe(7)	104.78(12)	S(7)-Fe(7)-Fe(5)	55.23(13)
Fe(6)-Fe(5)-Fe(7)	62.44(9)	S(8)-Fe(7)-Fe(5)	100.62(13)
Fe(8)-Fe(5)-Fe(7)	59.28(8)	S(6)-Fe(7)-Fe(5)	54.73(12)
S(1)-Fe(5)-Fe(1)	55.22(11)	P(3)-Fe(7)-Fe(5)	138.85(14)
S(7)-Fe(5)-Fe(1)	120.5(2)	Fe(8)-Fe(7)-Fe(5)	60.34(8)
S(6)-Fe(5)-Fe(1)	134.3(2)	S(7)-Fe(7)-Fe(6)	99.95(13)
S(5)-Fe(5)-Fe(1)	52.61(10)	S(8)-Fe(7)-Fe(6)	54.63(13)
Fe(6)-Fe(5)-Fe(1)	102.52(10)	S(6)-Fe(7)-Fe(6)	55.53(11)
Fe(8)-Fe(5)-Fe(1)	98.01(9)	P(3)-Fe(7)-Fe(6)	142.2(2)
Fe(7)-Fe(5)-Fe(1)	156.42(10)	Fe(8)-Fe(7)-Fe(6)	59.44(9)
S(6')-Fe(6)-S(8)	119.8(2)	Fe(5)-Fe(7)-Fe(6)	55.84(8)
S(6')-Fe(6)-S(5)	106.1(2)	S(7)-Fe(8)-S(8)	106.0(2)
S(8)-Fe(6)-S(5)	106.2(2)	S(7)-Fe(8)-S(5)	107.2(2)
S(6')-Fe(6)-S(6)	107.71(14)	S(8)-Fe(8)-S(5)	106.5(2)
S(8)-Fe(6)-S(6)	103.9(2)	S(7)-Fe(8)-P(4)	123.5(2)
S(5)-Fe(6)-S(6)	113.4(2)	S(8)-Fe(8)-P(4)	110.8(2)
S(6')-Fe(6)-Fe(5)	136.0(2)	S(5)-Fe(8)-P(4)	101.6(2)
S(8)-Fe(6)-Fe(5)	104.2(2)	S(7)-Fe(8)-Fe(7)	53.91(13)
S(5)-Fe(6)-Fe(5)	58.74(11)	S(8)-Fe(8)-Fe(7)	53.98(12)
S(6)-Fe(6)-Fe(5)	56.90(12)	S(5)-Fe(8)-Fe(7)	106.64(14)
S(6')-Fe(6)-Fe(8)	147.39(13)	P(4)-Fe(8)-Fe(7)	150.8(2)
S(8)-Fe(6)-Fe(8)	54.21(14)	S(7)-Fe(8)-Fe(6)	100.92(14)
S(5)-Fe(6)-Fe(8)	55.88(13)	S(8)-Fe(8)-Fe(6)	55.19(14)
S(6)-Fe(6)-Fe(8)	104.65(14)	S(5)-Fe(8)-Fe(6)	55.27(13)
Fe(5)-Fe(6)-Fe(8)	62.36(9)	P(4)-Fe(8)-Fe(6)	135.2(2)
S(6')-Fe(6)-Fe(7)	148.1(2)	Fe(7)-Fe(8)-Fe(6)	61.17(9)
S(8)-Fe(6)-Fe(7)	53.02(12)	S(7)-Fe(8)-Fe(5)	55.12(13)
S(5)-Fe(6)-Fe(7)	105.64(14)	S(8)-Fe(8)-Fe(5)	100.15(14)

Table S22. (Cont'd.)

S(5)-Fe(8)-Fe(5)	56.16(11)	C(3)-C(1)-P(1)	114.7(12)
P(4)-Fe(8)-Fe(5)	146.6(2)	C(5)-C(4)-C(6)	112(2)
Fe(7)-Fe(8)-Fe(5)	60.38(8)	C(5)-C(4)-P(1)	118(2)
Fe(6)-Fe(8)-Fe(5)	56.37(9)	C(6)-C(4)-P(1)	109.6(14)
Fe(5)-S(1)-Fe(4)	123.1(2)	C(9)-C(7)-C(8)	108(2)
Fe(5)-S(1)-Fe(2)	125.0(2)	C(9)-C(7)-P(1)	114.4(14)
Fe(4)-S(1)-Fe(2)	70.29(13)	C(8)-C(7)-P(1)	109.1(14)
Fe(5)-S(1)-Fe(1)	72.04(12)	C(10)-P(2)-C(13)	105.0(9)
Fe(4)-S(1)-Fe(1)	69.69(12)	C(10)-P(2)-C(16)	107.3(9)
Fe(2)-S(1)-Fe(1)	64.20(11)	C(13)-P(2)-C(16)	105.3(8)
Fe(2')-S(2)-Fe(1)	122.1(2)	C(10)-P(2)-Fe(4)	111.5(6)
Fe(2')-S(2)-Fe(3)	127.8(2)	C(13)-P(2)-Fe(4)	107.4(6)
Fe(1)-S(2)-Fe(3)	69.52(14)	C(16)-P(2)-Fe(4)	119.3(6)
Fe(2')-S(2)-Fe(2)	73.41(14)	C(12)-C(10)-C(11)	110(2)
Fe(1)-S(2)-Fe(2)	64.24(12)	C(12)-C(10)-P(2)	110.6(13)
Fe(3)-S(2)-Fe(2)	68.38(13)	C(11)-C(10)-P(2)	109.6(14)
Fe(3)-S(3)-Fe(4)	71.77(14)	C(14)-C(13)-C(15)	110(2)
Fe(3)-S(3)-Fe(1)	71.3(2)	C(14)-C(13)-P(2)	111.5(14)
Fe(4)-S(3)-Fe(1)	71.96(14)	C(15)-C(13)-P(2)	115.2(14)
Fe(3)-S(4)-Fe(4)	71.80(14)	C(18)-C(16)-C(17)	110(2)
Fe(3)-S(4)-Fe(2)	71.27(13)	C(18)-C(16)-P(2)	112.8(12)
Fe(4)-S(4)-Fe(2)	71.94(14)	C(17)-C(16)-P(2)	115.2(13)
Fe(1)-S(5)-Fe(6)	125.1(2)	C(19)-P(3)-C(25)	104.7(9)
Fe(1)-S(5)-Fe(8)	123.5(2)	C(19)-P(3)-C(22)	106.5(9)
Fe(6)-S(5)-Fe(8)	68.85(13)	C(25)-P(3)-C(22)	105.4(9)
Fe(1)-S(5)-Fe(5)	72.04(12)	C(19)-P(3)-Fe(7)	115.2(6)
Fe(6)-S(5)-Fe(5)	64.42(12)	C(25)-P(3)-Fe(7)	109.5(6)
Fe(8)-S(5)-Fe(5)	68.82(12)	C(22)-P(3)-Fe(7)	114.7(6)
Fe(6')-S(6)-Fe(5)	121.8(2)	C(20)-C(19)-C(21)	112(2)
Fe(6')-S(6)-Fe(7)	127.3(2)	C(20)-C(19)-P(3)	116.6(13)
Fe(5)-S(6)-Fe(7)	69.58(14)	C(21)-C(19)-P(3)	110.6(12)
Fe(6')-S(6)-Fe(6)	71.96(14)	C(24)-C(22)-C(23)	111(2)
Fe(5)-S(6)-Fe(6)	64.62(12)	C(24)-C(22)-P(3)	109.9(13)
Fe(7)-S(6)-Fe(6)	69.42(13)	C(23)-C(22)-P(3)	109.7(14)
Fe(7)-S(7)-Fe(8)	71.66(14)	C(27)-C(25)-C(26)	116(2)
Fe(7)-S(7)-Fe(5)	71.7(2)	C(27)-C(25)-P(3)	111.3(13)
Fe(8)-S(7)-Fe(5)	71.41(14)	C(26)-C(25)-P(3)	113(2)
Fe(7)-S(8)-Fe(8)	71.39(14)	C(28)-P(4)-C(34)	107.6(11)
Fe(7)-S(8)-Fe(6)	72.35(14)	C(28)-P(4)-C(31)	106.1(11)
Fe(8)-S(8)-Fe(6)	70.60(14)	C(34)-P(4)-C(31)	105.4(9)
C(7)-P(1)-C(4)	107.0(10)	C(28)-P(4)-Fe(8)	113.4(7)
C(7)-P(1)-C(1)	107.7(8)	C(34)-P(4)-Fe(8)	113.1(7)
C(4)-P(1)-C(1)	103.8(9)	C(31)-P(4)-Fe(8)	110.6(7)
C(7)-P(1)-Fe(3)	113.9(6)	C(29)-C(28)-C(30)	111(2)
C(4)-P(1)-Fe(3)	109.9(6)	C(29)-C(28)-P(4)	120(2)
C(1)-P(1)-Fe(3)	113.8(5)	C(30)-C(28)-P(4)	112(2)
C(2)-C(1)-C(3)	109(2)	C(32)-C(31)-C(33)	117(2)
C(2)-C(1)-P(1)	111.3(12)	C(32)-C(31)-P(4)	110.9(13)

Table S22. (Cont'd.)

C(33)-C(31)-P(4)	112(2)
C(36)-C(34)-C(35)	111(2)
C(36)-C(34)-P(4)	109(2)
C(35)-C(34)-P(4)	110.8(14)
N(1)-C(38)-C(37)	168(3)

Table S23. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$)
for $[\text{Fe}_{16}\text{S}_{16}(\text{P}^i\text{Pr}_3)_8] \cdot 2\text{MeCN}$.

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	25(1)	18(1)	22(1)	-2(1)	-2(1)	0(1)
Fe(2)	23(1)	21(1)	22(1)	-2(1)	-1(1)	0(1)
Fe(3)	33(2)	23(1)	28(1)	2(1)	-1(1)	-2(1)
Fe(4)	28(2)	23(1)	28(1)	1(1)	0(1)	0(1)
Fe(5)	27(2)	18(1)	23(1)	1(1)	1(1)	-1(1)
Fe(6)	26(1)	20(1)	24(1)	-2(1)	1(1)	-1(1)
Fe(7)	38(2)	22(1)	31(1)	2(1)	-2(1)	1(1)
Fe(8)	32(2)	25(1)	28(1)	2(1)	-3(1)	4(1)
S(1)	27(3)	21(2)	21(2)	3(2)	1(2)	0(2)
S(2)	22(2)	25(2)	24(2)	0(2)	-1(2)	-1(2)
S(3)	21(2)	29(2)	34(2)	0(2)	-5(2)	4(2)
S(4)	31(3)	19(2)	34(2)	0(2)	2(2)	-2(2)
S(5)	31(3)	21(2)	21(2)	-3(2)	2(2)	-1(2)
S(6)	28(3)	21(2)	24(2)	2(2)	-2(2)	1(2)
S(7)	25(3)	24(2)	36(2)	4(2)	7(2)	-3(2)
S(8)	38(3)	20(2)	32(2)	-5(2)	-2(2)	-3(2)
P(1)	47(3)	29(2)	30(2)	11(2)	1(2)	3(3)
C(2)	88(18)	70(15)	53(12)	23(11)	18(13)	22(14)
C(4)	73(16)	46(13)	68(13)	39(11)	9(13)	14(13)
C(5)	152(31)	158(31)	143(26)	109(24)	-2(24)	-41(26)
C(7)	83(18)	40(12)	41(10)	9(9)	-16(12)	13(13)
C(8)	281(45)	86(19)	52(14)	-24(13)	-81(21)	41(25)
C(9)	80(20)	87(18)	79(16)	-4(13)	-49(16)	5(17)
P(2)	33(3)	32(2)	22(2)	-1(2)	5(2)	-1(3)
C(11)	151(27)	41(13)	100(18)	28(12)	32(18)	49(17)
C(12)	27(11)	81(15)	34(10)	0(10)	4(9)	-19(11)
C(13)	66(16)	49(12)	37(10)	-16(9)	11(11)	-21(12)
C(15)	143(25)	77(15)	53(13)	-22(12)	27(16)	-36(19)
C(16)	63(15)	43(11)	32(9)	11(8)	5(10)	-25(11)
C(17)	97(19)	52(12)	30(10)	15(9)	12(12)	-9(14)
P(3)	47(3)	25(2)	29(2)	5(2)	3(2)	0(3)
C(19)	75(16)	26(10)	53(11)	-2(8)	0(12)	-8(12)
C(20)	100(21)	40(13)	116(19)	28(13)	6(17)	-33(15)
C(21)	48(14)	65(14)	68(13)	11(11)	-2(12)	-27(12)
C(22)	80(17)	42(11)	31(10)	-10(8)	20(11)	-7(13)
C(23)	103(22)	76(16)	65(14)	24(12)	45(14)	50(16)
C(24)	224(36)	73(16)	24(10)	-7(11)	15(16)	-3(21)
C(25)	51(13)	36(11)	48(10)	4(8)	-19(11)	11(11)
C(26)	85(20)	76(16)	72(15)	-3(12)	-28(14)	34(15)
P(4)	43(3)	37(3)	40(3)	3(2)	-13(3)	0(3)
C(28)	114(24)	63(15)	88(17)	17(13)	-52(17)	-28(16)
C(29)	192(40)	252(48)	191(37)	96(33)	-95(32)	-176(39)
C(30)	84(20)	92(19)	118(20)	27(16)	-9(17)	-69(17)
C(31)	119(22)	44(12)	26(9)	-5(8)	3(12)	29(14)

Table S23. (Cont'd.)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(32)	125(25)	100(20)	53(13)	-13(13)	35(15)	28(19)
C(33)	200(30)	46(12)	40(11)	-12(10)	-49(16)	13(18)
C(34)	27(13)	99(19)	88(17)	34(14)	-32(13)	9(13)
C(35)	76(17)	54(13)	52(12)	10(10)	0(12)	45(13)
C(36)	135(30)	200(35)	81(19)	67(21)	20(21)	68(27)

Table S24. Hydrogen Atom Coordinates ($\times 10^4$) and Isotropic Thermal Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}_{16}\text{S}_{16}(\text{P}^i\text{Pr}_3)_8] \cdot 2\text{MeCN}$.

atom	x/a	y/b	z/c	U(iso)
H(1A)	2042(11)	-454(5)	8179(6)	80
H(2A)	3409(13)	-445(6)	7846(7)	80
H(2B)	2885(13)	-54(6)	7631(7)	80
H(2C)	3534(13)	13(6)	8094(7)	80
H(3A)	3098(13)	-781(7)	8706(7)	80
H(3B)	3211(13)	-338(7)	8995(7)	80
H(3C)	2367(13)	-595(7)	9057(7)	80
H(4A)	506(13)	324(6)	8800(8)	80
H(5A)	140(18)	-282(9)	9249(10)	80
H(5B)	1029(18)	-479(9)	9126(10)	80
H(5C)	951(18)	-76(9)	9498(10)	80
H(6A)	-184(13)	-215(7)	8322(8)	80
H(6B)	349(13)	80(7)	7943(8)	80
H(6C)	692(13)	-374(7)	8109(8)	80
H(7A)	2377(14)	227(6)	9408(7)	80
H(8A)	2097(21)	969(8)	9671(8)	80
H(8B)	1823(21)	1061(8)	9082(8)	80
H(8C)	1310(21)	734(8)	9430(8)	80
H(9A)	3503(15)	693(7)	9413(8)	80
H(9B)	3643(15)	365(7)	8947(8)	80
H(9C)	3304(15)	828(7)	8824(8)	80
H(10A)	4627(12)	740(6)	6085(7)	80
H(11A)	4623(16)	217(6)	6794(9)	80
H(11B)	3763(16)	407(6)	6992(9)	80
H(11C)	3812(16)	169(6)	6442(9)	80
H(12A)	5297(11)	953(6)	6872(6)	80
H(12B)	4892(11)	1347(6)	6577(6)	80
H(12C)	4448(11)	1150(6)	7079(6)	80
H(13A)	2668(13)	405(6)	5939(6)	80
H(14A)	1725(15)	619(7)	5287(8)	80
H(14B)	1610(15)	887(7)	5812(8)	80
H(14C)	2103(15)	1085(7)	5329(8)	80
H(15A)	3085(17)	301(7)	5045(7)	80
H(15B)	3531(17)	750(7)	5070(7)	80
H(15C)	3859(17)	370(7)	5424(7)	80
H(16A)	3136(13)	1553(5)	5518(6)	80
H(17A)	4485(13)	1739(6)	5246(6)	80
H(17B)	4857(13)	1447(6)	5699(6)	80
H(17C)	4366(13)	1238(6)	5223(6)	80
H(18A)	3732(13)	2173(6)	5857(7)	80
H(18B)	3041(13)	1976(6)	6231(7)	80
H(18C)	3998(13)	1909(6)	6362(7)	80
H(19A)	2053(14)	4443(5)	6596(7)	80
H(20A)	3067(15)	4696(6)	6022(9)	80
H(20B)	3083(15)	4249(6)	5733(9)	80

Table S24. (Cont'd.)

atom	x/a	y/b	z/c	U(iso)
H(20C)	2279(15)	4540(6)	5699(9)	80
H(21A)	3444(12)	4387(6)	6881(7)	80
H(21B)	2861(12)	4046(6)	7156(7)	80
H(21C)	3434(12)	3910(6)	6675(7)	80
H(22A)	1990(14)	3762(6)	5397(6)	80
H(23A)	3042(14)	3233(7)	5323(8)	80
H(23B)	3275(14)	3574(7)	5760(8)	80
H(23C)	2923(14)	3122(7)	5928(8)	80
H(24A)	1509(19)	3074(7)	5153(7)	80
H(24B)	1370(19)	2972(7)	5759(7)	80
H(24C)	845(19)	3336(7)	5482(7)	80
H(25A)	289(12)	3733(6)	6164(6)	80
H(26A)	-23(14)	4372(7)	5750(7)	80
H(26B)	915(14)	4515(7)	5835(7)	80
H(26C)	705(14)	4134(7)	5446(7)	80
H(27A)	-246(13)	4246(6)	6713(7)	80
H(27B)	326(13)	3920(6)	7024(7)	80
H(27C)	678(13)	4375(6)	6868(7)	80
H(28A)	3721(17)	3580(7)	8846(9)	80
H(29A)	5157(20)	3637(11)	8901(13)	80
H(29B)	4823(20)	3275(11)	9282(13)	80
H(29C)	5236(20)	3152(11)	8735(13)	80
H(30A)	4453(15)	3852(8)	8108(9)	80
H(30B)	4377(15)	3395(8)	7847(9)	80
H(30C)	3565(15)	3670(8)	7952(9)	80
H(31A)	2463(15)	2624(6)	9296(6)	80
H(32A)	1756(16)	3221(7)	9601(8)	80
H(32B)	2314(16)	3502(7)	9220(8)	80
H(32C)	1691(16)	3160(7)	8983(8)	80
H(33A)	3008(17)	2902(6)	10087(7)	80
H(33B)	3681(17)	2649(6)	9754(7)	80
H(33C)	3681(17)	3153(6)	9751(7)	80
H(34A)	4482(12)	2469(7)	8927(9)	80
H(35A)	3928(14)	1771(6)	8839(7)	80
H(35B)	3307(14)	2062(6)	9164(7)	80
H(35C)	3127(14)	1963(6)	8562(7)	80
H(36A)	4830(17)	2104(10)	8155(9)	80
H(36B)	4060(17)	2310(10)	7858(9)	80
H(36C)	4808(17)	2601(10)	8050(9)	80
H(37A)	-411(14)	1713(6)	5904(7)	80
H(37B)	464(14)	1865(6)	5683(7)	80
H(37C)	-10(14)	2143(6)	6110(7)	80

Table S25. Summary of Crystal and Data Collection^a Parameters for [Fe₈S₆Cl₄(PCy₃)₄].3THF.

formula	C ₈₄ H ₁₅₆ Cl ₄ Fe ₈ O ₃ P ₄ S ₆
formula wt	2118.93
crystal system	tetragonal
space group	$I\bar{4}$
Z	2
a, Å	16.826(8)
c, Å	18.126(9)
V, Å ³	5132(4)
T, K	223
color	black
crystal habit	rhombahedron
d_{calc} , g/cm ³	1.371
μ , mm ⁻¹	1.427
scan type	ω
scan width, °	1.3
scan speed, °/min	10
2 θ range, °	3→45
data collected	7087
unique data	3380
data observed ($I > 2\sigma I$)	1975
no. of variables	231
wR2 ^b	.1808
R1 ^c	.0696

^aGraphite monochromated Mo K α ($\lambda = 0.71073$ Å) radiation.^bwR2 = $\{\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$. ^cR1 = $\sum||F_o| - |F_c||/\sum|F_o|$.

Table S26. Atomic Coordinates ($\times 10^4$) and Isotropic Thermal Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}_8\text{S}_6\text{Cl}_4(\text{PCy}_3)_4] \cdot 3\text{THF}$.

atom	x/a	y/b	z/c	U(iso)
Fe(1)	5785(1)	5783(1)	708(1)	33(1)
Fe(2)	5835(2)	4163(2)	746(1)	43(1)
S(1)	5000	5000	1424(2)	34(1)
S(2)	5001(2)	3406(2)	5(3)	34(1)
Cl	6618(4)	3388(4)	1418(3)	71(2)
P	6591(3)	6591(3)	1522(2)	33(1)
C(1)	5957(9)	7240(8)	2094(9)	51(4)
C(2)	5320(13)	6777(14)	2511(12)	105(8)
C(3)	4763(13)	7414(15)	2864(14)	108(9)
C(4)	5140(16)	8051(18)	3289(20)	134(13)
C(5)	5746(17)	8437(14)	2895(15)	161(14)
C(6)	6329(13)	7881(12)	2540(12)	101(8)
C(7)	7279(8)	7275(9)	1024(7)	42(4)
C(8)	6805(10)	7885(10)	579(10)	68(5)
C(9)	7420(12)	8443(11)	157(16)	99(8)
C(10)	8043(13)	8035(14)	-276(9)	91(7)
C(11)	8449(11)	7444(12)	172(12)	82(7)
C(12)	7882(10)	6818(10)	567(9)	68(5)
C(13)	7232(9)	5978(9)	2109(9)	52(4)
C(14)	7893(13)	6350(13)	2570(13)	110(8)
C(15)	8431(13)	5730(17)	2914(15)	163(14)
C(16)	8047(17)	5120(16)	3316(19)	117(11)
C(17)	7388(16)	4739(13)	2920(13)	105(8)
C(18)	6828(13)	5351(12)	2565(11)	83(6)
O(1)	5000	10000	5511(40)	350(34)
C(19)	4536(22)	10078(25)	4452(27)	196(16)
C(20)	4200(28)	9945(29)	5264(26)	264(24)
X(1) ^a	10269(72)	9830(83)	-972(32)	237(34)
X(2) ^a	10201(45)	9538(32)	-291(25)	177(26)

^as.o.f. = 0.5 C and 0.125 O.

Table S27. Interatomic Distances (Å) for
[Fe₈S₆Cl₄(PCy₃)₄]·3THF.

Fe(1)-S(1)	2.272(3)	X(2)-X(2G)	1.60(6)
Fe(1)-S(2A)	2.288(4)	X(2)-X(2E)	1.69(8)
Fe(1)-S(2B)	2.292(5)	X(2)-X(1E)	1.81(7)
Fe(1)-P	2.422(5)		
Fe(1)-Fe(2B)	2.638(3)		
Fe(1)-Fe(2)	2.727(4)		
Fe(1)-Fe(2A)	2.727(4)		
Fe(2)-Cl	2.219(6)		
Fe(2)-S(2)	2.323(5)		
Fe(2)-S(1)	2.338(3)		
Fe(2)-S(2B)	2.338(5)		
Fe(2)-Fe(1C)	2.638(3)		
Fe(2)-Fe(1A)	2.727(4)		
S(1)-Fe(1A)	2.272(3)		
S(1)-Fe(2A)	2.338(3)		
S(2)-Fe(1A)	2.288(4)		
S(2)-Fe(1C)	2.292(5)		
S(2)-Fe(2C)	2.338(5)		
P-C(13)	1.833(14)		
P-C(1)	1.844(14)		
P-C(7)	1.866(13)		
C(1)-C(6)	1.49(2)		
C(1)-C(2)	1.53(2)		
C(2)-C(3)	1.56(3)		
C(3)-C(4)	1.46(3)		
C(4)-C(5)	1.40(3)		
C(5)-C(6)	1.50(3)		
C(7)-C(12)	1.52(2)		
C(7)-C(8)	1.53(2)		
C(8)-C(9)	1.59(2)		
C(9)-C(10)	1.48(3)		
C(10)-C(11)	1.45(2)		
C(11)-C(12)	1.59(2)		
C(13)-C(18)	1.50(2)		
C(13)-C(14)	1.53(2)		
C(14)-C(15)	1.52(3)		
C(15)-C(16)	1.41(3)		
C(16)-C(17)	1.47(3)		
C(17)-C(18)	1.54(3)		
O(1)-C(20)	1.42(5)		
O(1)-C(20D)	1.42(5)		
C(19)-C(19D)	1.58(7)		
C(19)-C(20)	1.59(6)		
X(1)-X(1E)	1.1(2)		
X(1)-X(2)	1.33(8)		
X(1)-X(2E)	1.81(7)		
X(2)-X(2F)	1.60(6)		

Table S28. Bond Angles (deg) for $[\text{Fe}_8\text{S}_6\text{Cl}_4(\text{PCy}_3)_4] \cdot 3\text{THF}$.

S(1)-Fe(1)-S(2A)	109.17(14)	Fe(1A)-S(2)-Fe(1C)	106.95(14)
S(1)-Fe(1)-S(2B)	109.52(14)	Fe(1A)-S(2)-Fe(2)	72.52(14)
S(2A)-Fe(1)-S(2B)	111.80(11)	Fe(1C)-S(2)-Fe(2)	69.73(10)
S(1)-Fe(1)-P	107.7(2)	Fe(1A)-S(2)-Fe(2C)	69.52(10)
S(2A)-Fe(1)-P	109.2(2)	Fe(1C)-S(2)-Fe(2C)	72.2(2)
S(2B)-Fe(1)-P	109.4(2)	Fe(2)-S(2)-Fe(2C)	113.6(2)
S(1)-Fe(1)-Fe(2B)	127.51(14)	C(13)-P-C(1)	110.3(8)
S(2A)-Fe(1)-Fe(2B)	56.1(2)	C(13)-P-C(7)	105.3(7)
S(2B)-Fe(1)-Fe(2B)	55.7(2)	C(1)-P-C(7)	105.4(7)
P-Fe(1)-Fe(2B)	124.8(2)	C(13)-P-Fe(1)	111.5(5)
S(1)-Fe(1)-Fe(2)	54.85(9)	C(1)-P-Fe(1)	110.5(5)
S(2A)-Fe(1)-Fe(2)	128.87(14)	C(7)-P-Fe(1)	113.5(5)
S(2B)-Fe(1)-Fe(2)	54.70(11)	C(6)-C(1)-C(2)	113.3(14)
P-Fe(1)-Fe(2)	121.9(2)	C(6)-C(1)-P	119.5(12)
Fe(2B)-Fe(1)-Fe(2)	93.26(13)	C(2)-C(1)-P	112.5(11)
S(1)-Fe(1)-Fe(2A)	54.86(9)	C(1)-C(2)-C(3)	106(2)
S(2A)-Fe(1)-Fe(2A)	54.33(11)	C(4)-C(3)-C(2)	117(2)
S(2B)-Fe(1)-Fe(2A)	128.8(2)	C(5)-C(4)-C(3)	113(2)
P-Fe(1)-Fe(2A)	121.7(2)	C(4)-C(5)-C(6)	114(2)
Fe(2B)-Fe(1)-Fe(2A)	93.27(13)	C(5)-C(6)-C(1)	114(2)
Fe(2)-Fe(1)-Fe(2A)	93.64(11)	C(12)-C(7)-C(8)	113.6(13)
Cl-Fe(2)-S(2)	110.7(2)	C(12)-C(7)-P	111.5(10)
Cl-Fe(2)-S(1)	115.0(2)	C(8)-C(7)-P	110.2(10)
S(2)-Fe(2)-S(1)	105.76(13)	C(7)-C(8)-C(9)	108.1(14)
Cl-Fe(2)-S(2B)	110.4(2)	C(10)-C(9)-C(8)	116(2)
S(2)-Fe(2)-S(2B)	108.92(12)	C(11)-C(10)-C(9)	111(2)
S(1)-Fe(2)-S(2B)	105.72(14)	C(10)-C(11)-C(12)	115(2)
Cl-Fe(2)-Fe(1C)	126.0(2)	C(7)-C(12)-C(11)	108.1(13)
S(2)-Fe(2)-Fe(1C)	54.59(14)	C(18)-C(13)-C(14)	108.4(14)
S(1)-Fe(2)-Fe(1C)	119.04(14)	C(18)-C(13)-P	116.7(12)
S(2B)-Fe(2)-Fe(1C)	54.34(14)	C(14)-C(13)-P	121.1(12)
Cl-Fe(2)-Fe(1)	128.3(2)	C(15)-C(14)-C(13)	112(2)
S(2)-Fe(2)-Fe(1)	121.0(2)	C(16)-C(15)-C(14)	116(2)
S(1)-Fe(2)-Fe(1)	52.61(9)	C(15)-C(16)-C(17)	114(2)
S(2B)-Fe(2)-Fe(1)	53.13(10)	C(16)-C(17)-C(18)	112(2)
Fe(1C)-Fe(2)-Fe(1)	86.61(13)	C(13)-C(18)-C(17)	115(2)
Cl-Fe(2)-Fe(1A)	128.8(2)	C(20)-O(1)-C(20D)	143(8)
S(2)-Fe(2)-Fe(1A)	53.15(10)	C(19D)-C(19)-C(20)	109(2)
S(1)-Fe(2)-Fe(1A)	52.62(9)	O(1)-C(20)-C(19)	87(4)
S(2B)-Fe(2)-Fe(1A)	120.8(2)	X(1E)-X(1)-X(2)	97(9)
Fe(1C)-Fe(2)-Fe(1A)	86.62(13)	X(1E)-X(1)-X(2E)	47(5)
Fe(1)-Fe(2)-Fe(1A)	86.29(11)	X(2)-X(1)-X(2E)	63(4)
Fe(1A)-S(1)-Fe(1)	110.4(2)	X(1)-X(2)-X(2F)	109(8)
Fe(1A)-S(1)-Fe(2)	72.52(13)	X(1)-X(2)-X(2G)	125(6)
Fe(1)-S(1)-Fe(2)	72.53(13)	X(2F)-X(2)-X(2G)	64(3)
Fe(1A)-S(1)-Fe(2A)	72.53(13)	X(1)-X(2)-X(2E)	72(5)
Fe(1)-S(1)-Fe(2A)	72.52(13)	X(2F)-X(2)-X(2E)	58(2)
Fe(2)-S(1)-Fe(2A)	116.5(2)	X(2G)-X(2)-X(2E)	58(2)

Table S28. (Cont'd.)

X(1)-X(2)-X(1E)	36(6)
X(2F)-X(2)-X(1E)	99(5)
X(2G)-X(2)-X(1E)	89(4)
X(2E)-X(2)-X(1E)	45(3)

Table S29. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$)
for $[\text{Fe}_8\text{S}_6\text{Cl}_4(\text{PCy}_3)_4] \cdot 3\text{THF}$.

atom.	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	32(2)	32(2)	34(2)	-2(1)	-1(1)	-2(1)
Fe(2)	41(2)	43(2)	44(2)	-2(1)	1(1)	0(1)
S(1)	36(5)	39(5)	28(2)	0	0	-8(4)
S(2)	39(2)	29(2)	35(2)	-2(3)	7(3)	-1(1)
Cl	77(4)	73(4)	63(4)	13(3)	-10(3)	20(3)
P	32(3)	33(3)	33(2)	-2(2)	1(2)	-1(2)
C(1)	68(11)	30(8)	54(11)	-18(8)	23(9)	-4(8)
C(2)	80(16)	123(20)	112(18)	-43(15)	51(14)	15(14)
C(3)	60(15)	148(22)	117(20)	-82(18)	-3(14)	9(14)
C(4)	94(21)	156(28)	152(27)	-118(24)	35(19)	-12(18)
C(5)	209(29)	99(19)	175(27)	-109(19)	119(25)	-85(20)
C(6)	111(17)	90(16)	104(17)	-56(13)	53(13)	-13(13)
C(7)	26(8)	51(10)	49(9)	0(8)	6(7)	-9(7)
C(8)	68(12)	59(11)	76(13)	16(10)	-12(10)	-16(9)
C(9)	128(18)	67(12)	102(23)	13(13)	1(16)	-49(12)
C(10)	90(16)	128(20)	54(13)	11(13)	23(12)	-21(14)
C(11)	68(12)	107(15)	71(20)	2(12)	18(11)	-25(11)
C(12)	86(13)	65(12)	52(11)	-2(9)	33(10)	-12(10)
C(13)	54(10)	48(10)	55(11)	15(8)	-27(9)	2(8)
C(14)	105(17)	100(17)	126(19)	36(14)	-62(15)	-38(14)
C(15)	98(19)	207(29)	185(27)	120(25)	-118(20)	-72(20)
C(16)	136(26)	85(19)	130(24)	24(17)	-73(21)	-21(17)
C(17)	169(25)	58(15)	88(18)	27(14)	-23(17)	33(16)
C(18)	89(16)	86(16)	73(14)	12(12)	-12(11)	1(12)

Table S30. Hydrogen Atom Coordinates ($\times 10^4$) and Isotropic Thermal Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}_8\text{S}_6\text{Cl}_4(\text{PCy}_3)_4] \cdot 3\text{THF}$.

atom	x/a	y/b	z/c	U(iso)
H(1A)	5652(9)	7531(8)	1738(9)	80
H(2A)	5554(13)	6481(14)	2909(12)	80
H(2B)	5048(13)	6419(14)	2185(12)	80
H(3A)	4360(13)	7178(15)	3167(14)	80
H(3B)	4505(13)	7663(15)	2452(14)	80
H(4A)	5382(16)	7807(18)	3712(20)	80
H(4B)	4765(16)	8439(18)	3462(20)	80
H(5A)	6014(17)	8822(14)	3198(15)	80
H(5B)	5497(17)	8716(14)	2496(15)	80
H(6A)	6699(13)	8164(12)	2235(12)	80
H(6B)	6619(13)	7640(12)	2937(12)	80
H(7A)	7583(8)	7564(9)	1382(7)	80
H(8A)	6459(10)	8183(10)	896(10)	80
H(8B)	6488(10)	7608(10)	222(10)	80
H(9A)	7694(12)	8749(11)	524(16)	80
H(9B)	7133(12)	8806(11)	-153(16)	80
H(10A)	8408(13)	8405(14)	-493(9)	80
H(10B)	7780(13)	7753(14)	-666(9)	80
H(11A)	8721(11)	7731(12)	554(12)	80
H(11B)	8840(11)	7167(12)	-116(12)	80
H(12A)	7593(10)	6537(10)	192(9)	80
H(12B)	8168(10)	6439(10)	861(9)	80
H(13A)	7528(9)	5664(9)	1762(9)	80
H(14A)	7648(13)	6628(13)	2973(13)	80
H(14B)	8181(13)	6728(13)	2278(13)	80
H(15A)	8825(13)	5984(17)	3216(15)	80
H(15B)	8700(13)	5480(17)	2509(15)	80
H(16A)	7848(17)	5359(16)	3760(19)	80
H(16B)	8424(17)	4719(16)	3455(19)	80
H(17A)	7106(16)	4399(13)	3255(13)	80
H(17B)	7600(16)	4411(13)	2534(13)	80
H(18A)	6450(13)	5072(12)	2265(11)	80
H(18B)	6543(13)	5616(12)	2952(11)	80

Table S31. Summary of Crystal and Data Collection^a Parameters for [Fe₄S₄(PPrⁱ₃)₄](BPh₄).

formula	C ₆₀ H ₁₀₄ BFe ₄ P ₄ S ₄
formula wt	1311.76
crystal system	monoclinic
space group	<i>P</i> 2 ₁ / <i>c</i>
<i>Z</i>	4
<i>a</i> , Å	17.9899(2)
<i>b</i> , Å	17.3893(2)
<i>c</i> , Å	23.1191(1)
β , °	108.483(1)
<i>V</i> , Å ³	6859.3(1)
<i>T</i> , K	213
color	black
crystal habit	elongated hexagon
<i>d</i> _{calc} , g/cm ³	1.270
μ , mm ⁻¹	1.078
detector distance, cm	4.900
exposure time, s	30
2 θ range, °	3→54
data collected	40306
unique data	14740
data observed (<i>I</i> > 2 σ <i>I</i>)	11770
no. of variables	659
<i>wR</i> ^{2b}	.1043
<i>R</i> ^c	.0457

^aGraphite monochromated Mo K α (λ = 0.71073 Å) radiation.^b*wR*² = { $\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]$ }^{1/2}. ^c*R* = $\sum||F_o| - |F_c|| / \sum|F_o|$.

Table S32. Atomic Coordinates ($\times 10^4$) and Isotropic Thermal Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}_4\text{S}_4(\text{PPr}^i_3)_4](\text{BPh}_4)$.

atom	x/a	y/b	z/c	U(iso)
Fe(1)	2819(1)	3103(1)	1272(1)	30(1)
Fe(2)	2487(1)	1999(1)	1958(1)	29(1)
Fe(3)	2848(1)	1611(1)	953(1)	29(1)
Fe(4)	1478(1)	2315(1)	847(1)	33(1)
S(1)	3651(1)	2185(1)	1808(1)	31(1)
S(2)	1832(1)	3112(1)	1677(1)	38(1)
S(3)	2311(1)	2597(1)	315(1)	34(1)
S(4)	1846(1)	1126(1)	1231(1)	36(1)
P(1)	3362(1)	4349(1)	1248(1)	30(1)
P(2)	2571(1)	1550(1)	2952(1)	33(1)
P(3)	3566(1)	728(1)	545(1)	34(1)
P(4)	97(1)	2387(1)	319(1)	51(1)
C(1)	4178(2)	4273(2)	919(2)	51(1)
C(2)	4850(2)	3799(3)	1334(2)	68(1)
C(3)	4476(3)	5031(3)	719(3)	83(2)
C(4)	2667(2)	5058(2)	765(2)	42(1)
C(5)	1962(2)	5186(2)	991(2)	58(1)
C(6)	2396(3)	4808(3)	91(2)	69(1)
C(7)	3691(2)	4805(2)	2010(1)	43(1)
C(8)	4035(3)	4238(2)	2528(2)	56(1)
C(9)	4210(3)	5515(2)	2076(2)	77(2)
C(10)	2428(2)	490(2)	2901(2)	44(1)
C(11)	3137(2)	103(2)	2791(2)	57(1)
C(12)	2195(3)	85(2)	3410(2)	63(1)
C(13)	3545(2)	1716(2)	3543(2)	51(1)
C(14)	3585(3)	1495(3)	4197(2)	72(1)
C(15)	3869(3)	2514(3)	3504(2)	70(1)
C(16)	1788(2)	1929(2)	3232(2)	51(1)
C(17)	1868(3)	2796(2)	3360(2)	68(1)
C(18)	991(2)	1744(3)	2757(2)	71(1)
C(19)	3757(4)	-201(2)	945(4)	117(3)
C(20)	4371(3)	-721(2)	801(2)	72(1)
C(21)	3401(6)	-435(4)	1320(4)	185(5)
C(22)	4533(2)	1095(2)	550(1)	38(1)
C(23)	4440(3)	1873(2)	220(2)	65(1)
C(24)	5113(2)	1176(2)	1189(2)	53(1)
C(25)	3030(3)	553(5)	-273(2)	125(3)
C(26)	2209(3)	464(3)	-445(2)	84(2)
C(27)	3474(3)	188(3)	-654(2)	83(2)
C(28)	-439(3)	3083(3)	683(2)	72(1)
C(29)	-1323(3)	3103(4)	385(3)	111(2)
C(30)	-103(3)	3902(3)	767(3)	93(2)
C(31)	-352(3)	1448(3)	343(3)	89(2)
C(32)	-1149(4)	1291(5)	-165(4)	154(3)
C(33)	-362(3)	1264(3)	997(3)	97(2)

Table S32. (Cont'd.)

atom	x/a	y/b	z/c	U(iso)
C(34)	-129(3)	2677(5)	-484(2)	112(2)
C(35)	235(3)	2076(5)	-806(2)	131(3)
C(36)	194(4)	3492(5)	-554(3)	141(3)
C(37)	2902(2)	7360(2)	2299(1)	29(1)
C(38)	3708(2)	7517(2)	2519(1)	32(1)
C(39)	4176(2)	7552(2)	2141(2)	38(1)
C(40)	3851(2)	7436(2)	1519(2)	38(1)
C(41)	3056(2)	7273(2)	1279(1)	40(1)
C(42)	2602(2)	7235(2)	1665(1)	35(1)
C(43)	1915(2)	6439(2)	2592(1)	31(1)
C(44)	1121(2)	6285(2)	2286(2)	43(1)
C(45)	822(2)	5535(2)	2185(2)	53(1)
C(46)	1307(2)	4913(2)	2387(2)	49(1)
C(47)	2094(2)	5040(2)	2682(2)	43(1)
C(48)	2387(2)	5784(2)	2780(1)	36(1)
C(49)	1629(2)	7991(2)	2498(1)	32(1)
C(50)	1619(2)	8577(2)	2079(1)	36(1)
C(51)	1057(2)	9163(2)	1936(2)	45(1)
C(52)	472(2)	9175(2)	2204(2)	54(1)
C(53)	455(2)	8612(2)	2616(2)	54(1)
C(54)	1026(2)	8038(2)	2763(2)	43(1)
C(55)	2746(2)	7457(2)	3449(1)	31(1)
C(56)	3134(2)	8154(2)	3650(1)	39(1)
C(57)	3478(2)	8336(2)	4266(2)	48(1)
C(58)	3445(2)	7821(2)	4710(2)	52(1)
C(59)	3066(2)	7130(2)	4536(2)	52(1)
C(60)	2721(2)	6953(2)	3919(2)	41(1)
B(1)	2301(2)	7306(2)	2712(2)	30(1)

Table S33. Interatomic Distances (Å) for
[Fe₄S₄(PPrⁱ₃)₄](BPh₄).

Fe(1)-S(2)	2.2541(9)	C(22)-C(24)	1.522(5)
Fe(1)-S(1)	2.2695(8)	C(22)-C(23)	1.535(5)
Fe(1)-S(3)	2.2854(8)	C(25)-C(26)	1.410(6)
Fe(1)-P(1)	2.3844(9)	C(25)-C(27)	1.505(6)
Fe(1)-Fe(2)	2.6763(6)	C(28)-C(29)	1.521(6)
Fe(1)-Fe(4)	2.6768(6)	C(28)-C(30)	1.535(7)
Fe(1)-Fe(3)	2.7023(6)	C(31)-C(33)	1.552(8)
Fe(2)-S(2)	2.2510(9)	C(31)-C(32)	1.563(7)
Fe(2)-S(1)	2.2520(8)	C(34)-C(35)	1.544(9)
Fe(2)-S(4)	2.2884(9)	C(34)-C(36)	1.560(10)
Fe(2)-P(2)	2.3854(8)	C(37)-C(38)	1.402(4)
Fe(2)-Fe(4)	2.6908(6)	C(37)-C(42)	1.408(4)
Fe(2)-Fe(3)	2.6911(6)	C(37)-B(1)	1.657(4)
Fe(3)-S(4)	2.2611(9)	C(38)-C(39)	1.396(4)
Fe(3)-S(3)	2.2682(8)	C(39)-C(40)	1.385(5)
Fe(3)-S(1)	2.2763(8)	C(40)-C(41)	1.389(5)
Fe(3)-P(3)	2.3848(9)	C(41)-C(42)	1.390(4)
Fe(3)-Fe(4)	2.6936(6)	C(43)-C(48)	1.404(4)
Fe(4)-S(4)	2.2643(9)	C(43)-C(44)	1.405(4)
Fe(4)-S(3)	2.2758(9)	C(43)-B(1)	1.647(4)
Fe(4)-S(2)	2.2871(9)	C(44)-C(45)	1.402(5)
Fe(4)-P(4)	2.3980(9)	C(45)-C(46)	1.375(5)
P(1)-C(7)	1.850(3)	C(46)-C(47)	1.380(5)
P(1)-C(4)	1.857(3)	C(47)-C(48)	1.388(4)
P(1)-C(1)	1.859(3)	C(49)-C(50)	1.401(4)
P(2)-C(16)	1.848(4)	C(49)-C(54)	1.407(4)
P(2)-C(10)	1.860(3)	C(49)-B(1)	1.658(4)
P(2)-C(13)	1.871(4)	C(50)-C(51)	1.401(4)
P(3)-C(19)	1.840(4)	C(51)-C(52)	1.380(5)
P(3)-C(22)	1.849(3)	C(52)-C(53)	1.373(5)
P(3)-C(25)	1.855(4)	C(53)-C(54)	1.395(5)
P(4)-C(31)	1.829(5)	C(55)-C(56)	1.401(4)
P(4)-C(34)	1.841(5)	C(55)-C(60)	1.407(4)
P(4)-C(28)	1.902(5)	C(55)-B(1)	1.657(4)
C(1)-C(2)	1.525(5)	C(56)-C(57)	1.397(4)
C(1)-C(3)	1.548(5)	C(57)-C(58)	1.379(5)
C(4)-C(5)	1.533(5)	C(58)-C(59)	1.376(6)
C(4)-C(6)	1.541(5)	C(59)-C(60)	1.398(5)
C(7)-C(8)	1.522(5)		
C(7)-C(9)	1.526(5)		
C(10)-C(11)	1.534(5)		
C(10)-C(12)	1.538(5)		
C(13)-C(15)	1.519(5)		
C(13)-C(14)	1.539(5)		
C(16)-C(17)	1.535(5)		
C(16)-C(18)	1.537(6)		
C(19)-C(21)	1.296(7)		
C(19)-C(20)	1.544(5)		

Table S34. Bond Angles (deg) for $[\text{Fe}_4\text{S}_4(\text{PPr}^i_3)_4](\text{BPh}_4)$.

S(2)-Fe(1)-S(1)	104.33(3)	S(4)-Fe(3)-Fe(2)	54.21(2)
S(2)-Fe(1)-S(3)	106.22(3)	S(3)-Fe(3)-Fe(2)	101.69(3)
S(1)-Fe(1)-S(3)	104.48(3)	S(1)-Fe(3)-Fe(2)	53.12(2)
S(2)-Fe(1)-P(1)	112.72(3)	P(3)-Fe(3)-Fe(2)	144.35(3)
S(1)-Fe(1)-P(1)	116.57(3)	S(4)-Fe(3)-Fe(4)	53.53(2)
S(3)-Fe(1)-P(1)	111.62(3)	S(3)-Fe(3)-Fe(4)	53.78(2)
S(2)-Fe(1)-Fe(2)	53.50(2)	S(1)-Fe(3)-Fe(4)	100.95(2)
S(1)-Fe(1)-Fe(2)	53.41(2)	P(3)-Fe(3)-Fe(4)	148.35(3)
S(3)-Fe(1)-Fe(2)	101.68(3)	Fe(2)-Fe(3)-Fe(4)	59.96(2)
P(1)-Fe(1)-Fe(2)	146.66(3)	S(4)-Fe(3)-Fe(1)	101.21(3)
S(2)-Fe(1)-Fe(4)	54.45(2)	S(3)-Fe(3)-Fe(1)	53.89(2)
S(1)-Fe(1)-Fe(4)	101.64(3)	S(1)-Fe(3)-Fe(1)	53.41(2)
S(3)-Fe(1)-Fe(4)	53.90(2)	P(3)-Fe(3)-Fe(1)	141.84(3)
P(1)-Fe(1)-Fe(4)	141.78(3)	Fe(2)-Fe(3)-Fe(1)	59.50(2)
Fe(2)-Fe(1)-Fe(4)	60.35(2)	Fe(4)-Fe(3)-Fe(1)	59.48(2)
S(2)-Fe(1)-Fe(3)	101.88(3)	S(4)-Fe(4)-S(3)	104.34(3)
S(1)-Fe(1)-Fe(3)	53.64(2)	S(4)-Fe(4)-S(2)	104.82(3)
S(3)-Fe(1)-Fe(3)	53.30(2)	S(3)-Fe(4)-S(2)	105.44(3)
P(1)-Fe(1)-Fe(3)	145.31(3)	S(4)-Fe(4)-P(4)	112.02(4)
Fe(2)-Fe(1)-Fe(3)	60.04(2)	S(3)-Fe(4)-P(4)	117.84(3)
Fe(4)-Fe(1)-Fe(3)	60.10(2)	S(2)-Fe(4)-P(4)	111.32(4)
S(2)-Fe(2)-S(1)	105.01(3)	S(4)-Fe(4)-Fe(1)	101.90(3)
S(2)-Fe(2)-S(4)	105.21(3)	S(3)-Fe(4)-Fe(1)	54.23(2)
S(1)-Fe(2)-S(4)	104.97(3)	S(2)-Fe(4)-Fe(1)	53.31(2)
S(2)-Fe(2)-P(2)	115.31(3)	P(4)-Fe(4)-Fe(1)	145.82(3)
S(1)-Fe(2)-P(2)	114.66(3)	S(4)-Fe(4)-Fe(2)	54.19(2)
S(4)-Fe(2)-P(2)	110.74(3)	S(3)-Fe(4)-Fe(2)	101.50(3)
S(2)-Fe(2)-Fe(1)	53.61(2)	S(2)-Fe(4)-Fe(2)	53.02(2)
S(1)-Fe(2)-Fe(1)	54.01(2)	P(4)-Fe(4)-Fe(2)	140.65(3)
S(4)-Fe(2)-Fe(1)	101.26(3)	Fe(1)-Fe(4)-Fe(2)	59.81(2)
P(2)-Fe(2)-Fe(1)	148.00(3)	S(4)-Fe(4)-Fe(3)	53.42(2)
S(2)-Fe(2)-Fe(4)	54.26(2)	S(3)-Fe(4)-Fe(3)	53.51(2)
S(1)-Fe(2)-Fe(4)	101.69(2)	S(2)-Fe(4)-Fe(3)	101.25(3)
S(4)-Fe(2)-Fe(4)	53.36(2)	P(4)-Fe(4)-Fe(3)	147.21(3)
P(2)-Fe(2)-Fe(4)	143.49(3)	Fe(1)-Fe(4)-Fe(3)	60.42(2)
Fe(1)-Fe(2)-Fe(4)	59.83(2)	Fe(2)-Fe(4)-Fe(3)	59.97(2)
S(2)-Fe(2)-Fe(3)	102.30(3)	Fe(2)-S(1)-Fe(1)	72.58(3)
S(1)-Fe(2)-Fe(3)	53.95(2)	Fe(2)-S(1)-Fe(3)	72.92(3)
S(4)-Fe(2)-Fe(3)	53.27(2)	Fe(1)-S(1)-Fe(3)	72.95(3)
P(2)-Fe(2)-Fe(3)	142.29(3)	Fe(2)-S(2)-Fe(1)	72.89(3)
Fe(1)-Fe(2)-Fe(3)	60.46(2)	Fe(2)-S(2)-Fe(4)	72.73(3)
Fe(4)-Fe(2)-Fe(3)	60.07(2)	Fe(1)-S(2)-Fe(4)	72.23(3)
S(4)-Fe(3)-S(3)	104.69(3)	Fe(3)-S(3)-Fe(4)	72.71(3)
S(4)-Fe(3)-S(1)	105.07(3)	Fe(3)-S(3)-Fe(1)	72.80(3)
S(3)-Fe(3)-S(1)	104.82(3)	Fe(4)-S(3)-Fe(1)	71.87(3)
S(4)-Fe(3)-P(3)	116.89(3)	Fe(3)-S(4)-Fe(4)	73.06(3)
S(3)-Fe(3)-P(3)	113.69(3)	Fe(3)-S(4)-Fe(2)	72.53(3)
S(1)-Fe(3)-P(3)	110.64(3)	Fe(4)-S(4)-Fe(2)	72.46(3)

Table S34. (Cont'd.)

C(7)-P(1)-C(4)	103.8(2)	C(26)-C(25)-C(27)	119.5(4)
C(7)-P(1)-C(1)	111.3(2)	C(26)-C(25)-P(3)	117.7(4)
C(4)-P(1)-C(1)	105.7(2)	C(27)-C(25)-P(3)	117.7(3)
C(7)-P(1)-Fe(1)	112.17(11)	C(29)-C(28)-C(30)	110.5(4)
C(4)-P(1)-Fe(1)	114.48(12)	C(29)-C(28)-P(4)	114.7(4)
C(1)-P(1)-Fe(1)	109.13(12)	C(30)-C(28)-P(4)	114.3(3)
C(16)-P(2)-C(10)	105.6(2)	C(33)-C(31)-C(32)	113.9(5)
C(16)-P(2)-C(13)	109.3(2)	C(33)-C(31)-P(4)	110.8(4)
C(10)-P(2)-C(13)	106.2(2)	C(32)-C(31)-P(4)	116.2(5)
C(16)-P(2)-Fe(2)	113.44(13)	C(35)-C(34)-C(36)	109.6(5)
C(10)-P(2)-Fe(2)	107.32(11)	C(35)-C(34)-P(4)	108.0(5)
C(13)-P(2)-Fe(2)	114.33(12)	C(36)-C(34)-P(4)	112.6(4)
C(19)-P(3)-C(22)	105.9(2)	C(38)-C(37)-C(42)	114.8(3)
C(19)-P(3)-C(25)	108.8(4)	C(38)-C(37)-B(1)	126.1(3)
C(22)-P(3)-C(25)	104.3(2)	C(42)-C(37)-B(1)	119.1(2)
C(19)-P(3)-Fe(3)	113.9(2)	C(39)-C(38)-C(37)	122.7(3)
C(22)-P(3)-Fe(3)	113.67(10)	C(40)-C(39)-C(38)	120.3(3)
C(25)-P(3)-Fe(3)	109.7(2)	C(39)-C(40)-C(41)	119.1(3)
C(31)-P(4)-C(34)	108.4(3)	C(40)-C(41)-C(42)	119.6(3)
C(31)-P(4)-C(28)	105.3(2)	C(41)-C(42)-C(37)	123.4(3)
C(34)-P(4)-C(28)	106.9(3)	C(48)-C(43)-C(44)	114.8(3)
C(31)-P(4)-Fe(4)	109.5(2)	C(48)-C(43)-B(1)	120.6(3)
C(34)-P(4)-Fe(4)	113.0(2)	C(44)-C(43)-B(1)	124.6(3)
C(28)-P(4)-Fe(4)	113.4(2)	C(45)-C(44)-C(43)	122.5(3)
C(2)-C(1)-C(3)	111.6(3)	C(46)-C(45)-C(44)	120.4(3)
C(2)-C(1)-P(1)	110.6(3)	C(45)-C(46)-C(47)	118.8(3)
C(3)-C(1)-P(1)	117.1(3)	C(46)-C(47)-C(48)	120.5(3)
C(5)-C(4)-C(6)	110.8(3)	C(47)-C(48)-C(43)	123.0(3)
C(5)-C(4)-P(1)	111.3(2)	C(50)-C(49)-C(54)	114.6(3)
C(6)-C(4)-P(1)	111.0(2)	C(50)-C(49)-B(1)	125.2(3)
C(8)-C(7)-C(9)	111.3(3)	C(54)-C(49)-B(1)	120.1(3)
C(8)-C(7)-P(1)	113.5(2)	C(49)-C(50)-C(51)	122.8(3)
C(9)-C(7)-P(1)	116.3(3)	C(52)-C(51)-C(50)	120.1(3)
C(11)-C(10)-C(12)	111.6(3)	C(53)-C(52)-C(51)	119.2(3)
C(11)-C(10)-P(2)	109.8(2)	C(52)-C(53)-C(54)	120.2(3)
C(12)-C(10)-P(2)	118.1(3)	C(53)-C(54)-C(49)	123.0(3)
C(15)-C(13)-C(14)	112.8(3)	C(56)-C(55)-C(60)	114.7(3)
C(15)-C(13)-P(2)	112.7(3)	C(56)-C(55)-B(1)	120.3(3)
C(14)-C(13)-P(2)	114.9(3)	C(60)-C(55)-B(1)	124.8(3)
C(17)-C(16)-C(18)	110.6(4)	C(57)-C(56)-C(55)	123.1(3)
C(17)-C(16)-P(2)	112.4(3)	C(58)-C(57)-C(56)	120.2(3)
C(18)-C(16)-P(2)	108.5(3)	C(59)-C(58)-C(57)	118.9(3)
C(21)-C(19)-C(20)	120.0(4)	C(58)-C(59)-C(60)	120.6(3)
C(21)-C(19)-P(3)	124.0(4)	C(59)-C(60)-C(55)	122.5(3)
C(20)-C(19)-P(3)	116.0(3)	C(43)-B(1)-C(49)	112.2(2)
C(24)-C(22)-C(23)	109.5(3)	C(43)-B(1)-C(37)	105.7(2)
C(24)-C(22)-P(3)	113.1(2)	C(49)-B(1)-C(37)	109.6(2)
C(23)-C(22)-P(3)	110.3(2)	C(43)-B(1)-C(55)	111.0(2)

Table S34. (Cont'd.)

C(49)-B(1)-C(55)	105.2(2)
C(37)-B(1)-C(55)	113.2(2)

Table S35. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$)
for $[\text{Fe}_4\text{S}_4(\text{PPr}^i_3)_4](\text{BPh}_4)$.

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	32(1)	25(1)	31(1)	0(1)	9(1)	1(1)
Fe(2)	32(1)	30(1)	27(1)	1(1)	10(1)	2(1)
Fe(3)	30(1)	27(1)	29(1)	-2(1)	9(1)	2(1)
Fe(4)	25(1)	40(1)	33(1)	2(1)	5(1)	2(1)
S(1)	27(1)	33(1)	30(1)	-1(1)	5(1)	2(1)
S(2)	39(1)	35(1)	41(1)	-1(1)	16(1)	9(1)
S(3)	35(1)	36(1)	29(1)	3(1)	7(1)	3(1)
S(4)	37(1)	35(1)	36(1)	-1(1)	11(1)	-6(1)
P(1)	35(1)	26(1)	29(1)	2(1)	10(1)	3(1)
P(2)	38(1)	34(1)	28(1)	-2(1)	13(1)	-6(1)
P(3)	34(1)	31(1)	37(1)	-7(1)	10(1)	1(1)
P(4)	27(1)	82(1)	41(1)	7(1)	4(1)	-1(1)
C(1)	53(2)	50(2)	61(2)	12(2)	34(2)	6(2)
C(2)	48(2)	69(3)	100(3)	20(3)	41(2)	11(2)
C(3)	86(3)	78(3)	106(4)	33(3)	58(3)	1(3)
C(4)	54(2)	31(2)	38(2)	7(1)	11(2)	7(1)
C(5)	49(2)	58(2)	63(2)	14(2)	13(2)	22(2)
C(6)	94(3)	64(3)	36(2)	7(2)	3(2)	30(2)
C(7)	54(2)	36(2)	33(2)	-5(1)	6(2)	6(2)
C(8)	82(3)	41(2)	34(2)	-1(2)	3(2)	-1(2)
C(9)	115(4)	34(2)	58(3)	-3(2)	-5(2)	-19(2)
C(10)	59(2)	36(2)	38(2)	1(1)	15(2)	-9(2)
C(11)	80(3)	38(2)	56(2)	2(2)	27(2)	6(2)
C(12)	96(3)	50(2)	48(2)	3(2)	30(2)	-19(2)
C(13)	54(2)	57(2)	36(2)	0(2)	6(2)	-12(2)
C(14)	94(3)	73(3)	36(2)	3(2)	2(2)	-24(3)
C(15)	74(3)	90(3)	44(2)	-10(2)	16(2)	-40(3)
C(16)	60(2)	58(2)	49(2)	-5(2)	34(2)	-2(2)
C(17)	84(3)	60(3)	75(3)	-17(2)	46(3)	5(2)
C(18)	49(2)	85(3)	90(3)	-2(3)	37(2)	1(2)
C(19)	117(4)	37(2)	255(8)	55(4)	141(5)	36(3)
C(20)	66(3)	34(2)	128(4)	6(2)	47(3)	16(2)
C(21)	329(11)	122(5)	199(8)	121(6)	221(9)	161(7)
C(22)	40(2)	37(2)	39(2)	-2(1)	16(1)	3(1)
C(23)	81(3)	52(2)	73(3)	16(2)	40(2)	-3(2)
C(24)	38(2)	61(2)	53(2)	-15(2)	5(2)	2(2)
C(25)	48(3)	244(8)	72(3)	-102(4)	2(2)	6(4)
C(26)	63(3)	127(5)	51(2)	-20(3)	4(2)	-1(3)
C(27)	72(3)	123(4)	53(2)	-48(3)	17(2)	-2(3)
C(28)	52(2)	86(3)	76(3)	23(3)	19(2)	11(2)
C(29)	45(3)	107(5)	180(7)	15(4)	35(3)	10(3)
C(30)	74(3)	73(3)	120(5)	7(3)	14(3)	14(3)
C(31)	56(3)	88(4)	109(4)	-14(3)	6(3)	-19(3)
C(32)	83(4)	178(8)	175(8)	-30(6)	4(5)	-64(5)
C(33)	71(3)	93(4)	132(5)	29(4)	38(3)	-19(3)

Table S35. (Cont'd.)

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(34)	43(3)	227(8)	57(3)	18(4)	2(2)	-9(4)
C(35)	80(4)	250(9)	65(3)	-65(5)	27(3)	-53(5)
C(36)	109(5)	186(8)	126(6)	106(6)	36(4)	20(5)
C(37)	28(1)	25(1)	31(1)	2(1)	7(1)	1(1)
C(38)	30(1)	32(2)	32(2)	0(1)	7(1)	-1(1)
C(39)	29(2)	34(2)	51(2)	0(1)	13(1)	-3(1)
C(40)	43(2)	36(2)	42(2)	6(1)	23(2)	2(1)
C(41)	47(2)	43(2)	30(2)	2(1)	13(1)	3(1)
C(42)	29(2)	42(2)	34(2)	0(1)	9(1)	-2(1)
C(43)	31(2)	33(2)	32(2)	1(1)	14(1)	0(1)
C(44)	31(2)	38(2)	57(2)	-1(2)	11(2)	-1(1)
C(45)	33(2)	49(2)	76(3)	-7(2)	15(2)	-11(2)
C(46)	51(2)	35(2)	70(2)	-6(2)	33(2)	-11(2)
C(47)	49(2)	32(2)	51(2)	3(1)	23(2)	5(1)
C(48)	35(2)	32(2)	41(2)	1(1)	12(1)	3(1)
C(49)	33(2)	30(2)	33(2)	-3(1)	8(1)	0(1)
C(50)	36(2)	33(2)	36(2)	-1(1)	7(1)	1(1)
C(51)	52(2)	34(2)	41(2)	2(1)	2(2)	7(2)
C(52)	51(2)	47(2)	57(2)	-6(2)	8(2)	24(2)
C(53)	47(2)	60(2)	60(2)	0(2)	23(2)	17(2)
C(54)	46(2)	41(2)	46(2)	3(2)	19(2)	9(2)
C(55)	29(1)	33(2)	34(2)	2(1)	12(1)	4(1)
C(56)	47(2)	40(2)	33(2)	-1(1)	15(1)	-4(1)
C(57)	50(2)	57(2)	39(2)	-14(2)	17(2)	-9(2)
C(58)	46(2)	81(3)	27(2)	-5(2)	9(2)	7(2)
C(59)	62(2)	62(2)	37(2)	14(2)	21(2)	15(2)
C(60)	50(2)	40(2)	38(2)	7(1)	20(2)	6(2)
B(1)	27(2)	33(2)	28(2)	1(1)	8(1)	1(1)

Table S36. Hydrogen Atom Coordinates ($\times 10^4$) and Isotropic Thermal Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}_4\text{S}_4(\text{PPr}^i_3)_4](\text{BPh}_4)$.

atom	x/a	y/b	z/c	U(iso)
H(1A)	3970(2)	3969(2)	546(2)	61
H(2A)	4646(2)	3335(3)	1450(2)	102
H(2B)	5114(2)	4091(3)	1693(2)	102
H(2C)	5213(2)	3672(3)	1121(2)	102
H(3A)	4040(3)	5315(3)	459(3)	125
H(3B)	4836(3)	4915(3)	501(3)	125
H(3C)	4737(3)	5333(3)	1073(3)	125
H(4A)	2943(2)	5550(2)	795(2)	50
H(5A)	2143(2)	5342(2)	1411(2)	86
H(5B)	1669(2)	4717(2)	953(2)	86
H(5C)	1631(2)	5580(2)	751(2)	86
H(6A)	2845(3)	4732(3)	-41(2)	103
H(6B)	2067(3)	5200(3)	-153(2)	103
H(6C)	2106(3)	4337(3)	48(2)	103
H(7A)	3210(2)	4993(2)	2074(1)	51
H(8A)	3697(3)	3798(2)	2475(2)	84
H(8B)	4080(3)	4481(2)	2910(2)	84
H(8C)	4544(3)	4077(2)	2525(2)	84
H(9A)	3980(3)	5861(2)	1745(2)	115
H(9B)	4720(3)	5363(2)	2070(2)	115
H(9C)	4256(3)	5767(2)	2455(2)	115
H(10A)	1989(2)	403(2)	2527(2)	53
H(11A)	3267(2)	369(2)	2472(2)	85
H(11B)	3013(2)	-423(2)	2674(2)	85
H(11C)	3576(2)	121(2)	3159(2)	85
H(12A)	1751(3)	341(2)	3467(2)	94
H(12B)	2627(3)	103(2)	3782(2)	94
H(12C)	2064(3)	-441(2)	3297(2)	94
H(13A)	3905(2)	1362(2)	3437(2)	61
H(14A)	3374(3)	988(3)	4197(2)	108
H(14B)	3286(3)	1856(3)	4347(2)	108
H(14C)	4121(3)	1503(3)	4456(2)	108
H(15A)	3830(3)	2623(3)	3088(2)	105
H(15B)	4409(3)	2535(3)	3754(2)	105
H(15C)	3573(3)	2888(3)	3645(2)	105
H(16A)	1818(2)	1663(2)	3612(2)	62
H(17A)	2368(3)	2900(2)	3657(2)	103
H(17B)	1458(3)	2964(2)	3514(2)	103
H(17C)	1829(3)	3066(2)	2989(2)	103
H(18A)	951(2)	1200(3)	2683(2)	106
H(18B)	948(2)	2010(3)	2384(2)	106
H(18C)	578(2)	1908(3)	2909(2)	106
H(19A)	4168(4)	35(2)	1283(4)	141
H(20A)	4578(3)	-464(2)	517(2)	108
H(20B)	4129(3)	-1195(2)	625(2)	108
H(20C)	4789(3)	-828(2)	1170(2)	108

Table S36. (Cont'd.)

atom	x/a	y/b	z/c	U(iso)
H(21A)	3041(6)	-46(4)	1359(4)	277
H(21B)	3779(6)	-531(4)	1712(4)	277
H(21C)	3119(6)	-899(4)	1168(4)	277
H(22A)	4752(2)	729(2)	325(1)	46
H(23A)	4074(3)	1822(2)	-183(2)	97
H(23B)	4938(3)	2035(2)	194(2)	97
H(23C)	4249(3)	2248(2)	444(2)	97
H(24A)	5171(2)	689(2)	1395(2)	79
H(24B)	4922(2)	1551(2)	1412(2)	79
H(24C)	5611(2)	1338(2)	1163(2)	79
H(25A)	3037(3)	1082(5)	-417(2)	150
H(26A)	2014(3)	730(3)	-159(2)	126
H(26B)	2082(3)	-72(3)	-447(2)	126
H(26C)	1974(3)	675(3)	-845(2)	126
H(27A)	4022(3)	300(3)	-480(2)	124
H(27B)	3286(3)	389(3)	-1061(2)	124
H(27C)	3397(3)	-359(3)	-665(2)	124
H(28A)	-354(3)	2887(3)	1097(2)	86
H(29A)	-1524(3)	2587(4)	335(3)	166
H(29B)	-1446(3)	3346(4)	-7(3)	166
H(29C)	-1557(3)	3388(4)	638(3)	166
H(30A)	455(3)	3880(3)	954(3)	139
H(30B)	-331(3)	4190(3)	1021(3)	139
H(30C)	-222(3)	4148(3)	376(3)	139
H(31A)	14(3)	1075(3)	266(3)	107
H(32A)	-1101(4)	1418(5)	-556(4)	231
H(32B)	-1551(4)	1602(5)	-92(4)	231
H(32C)	-1283(4)	758(5)	-160(4)	231
H(33A)	143(3)	1374(3)	1285(3)	146
H(33B)	-484(3)	731(3)	1023(3)	146
H(33C)	-752(3)	1575(3)	1088(3)	146
H(34A)	-699(3)	2677(5)	-677(2)	135
H(35A)	36(3)	1575(5)	-762(2)	196
H(35B)	795(3)	2079(5)	-625(2)	196
H(35C)	101(3)	2201(5)	-1231(2)	196
H(36A)	-33(4)	3865(5)	-353(3)	211
H(36B)	59(4)	3619(5)	-979(3)	211
H(36C)	753(4)	3496(5)	-374(3)	211
H(38A)	3939(2)	7602(2)	2935(1)	38
H(39A)	4709(2)	7655(2)	2307(2)	45
H(40A)	4160(2)	7466(2)	1265(2)	46
H(41A)	2829(2)	7190(2)	863(1)	48
H(42A)	2072(2)	7120(2)	1497(1)	42
H(44A)	781(2)	6695(2)	2146(2)	51
H(45A)	292(2)	5457(2)	1980(2)	64
H(46A)	1109(2)	4415(2)	2327(2)	58
H(47A)	2430(2)	4625(2)	2816(2)	51
H(48A)	2920(2)	5852(2)	2978(1)	43

Table S36. (Cont'd.)

atom	x/a	y/b	z/c	U(iso)
H(50A)	2003(2)	8575(2)	1888(1)	43
H(51A)	1077(2)	9545(2)	1660(2)	55
H(52A)	93(2)	9560(2)	2107(2)	65
H(53A)	61(2)	8613(2)	2797(2)	65
H(54A)	1008(2)	7670(2)	3050(2)	52
H(56A)	3165(2)	8511(2)	3359(1)	47
H(57A)	3729(2)	8807(2)	4376(2)	58
H(58A)	3675(2)	7938(2)	5121(2)	63
H(59A)	3041(2)	6778(2)	4832(2)	63
H(60A)	2465(2)	6484(2)	3815(2)	49

Table S7. Summary of Crystal and Data Collection^a Parameters for [Fe₄S₄(PCy₃)₄](BPh₄).

formula	C ₉₆ H ₁₅₂ B ₁ Fe ₄ P ₄ S ₄
formula wt	1792.64
crystal system	monoclinic
space group	<i>P</i> 2 ₁ / <i>c</i>
<i>Z</i>	4
<i>a</i> , Å	14.909(3)
<i>b</i> , Å	21.400(5)
<i>c</i> , Å	30.322(5)
β , °	94.52(2)
<i>V</i> , Å ³	9644(3)
<i>T</i> , K	223
color	black
crystal habit	brick
<i>d</i> _{calc} , g/cm ³	1.232
μ , mm ⁻¹	0.79
scan type	ω
scan width, °	1.2
scan speed, °/min	10
2 θ range, °	3→45
data collected	13308
unique data	12670
data observed (<i>I</i> > 2 σ <i>I</i>)	5256
no. of variables	636
w <i>R</i> ^{2b}	.1239
<i>R</i> ^c	.0650

^aGraphite monochromated Mo K α (λ = 0.71073 Å) radiation.^bw*R*² = { $\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]$ }^{1/2}. ^c*R* = $\sum||F_o| - |F_c|| / \sum|F_o|$.

Table S8. Atomic Coordinates ($\times 10^4$) and Isotropic Thermal Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}_4\text{S}_4(\text{PCy}_3)_4](\text{BPh}_4)$.

atom	x/a	y/b	z/c	U(iso)
Fe(1)	2672(1)	6745(1)	704(1)	25(1)
Fe(2)	4267(1)	7294(1)	657(1)	25(1)
Fe(3)	2782(1)	8005(1)	667(1)	27(1)
Fe(4)	3081(1)	7295(1)	-49(1)	26(1)
S(1)	3417(1)	7376(1)	1224(1)	29(1)
S(2)	3745(2)	6424(1)	284(1)	29(1)
S(3)	1763(1)	7387(1)	260(1)	30(1)
S(4)	3879(2)	8139(1)	218(1)	30(1)
P(1)	1998(2)	5934(1)	1103(1)	27(1)
P(3)	2311(2)	8966(1)	1006(1)	35(1)
P(2)	5843(1)	7332(1)	837(1)	25(1)
P(4)	3174(2)	7199(1)	-836(1)	29(1)
C(1)	2685(6)	5853(4)	1641(2)	32(2)
C(2)	2243(6)	5507(4)	2004(3)	41(3)
C(3)	2843(5)	5535(5)	2440(3)	40(3)
C(4)	3780(6)	5277(5)	2380(3)	49(3)
C(5)	4213(6)	5614(5)	2014(3)	53(3)
C(6)	3608(6)	5585(5)	1579(3)	42(3)
C(7)	853(5)	6110(4)	1265(3)	32(2)
C(8)	138(6)	6123(5)	861(3)	49(3)
C(9)	-797(6)	6243(5)	1027(3)	58(3)
C(10)	-785(7)	6869(5)	1282(3)	62(3)
C(11)	-67(6)	6890(5)	1648(3)	51(3)
C(12)	847(6)	6745(4)	1497(3)	39(3)
C(13)	1964(6)	5159(4)	817(3)	33(2)
C(14)	1774(6)	5214(4)	327(3)	43(3)
C(15)	1842(7)	4582(4)	92(3)	50(3)
C(16)	1264(6)	4092(4)	289(3)	41(3)
C(17)	1461(7)	4035(5)	788(3)	54(3)
C(18)	1371(7)	4657(4)	1009(3)	44(3)
C(19)	6059(5)	7889(4)	1292(3)	31(2)
C(20)	7041(6)	7965(5)	1471(3)	54(3)
C(21)	7098(8)	8399(5)	1877(4)	77(4)
C(22)	6718(7)	9016(5)	1767(4)	74(4)
C(23)	5767(7)	8974(5)	1576(3)	57(3)
C(24)	5665(6)	8543(4)	1181(3)	48(3)
C(25)	6493(5)	7622(4)	378(2)	28(2)
C(26)	6045(5)	7451(4)	-77(2)	34(2)
C(27)	6539(5)	7773(4)	-440(3)	35(2)
C(28)	7511(5)	7596(4)	-415(3)	39(2)
C(29)	7973(6)	7734(5)	32(3)	51(3)
C(30)	7479(5)	7432(4)	397(3)	35(2)
C(31)	6375(6)	6598(4)	1034(2)	25(2)
C(32)	6179(6)	6051(4)	703(3)	32(2)
C(33)	6635(6)	5448(4)	861(3)	38(3)

Table S8. (Cont'd.)

atom	x/a	y/b	z/c	U(iso)
C(34)	6347(6)	5275(4)	1322(3)	39(3)
C(35)	6540(6)	5806(4)	1647(3)	39(3)
C(36)	6089(6)	6406(4)	1488(3)	36(2)
C(37)	1069(8)	9038(6)	1045(4)	81(4)
C(38)	738(8)	9614(6)	1242(4)	94(4)
C(39)	-283(15)	9537(11)	1412(8)	81(9)
C(39')	-327(16)	9733(11)	1042(8)	54(8)
C(40)	-808(9)	9187(7)	1156(5)	109(5)
C(41)	-473(10)	8592(7)	1016(5)	118(5)
C(42)	595(12)	8463(9)	1144(6)	52(7)
C(42')	492(18)	8698(13)	748(9)	72(10)
C(43)	2651(6)	9666(4)	693(3)	41(3)
C(44)	2218(7)	9688(5)	213(3)	53(3)
C(45)	2520(7)	10271(5)	-19(3)	63(3)
C(46)	3501(7)	10326(5)	-13(3)	71(4)
C(47)	3961(7)	10317(5)	458(3)	67(3)
C(48)	3695(6)	9733(4)	704(3)	46(3)
C(49)	2883(6)	9082(4)	1569(3)	38(3)
C(50)	2894(6)	9753(4)	1762(3)	49(3)
C(51)	3569(7)	9779(5)	2176(3)	69(4)
C(52)	3317(8)	9308(5)	2514(3)	71(4)
C(53)	3273(8)	8633(5)	2334(3)	74(4)
C(54)	2590(7)	8615(5)	1917(3)	56(3)
C(55)	2314(8)	6636(5)	-1073(3)	79(4)
C(56)	1895(7)	6248(5)	-769(3)	59(3)
C(57)	1172(7)	5806(5)	-932(3)	55(3)
C(58)	910(8)	5793(6)	-1400(4)	91(4)
C(59)	1331(7)	6208(5)	-1691(3)	70(4)
C(60)	2020(6)	6656(4)	-1535(3)	47(3)
C(61)	4272(6)	6949(4)	-1012(3)	34(2)
C(62)	4567(6)	6302(4)	-844(3)	44(3)
C(63)	5521(7)	6136(5)	-958(3)	65(3)
C(64)	5602(7)	6182(5)	-1450(3)	52(3)
C(65)	5304(6)	6797(4)	-1634(3)	44(3)
C(66)	4362(5)	6967(4)	-1517(2)	33(2)
C(67)	2951(5)	7951(4)	-1116(2)	26(2)
C(68)	3723(6)	8427(4)	-1038(3)	33(2)
C(69)	3492(6)	9037(4)	-1268(3)	44(3)
C(70)	2627(6)	9316(5)	-1136(3)	57(3)
C(71)	1866(7)	8861(5)	-1209(3)	65(3)
C(72)	2082(6)	8245(4)	-973(3)	46(3)
C(73)	2642(5)	1756(4)	1857(3)	26(2)
C(74)	3094(6)	1485(4)	1517(3)	30(2)
C(75)	4030(6)	1360(4)	1561(3)	42(3)
C(76)	4517(6)	1518(4)	1943(3)	43(3)

Table S8. (Cont'd.)

atom	x/a	y/b	z/c	U(iso)
C(77)	4112(6)	1792(4)	2288(3)	43(3)
C(78)	3184(6)	1912(4)	2237(3)	38(2)
C(79)	1094(6)	1330(4)	2129(3)	29(2)
C(80)	156(6)	1224(5)	2064(3)	49(3)
C(81)	-267(7)	757(5)	2300(3)	55(3)
C(82)	229(6)	391(4)	2590(3)	43(3)
C(83)	1134(6)	477(4)	2661(3)	43(3)
C(84)	1540(6)	936(4)	2432(3)	38(2)
C(85)	1400(6)	2583(4)	2043(3)	31(2)
C(86)	733(6)	2732(5)	2323(3)	52(3)
C(87)	619(7)	3362(5)	2472(3)	61(3)
C(88)	1178(7)	3793(5)	2327(3)	58(3)
C(89)	1821(7)	3684(5)	2063(3)	63(3)
C(90)	1919(6)	3079(4)	1917(3)	46(3)
C(91)	1048(5)	1853(4)	1333(3)	29(2)
C(92)	1013(6)	1293(4)	1096(3)	35(2)
C(93)	551(6)	1233(5)	673(3)	45(3)
C(94)	132(6)	1751(4)	477(3)	42(3)
C(95)	155(6)	2304(5)	698(3)	40(2)
C(96)	618(5)	2358(4)	1115(2)	32(2)
B(1)	1539(7)	1870(5)	1839(3)	38(3)

Table S9. Interatomic Distances (Å) for
[Fe₄S₄(PCy₃)₄](BPh₄) .

Fe(1)-S(2)	2.229(3)	C(14)-C(15)	1.535(11)
Fe(1)-S(3)	2.291(3)	C(15)-C(16)	1.512(11)
Fe(1)-S(1)	2.296(3)	C(16)-C(17)	1.523(11)
Fe(1)-P(1)	2.383(3)	C(17)-C(18)	1.501(11)
Fe(1)-Fe(2)	2.665(2)	C(19)-C(20)	1.529(11)
Fe(1)-Fe(4)	2.679(2)	C(19)-C(24)	1.544(11)
Fe(1)-Fe(3)	2.704(2)	C(20)-C(21)	1.540(12)
Fe(2)-S(1)	2.222(2)	C(21)-C(22)	1.464(13)
Fe(2)-S(2)	2.282(3)	C(22)-C(23)	1.491(12)
Fe(2)-S(4)	2.293(3)	C(23)-C(24)	1.510(11)
Fe(2)-P(2)	2.371(2)	C(25)-C(30)	1.523(10)
Fe(2)-Fe(4)	2.667(2)	C(25)-C(26)	1.529(9)
Fe(2)-Fe(3)	2.690(2)	C(26)-C(27)	1.535(10)
Fe(3)-S(4)	2.229(3)	C(27)-C(28)	1.494(10)
Fe(3)-S(3)	2.299(3)	C(28)-C(29)	1.501(10)
Fe(3)-S(1)	2.304(2)	C(29)-C(30)	1.522(10)
Fe(3)-P(3)	2.427(3)	C(31)-C(36)	1.529(10)
Fe(3)-Fe(4)	2.717(2)	C(31)-C(32)	1.556(10)
Fe(4)-S(3)	2.250(2)	C(32)-C(33)	1.520(10)
Fe(4)-S(4)	2.277(3)	C(33)-C(34)	1.539(10)
Fe(4)-S(2)	2.305(3)	C(34)-C(35)	1.516(11)
Fe(4)-P(4)	2.408(2)	C(35)-C(36)	1.511(11)
P(1)-C(7)	1.852(8)	C(37)-C(42')	1.40(3)
P(1)-C(1)	1.863(8)	C(37)-C(42)	1.46(2)
P(1)-C(13)	1.871(8)	C(37)-C(38)	1.473(14)
P(3)-C(49)	1.863(8)	C(38)-C(39)	1.65(2)
P(3)-C(43)	1.865(9)	C(38)-C(39')	1.68(2)
P(3)-C(37)	1.871(12)	C(39)-C(40)	1.29(2)
P(2)-C(19)	1.833(8)	C(39')-C(40)	1.43(2)
P(2)-C(31)	1.838(8)	C(40)-C(41)	1.44(2)
P(2)-C(25)	1.862(7)	C(41)-C(42)	1.63(2)
P(4)-C(67)	1.836(8)	C(41)-C(42')	1.72(3)
P(4)-C(61)	1.842(8)	C(43)-C(44)	1.546(11)
P(4)-C(55)	1.863(9)	C(43)-C(48)	1.560(12)
C(1)-C(6)	1.516(11)	C(44)-C(45)	1.517(12)
C(1)-C(2)	1.521(10)	C(45)-C(46)	1.466(13)
C(2)-C(3)	1.537(10)	C(46)-C(47)	1.536(12)
C(3)-C(4)	1.526(11)	C(47)-C(48)	1.524(12)
C(4)-C(5)	1.510(11)	C(49)-C(54)	1.541(11)
C(5)-C(6)	1.539(11)	C(49)-C(50)	1.553(11)
C(7)-C(12)	1.529(11)	C(50)-C(51)	1.546(12)
C(7)-C(8)	1.560(10)	C(51)-C(52)	1.507(13)
C(8)-C(9)	1.540(12)	C(52)-C(53)	1.544(13)
C(9)-C(10)	1.545(13)	C(53)-C(54)	1.561(12)
C(10)-C(11)	1.482(11)	C(55)-C(56)	1.421(12)
C(11)-C(12)	1.504(11)	C(55)-C(60)	1.436(11)
C(13)-C(14)	1.493(10)	C(56)-C(57)	1.488(12)
C(13)-C(18)	1.535(11)	C(57)-C(58)	1.442(13)
