Contents

Table S1.1. Crystal data and details of the structure refinement for: $[Fe(C_5H_4)_2S_3O]$

Empirical formula	$C_{10}H_8FeS_3O$
Formula weight	296.19
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	
a = 7.7175(2) Å	α = 81.5030(10)°
b = 7.8289(2) Å	β = 74.8840(10)°
c =10.1986(2) Å	γ = 61.4000(10)°
Volume, Z	522.09(2) $Å^3$, 1
Density (calculated)	1.884 Mg/m^3
Absorption coefficient	2.007 mm^{-1}
F(000)	300
Crystal size	0.38 x 0.16 x 0.10 mm
Θ range for data collection	3.14 to 27.50°
Limiting indices	-10 < h < 6, -10 < k < 10 -13 < l < 12
Reflections collected	3915
Independent reflections	2323 (Rint = 0.0610)
Completeness to Θ = 27.50°	97.2 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2323 / 0 / 145
Goodness-of-fit on F^2	0.810
Final R indices [I>2σ(I)]	R1 = 0.0493, wR2 = 0.1240
R indices (all data)	R1 = 0.0775, wR2 = 0.1393
Largest diff. peak and hole	0.603 / -1.009 $eÅ^{-3}$

Table S1.2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for: [$Fe(C_5H_4)_2S_3O$]
(U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.)

	x	y	z	U(eq)
Fe	7326(1)	6219(1)	2570(1)	27(1)
S(1)	9012(2)	8861(2)	3706(1)	48(1)
S(2)	9351(2)	9668(2)	1663(1)	44(1)
S(3)	6372(2)	10795(2)	1344(2)	49(1)
C(1)	6135(6)	8650(5)	1415(4)	31(1)
C(2)	4561(7)	8304(7)	2282(5)	39(1)
C(3)	4881(7)	6459(7)	1960(5)	43(1)
C(4)	6620(7)	5681(7)	911(5)	42(1)
C(5)	7436(7)	7021(6)	552(4)	36(1)
C(6)	8840(6)	6705(5)	3703(4)	27(1)
C(7)	7296(7)	6313(6)	4567(5)	40(1)
C(8)	7727(7)	4404(6)	4255(5)	41(1)
C(9)	9494(7)	3674(6)	3233(5)	38(1)
C(10)	10191(6)	5075(6)	2882(5)	35(1)
O(1)	4887(9)	11973(8)	2372(6)	41(2)
O(1')	7470(14)	10137(11)	4587(9)	76(3)

Table S1.3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for: [$Fe(C_5H_4)_2S_3O$]

	x	y	z	U(eq)
H(2)	3453	9181	2968	47
H(3)	4043	5823	2405	52
H(4)	7201	4406	511	50
H(5)	8639	6865	-150	43
H(7)	6166	7173	5251	48
H(8)	6920	3730	4680	49
H(9)	10123	2404	2815	46
H(10)	11398	4946	2195	41

Table S1.4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for: $[Fe(C_5H_4)_2S_3O$
(The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)2U_{11}$ + ... + $2hka^*b^*U_{12}$])

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe	24(1)	28(1)	28(1)	1(1)	-11(1)	-9(1)
S(1)	78(1)	42(1)	37(1)	-3(1)	-17(1)	-35(1)
S(2)	49(1)	45(1)	46(1)	2(1)	-11(1)	-28(1)
S(3)	45(1)	27(1)	73(1)	6(1)	-24(1)	-10(1)
C(1)	27(2)	30(2)	35(2)	2(2)	-13(2)	-9(2)
C(2)	26(2)	43(2)	41(2)	2(2)	-16(2)	-7(2)
C(3)	39(3)	52(3)	53(3)	5(2)	-26(2)	-26(2)
C(4)	53(3)	44(2)	38(2)	2(2)	-27(2)	-22(2)
C(5)	41(2)	39(2)	29(2)	0(2)	-18(2)	-15(2)
C(6)	31(2)	29(2)	25(2)	1(2)	-12(2)	-14(2)
C(7)	42(3)	41(2)	31(2)	1(2)	-14(2)	-13(2)
C(8)	50(3)	43(2)	40(3)	14(2)	-24(2)	-25(2)
C(9)	37(2)	28(2)	48(3)	6(2)	-26(2)	-8(2)
C(10)	25(2)	33(2)	44(2)	-4(2)	-17(2)	-6(2)
O(1)	39(3)	28(3)	43(4)	-9(3)	-7(3)	-3(3)
O(1')	88(6)	50(4)	73(6)	-21(4)	-4(5)	-19(4)

Table S1.5. Bond lengths [Å] for: $[Fe(C_5H_4)_2S_3O]$

Fe-C(1)	2.020(4)	S(3)-C(1)	1.763(4)
Fe-C(2)	2.038(4)	S(1)-C(6)	1.755(4)
Fe-C(3)	2.055(4)	C(1)-C(2)	1.419(6)
Fe-C(4)	2.060(4)	C(1)-C(5)	1.433(5)
Fe-C(5)	2.053(4)	C(2)-C(3)	1.418(7)
Fe-C(6)	2.026(4)	C(3)-C(4)	1.406(7)
Fe-C(7)	2.043(4)	C(4)-C(5)	1.425(7)
Fe-C(8)	2.050(4)	C(6)-C(7)	1.418(6)
Fe-C(9)	2.056(4)	C(6)-C(10)	1.415(5)
Fe-C(10)	2.044(4)	C(7)-C(8)	1.434(6)
S(1)-S(2)	2.0722(18)	C(8)-C(9)	1.401(7)
S(2)-S(3)	2.1290(17)	C(9)-C(10)	1.403(7)
S(1)-O(1')	1.338(8)		
S(3)-O(1)	1.383(6)		

Table S1.6. Bond angles [°] for: $[Fe(C_5H_4)_2S_3O]$

S(1)-S(2)-S(3)	102.76(8)
O(1')-S(1)-S(2)	118.0(4)
O(1')-S(1)-C(6)	112.2(4)
C(6)-S(1)-S(2)	101.98(14)
O(1)-S(3)-S(2)	113.4(3)
O(1)-S(3)-C(1)	107.8(3)
C(1)-S(3)-S(2)	101.49(14)
C(2)-C(1)-S(3)	125.5(3)
C(5)-C(1)-S(3)	125.4(4)
C(2)-C(1)-C(5)	109.0(4)
C(3)-C(2)-C(1)	107.2(4)
C(4)-C(3)-C(2)	108.6(5)
C(3)-C(4)-C(5)	109.0(4)
C(4)-C(5)-C(1)	106.2(4)
C(10)-C(6)-C(7)	108.6(4)
C(10)-C(6)-S(1)	127.0(3)
C(7)-C(6)-S(1)	124.4(3)
C(6)-C(7)-C(8)	106.6(4)
C(9)-C(8)-C(7)	108.2(5)
C(8)-C(9)-C(10)	108.9(4)
C(9)-C(10)-C(6)	107.7(4)

Table S1.7. Torsion angles [°] for: $[Fe(C_5H_4)_2S_3O]$

S(1)-S(2)-S(3)-O(1)	43.0(3)
S(1)-S(2)-S(3)-C(1)	-72.33(16)
S(1)-C(6)-C(7)-C(8)	-179.2(3)
S(1)-C(6)-C(10)-C(9)	178.9(3)
S(2)-S(1)-C(6)-C(7)	-129.6(3)
S(2)-S(1)-C(6)-C(10)	51.6(4)
S(2)-S(3)-C(1)-C(2)	125.6(3)
S(2)-S(3)-C(1)-C(5)	-58.3(4)
S(3)-C(1)-C(2)-C(3)	176.7(3)
S(3)-C(1)-C(5)-C(4)	-176.6(3)
O(1)-S(3)-C(1)-C(2)	6.2(5)
O(1)-S(3)-C(1)-C(5)	-177.7(4)
O(1')-S(1)-S(2)-S(3)	-47.8(5)
O(1')-S(1)-C(6)-C(7)	-2.3(6)
O(1')-S(1)-C(6)-C(10)	178.9(6)
C(1)-C(2)-C(3)-C(4)	-0.1(5)
C(2)-C(1)-C(5)-C(4)	0.0(5)
C(2)-C(3)-C(4)-C(5)	0.1(5)
C(3)-C(4)-C(5)-C(1)	-0.1(5)
C(6)-S(1)-S(2)-S(3)	75.65(15)
C(7)-C(6)-C(10)-C(9)	0.0(5)
C(7)-C(8)-C(9)-C(10)	-0.3(5)
C(8)-C(9)-C(10)-C(6)	0.2(5)
C(10)-C(6)-C(7)-C(8)	-0.2(5)

Table S2.1. Crystal data and details of the structure refinement for: $[Fe(C_5H_4)_2S_3O_2]$

Empirical formula	$C_{10}H_8S_3O_2Fe$
Formula weight	312.20
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	$P2_1/n$
Unit cell dimensions	
a = 9.33880(10) Å,	α = 90°
b = 9.8378(2) Å,	β = 94.8330(10)°
c = 12.00280(10) Å,	γ = 90°
Volume, Z	1098.82(3) $Å^3$, 4
Density (calculated)	1.887 Mg/m^3
Absorption coefficient	1.919 mm^{-1}
Crystal size	0.12 0.38 x 0.42 mm
θ range for data collection	2.66 to 27.49°
Limiting indices	-8 < h < 12, -12 < k < 12 -15 < l < 15
Reflections collected	7911
Independent reflections	2512 (R_{int} = 0.0832)
Completeness to θ = 27.49°	99.4 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2512 / 0 / 145
Goodness-of-fit on F^2	1.078
Final R indices [I>2σ(I)]	R1 = 0.0375, wR2 = 0.0912
R indices (all data)	R1 = 0.0487, wR2 = 0.0987
Largest diff. peak and hole	0.781 / -0.558 $eÅ^{-3}$

Table S2.2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for: [$Fe(C_5H_4)_2S_3O_2$]
(U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.)

	x	y	z	U(eq)
Fe	404(1)	7161(1)	2495(1)	21(1)
S(1)	-2608(1)	6567(1)	3746(1)	33(1)
S(2)	-1994(1)	8450(1)	4496(1)	36(1)
S(3)	43(1)	8051(1)	5140(1)	34(1)
C(1)	-1569(3)	6344(3)	2620(2)	26(1)
C(2)	-1592(3)	7199(3)	1653(2)	31(1)
C(3)	-584(3)	6644(3)	952(3)	36(1)
C(4)	59(3)	5479(3)	1488(2)	33(1)
C(5)	-521(3)	5284(3)	2531(3)	31(1)
C(6)	1002(3)	8155(3)	3938(2)	26(1)
C(7)	833(3)	9099(3)	3035(2)	31(1)
C(8)	1798(3)	8714(3)	2238(3)	37(1)
C(9)	2580(3)	7547(4)	2648(3)	37(1)
C(10)	2084(3)	7192(3)	3700(2)	30(1)
O(1)	-4083(2)	6825(3)	3343(2)	56(1)
O(1A)	-2275(3)	5476(3)	4513(2)	52(1)

Table S2.3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for: [$Fe(C_5H_4)_2S_3O_2$]

	x	y	z	U(eq)
H(2)	-2197	8002	1498	37
H(3)	-352	7017	232	43
H(4)	812	4921	1197	39
H(5)	-279	4557	3072	37
H(7)	165	9868	2973	37
H(8)	1902	9169	1523	44
H(9)	3310	7060	2264	44
H(10)	2422	6427	4175	36

Table S2.4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for: [$Fe(C_5H_4)_2S_3O_2$]
(The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$])

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe	20(1)	22(1)	20(1)	-2(1)	-2(1)	0(1)
S(1)	26(1)	36(1)	37(1)	-2(1)	7(1)	-5(1)
S(2)	32(1)	37(1)	38(1)	-8(1)	6(1)	7(1)
S(3)	37(1)	43(1)	22(1)	-6(1)	-1(1)	3(1)
C(1)	23(1)	28(1)	28(1)	-5(1)	-2(1)	-5(1)
C(2)	25(1)	37(2)	29(1)	-2(1)	-8(1)	0(1)
C(3)	34(2)	49(2)	24(1)	-6(1)	-6(1)	-6(1)
C(4)	31(1)	32(2)	34(2)	-15(1)	-1(1)	0(1)
C(5)	32(1)	22(1)	38(2)	-5(1)	-2(1)	-3(1)
C(6)	26(1)	28(1)	21(1)	-6(1)	-5(1)	-3(1)
C(7)	35(1)	23(1)	34(2)	-2(1)	-4(1)	-4(1)
C(8)	40(2)	38(2)	34(2)	1(1)	4(1)	-17(1)
C(9)	24(1)	47(2)	40(2)	-10(1)	2(1)	-4(1)
C(10)	23(1)	35(2)	31(2)	-8(1)	-9(1)	3(1)
O(1)	24(1)	73(2)	70(2)	-19(2)	4(1)	-5(1)
O(1A)	66(2)	44(1)	48(2)	10(1)	19(1)	-5(1)

Table S2.5. Bond lengths [Å] for: [$Fe(C_5H_4)_2S_3O_2$]

Fe-C(1)	2.027(3)	S(1)-C(1)	1.743(3)
Fe-C(2)	2.044(3)	S(3)-C(6)	1.764(3)
Fe-C(3)	2.063(3)	C(1)-C(2)	1.432(4)
Fe-C(4)	2.059(3)	C(1)-C(5)	1.440(4)
Fe-C(5)	2.041(3)	C(2)-C(3)	1.423(4)
Fe-C(6)	2.026(3)	C(3)-C(4)	1.422(5)
Fe-C(7)	2.042(3)	C(4)-C(5)	1.418(4)
Fe-C(8)	2.047(3)	C(6)-C(7)	1.426(4)
Fe-C(9)	2.060(3)	C(6)-C(10)	1.431(4)
Fe-C(10)	2.042(3)	C(7)-C(8)	1.420(4)
S(1)-S(2)	2.1168(11)	C(8)-C(9)	1.426(5)
S(2)-S(3)	2.0305(11)	C(9)-C(10)	1.425(4)
S(1)-O(1)	1.443(2)		
S(1)-O(1A)	1.430(3)		

Table S2.6. Bond angles [°] for: $[Fe(C_5H_4)_2S_3O_2]$

O(1A)-S(1)-O(1)	119.79(17)
O(1A)-S(1)-C(1)	107.43(14)
O(1)-S(1)-C(1)	109.88(15)
O(1A)-S(1)-S(2)	110.28(13)
O(1)-S(1)-S(2)	101.85(13)
C(1)-S(1)-S(2)	106.92(9)
S(3)-S(2)-S(1)	101.79(4)
C(6)-S(3)-S(2)	101.60(9)
C(2)-C(1)-C(5)	109.2(2)
C(2)-C(1)-S(1)	125.7(2)
C(5)-C(1)-S(1)	125.1(2)
C(3)-C(2)-C(1)	106.8(3)
C(4)-C(3)-C(2)	108.4(3)
C(5)-C(4)-C(3)	109.3(3)
C(4)-C(5)-C(1)	106.3(3)
C(7)-C(6)-C(10)	108.3(2)
C(7)-C(6)-S(3)	128.9(2)
C(10)-C(6)-S(3)	122.7(2)
C(8)-C(7)-C(6)	107.6(3)
C(7)-C(8)-C(9)	108.5(3)
C(10)-C(9)-C(8)	108.0(3)
C(9)-C(10)-C(6)	107.6(3)

Table S2.7. Torsion angles [°] for: $[Fe(C_5H_4)_2S_3O_2]$

O(1A)-S(1)-S(2)-S(3)	48.65(12)
O(1)-S(1)-S(2)-S(3)	176.87(13)
C(1)-S(1)-S(2)-S(3)	-67.85(11)
S(1)-S(2)-S(3)-C(6)	78.00(10)
O(1A)-S(1)-C(1)-C(2)	178.8(2)
O(1)-S(1)-C(1)-C(2)	46.9(3)
S(2)-S(1)-C(1)-C(2)	-62.9(2)
O(1A)-S(1)-C(1)-C(5)	-2.9(3)
O(1)-S(1)-C(1)-C(5)	-134.8(2)
S(2)-S(1)-C(1)-C(5)	115.4(2)
C(5)-C(1)-C(2)-C(3)	1.5(3)
S(1)-C(1)-C(2)-C(3)	-179.9(2)
C(1)-C(2)-C(3)-C(4)	-0.8(3)
C(2)-C(3)-C(4)-C(5)	-0.3(3)
C(3)-C(4)-C(5)-C(1)	1.2(3)
C(2)-C(1)-C(5)-C(4)	-1.7(3)
S(1)-C(1)-C(5)-C(4)	179.7(2)
S(2)-S(3)-C(6)-C(7)	40.2(3)
S(2)-S(3)-C(6)-C(10)	-136.5(2)
C(10)-C(6)-C(7)-C(8)	0.4(3)
S(3)-C(6)-C(7)-C(8)	-176.6(2)
C(6)-C(7)-C(8)-C(9)	-0.7(3)
C(7)-C(8)-C(9)-C(10)	0.8(3)
C(8)-C(9)-C(10)-C(6)	-0.5(3)
C(7)-C(6)-C(10)-C(9)	0.1(3)
S(3)-C(6)-C(10)-C(9)	177.3(2)