Electronic Supporting Information of the Manuscript: “The Isopropylsulfinyl Group: a Useful Chiral Controller for the Asymmetric Aziridination of Sulfinylimines and the Organocatalytic allylation of Hydrazones”

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General Methods.

All reactions were run under an atmosphere of dry argon using oven-dried glassware and freshly distilled and dried solvents. THF and diethyl ether were distilled from sodium benzophenone ketyl. Dichloromethane was distilled from calcium hydride. TLC was performed on Silica Gel GF₂₅₄ (Merck) with detection by charring with phosphomolybdic acid/EtOH. For flash chromatography, silica Gel (Merck 230-400 mesh) was used. Column were eluted with positive air pressure. Chromatographic eluents are given as volume to volume ratios (v/v). NMR spectra were recorded with a Bruker AMX₅₀₀ (¹H, 500 MHz) and Bruker Avance DRX₅₀₀ (¹H, 500 MHz) spectrometers. Chemical shifts are reported in ppm, and coupling constants are reported in Hz. Routine spectra were referenced to the residual proton or carbon signals of the solvent. High-resolution mass spectra were recorded on a Kratos MS-80RFA 241-MC apparatus. Optical rotations were determined with a Perkin-Elmer 341 polarimeter. Elemental analyses were recorded on a leco CHNS-932 apparatus. The organic extracts were dried over anhydrous sodium sulfate and concentrated in vacuo.

(S)-(1,2:5,6-Di-O-cyclohexylidene- α -D-glucofuranosyl) isopropanesulfinate, 2(S_S).

To a solution of 1,2:5,6-Di-O-cyclohexylidene- α -D-glucofuranosyl (DCG) **1** (5 g, 15.27 mmol) in a mixture of toluene (210 mL) and methylene chloride (20 mL) was added diisopropylethyl amine (4.8 mL, 27.5 mmol). The solution was stirred for 30 min at -78°C, before adding isopropylsulfinyl chloride (2.5 mL, 27.5 mmol). After 1 hour at -78°C the reaction was hydrolysed with a 10% HCl aqueous solution (100 mL) and the

aqueous phase was extracted with methylene chloride (3 x 60 mL). The organic layer was washed with saturated NaHCO₃ aqueous solution and saturated NaCl aqueous solution and dried over Na₂SO₄. After removing the solvent under vacuum, the sulfinate ester **2(S_S)** was obtained (in almost quantitative yield) as an oil in a 96% d.e. The crude of reaction can be used in the following reaction without previous purification and optically pure sulfinate can be obtained by column chromatography (AcOEt:Hexanes, 1:7). $[\alpha]_D^{25}$: -52 [c. 0.6, acetone]. ¹H NMR(CDCl₃, 500 MHz) δ : 5.87 (d, 1H, J= 3.5 Hz, H-1), 4.71 (d, 1H, J= 2.5 Hz, H-3), 4.56 (d, 1H, J= 3.5 Hz, H-2), 4.29-4.22 (m, 2H, H-4 y H-5), 4.16-3.92 (m, 2H, H-6 y H-6'), 2.77(m, 1H, J= 7.0 Hz, SCH(CH₃)₂), 1.72-1.25 (m, 20H), 1.22 (d, 6H, J = 7.0 Hz, SCH(CH₃)₂). ¹³C NMR(CDCl₃, 125 MHz): 113.1, 109.7, 104.6, 82.9, 80.7, 79.9, 72.0, 66.5, 60.4, 55.6, 36.4, 35.7, 34.6, 25.2, 24.8, 24.0, 23.8, 23.7, 23.5, 13.9. HRMS Calcd. For C₂₁H₃₄O₇S (M)⁺: 430.2025. Found: 430.2016 (2.0 ppm).

(R)-(1,2:5,6-Di-O-cyclohexylidene- α -D-glucofuranosyl) isopropanesulfinate, 2(R_S).

To a solution of 1,2:5,6-Di-O-cyclohexylidene- α -D-glucofuranosyl (DCG) **1** (5 g, 15.27mmol) in THF (200 mL) was added pyridine (3.3 mL, 27.5 mmol). The solution was stirred for 30 min at -78°C, before adding isopropylsulfinyl chloride (3.7 mL, 27.5 mmol). After 1 hour at -78°C the reaction was hydrolysed with a 10% HCl aqueous solution (100 mL), and the aqueous phase was extracted with methylene chloride (3 x 60 mL). The organic layer was washed with saturated NaHCO₃ aqueous solution and saturated NaCl aqueous solution and dried over Na₂SO₄. After removing the solvent under vacuum, the sulfinate ester **2(S_S)** was obtained (in almost quantitative yield) as an oil in a 78 % d.e. The resulting mixture of diastereomers can be separated by silica gel column chromatography (AcOEt: Hexane 1:7). $[\alpha]_D^{20}$: +15 [c. 0.8, acetone]. ¹H NMR(CDCl₃, 400 MHz) δ : 5.87 (d, 1H, J= 3.5 Hz, H-1), 4.73 (d, 1H, J= 3.5 Hz, H-2), 4.69 (d, 1H, J= 1.3 Hz, H-3), 4.23-4.04 (m, 3H, H-4, H-5 y H-6), 3.94-3.90 (m, 1H, H-6') 2.79(m, 1H, J= 7.0 Hz, SCH(CH₃)₂), 1.82-1.34 (m, 20H), 1.24 (d, 3H, J = 7.0 Hz, SCH(CH₃)₂), 1.23 (d, 3H, J = 7.0 Hz, SCH(CH₃)₂). ¹³C NMR(CDCl₃, 100 MHz): 113.0, 110.0, 105.0, 83.3, 83.1, 81.2, 71.7, 67.5, 56.0, 36.6, 36.4, 35.6, 34.8, 25.1, 24.8, 24.0, 23.9, 23.8, 23.5, 13.8, 13.7. HRMS: Calcd. For C₂₁H₃₄O₇S (M)⁺: 430.2025. Found: 430.2020 (1.2 ppm).

(S)-Isopropylsulfinamide, 3(S).

To a solution of sulfinate ester **2(S_S)** (5.45g, 12.6 mmol) in THF (50 mL) at 0°C was added a 1M LiHMDS solution in THF (19 mL, 19 mmol). The reaction was stirred for 1 hour then MeOH (20mL) was added followed by silica gel and the mixture was stirred for 15 min. After evaporation of the solvent the residue was purified by column chromatography (80% yield) (AcOEt 100% to AcOEt: MeOH 9:1). Recrystallization from hexanes afforded **3S_S** as a white solid. m.p. 42°C. $[\alpha]_D^{20}$: -18 [c. 0.7, CHCl₃]. ¹H NMR (CDCl₃, 200 MHz): 4.10 (brs, 2H, NH₂), 2.70 (m, 1H, *J* = 6.9 Hz, CHMe₂), 1.29 (d, 3H, *J* = 6.9Hz, CHMe₂), 1.20 (d, 3H, *J* = 6.9 Hz, CHMe₂). ¹³C NMR (CDCl₃, 125 MHz) δ: 54.4, 15.7, 15.6. HRMS. Calcd for C₃H₉NOS (M)⁺: 107.0405. Found: 107.0406 (1.0 ppm).

(S)-(E)-N-(Benzylidene)-isopropanesulfinamide, 4(S).

To a solution of sulfinate ester **2(S_S)** (5.45g, 12.6 mmol) in THF (50 mL) at 0°C was added a 1M LiHMDS solution in THF (19mL, 19 mmol). The reaction was stirred for 1 hour, and transferred via canula to a second flask containing benzaldehyde (25.2 mmol) and CsF (12.6 mmol) in THF (20 mL). After being stirred for 1 h at room temperature, the reaction mixture was quenched with saturated aqueous NH₄Cl solution and the aqueous layer was extracted with AcOEt (4 x 40 mL). The organic layer was washed with saturated NaHCO₃ aqueous solution and with saturated NaCl aqueous solution and dried over Na₂SO₄. The solvent was removed under reduced pressure, and the residue was purified by flash chromatography (AcOEt: Hexanes, 1:9), to give **4(S)** (75 %) as a white solid. m.p. 37-39°C. $[\alpha]_D^{20}$: +54 [c.0.5, CHCl₃]. ¹H NMR (CDCl₃, 500 MHz) δ: 8.60 (s, 1H, N=CHPh), 7.83 (d, 2H, *J* = 7.0 Hz, Ph), 7.50-7.43 (m, 3H, Ph), 2.95 (m, 1H, *J* = 6.8Hz, CHMe₂), 1.28 (d, 3H, *J* = 6.8Hz, CHMe₂) 1.20 (d, 3H, *J* = 6.8 Hz, CHMe₂). ¹³C NMR (CDCl₃, 125 MHz) δ: 162.6 (C=N), 134.0, 132.5, 129.4, 128.9, 53.9, 14.8, 13.6; HRMS Calc. for C₁₀H₁₄NOS (M+1)⁺: 196.0796. Found: 196.0797 (0.5 ppm).

(S)-Isopropylsulfinylferrocene, 15(S).

To a solution of ferrocene (22.8 mmol) in THF (70mL) at 0°C, was added a 1.7 M solution of *tert*-BuLi in THF (11.7 mL, 20 mmol). The reaction was stirred 2hrs at 0°C, and the obtained suspension of ferrocenyllithium was transferred via canula to a second flask containing (S)-isopropylsulfinate **2(S_S)** (6.5g, 15.2mmol) in THF (50 mL)

previously cooled to -78°C . After being stirred 5 min at -78°C , the reaction mixture was quenched with saturated NaCl aqueous solution and the aqueous layer was extracted with AcOEt (5 x 40 mL). After drying the organic layer over Na_2SO_4 , and evaporation of the solvent under vacuum, the residue was purified by flash chromatography (AcOEt: Hexanes, 1:2), to give 1.6 g of **15(S)** (50 %) as a yellow solid. HPLC analysis of the sulfoxide using chiralpack AD column (flow rate 0.8mL/min, *i*PrOH:Hexane 3:97, 30°C , $t_R = 37.1$ min (**15R**) and $t_R = 39.9$ min (**15S**)) shows that the ee of the product is 90%. A single recrystallization from AcOEt:hexane afforded optically pure **15(S)**, 1.12 g (35%). m.p. 114°C . $[\alpha]_{\text{D}}^{20}$: +347 (c. 0.5, CHCl_3). ^1H NMR (CDCl_3 , 500 MHz) δ : 4.68 (s, 1H), 4.40 (s ancho, 2H), 4.36 (s, 5H), 4.32 (s, 1H), 2.75 (m, 1H, $J = 6.8\text{Hz}$, CHMe_2), 1.16 (d, 3H, $J = 8.6\text{ Hz}$, CHMe_2), 0.98 (d, 3H, $J = 8.6\text{ Hz}$, CHMe_2). ^{13}C NMR (CDCl_3 , 125 MHz) δ : 88.4, 70.0, 69.9, 69.6, 68.8, 64.7, 54.4, 15.3, 15.1. Anal. Calcd. for $\text{C}_{13}\text{H}_{16}\text{FeOS}$: C: 56,54%, H: 5,84%. Found: C: 56,24%, H: 5,75%.

General Procedure for the Asymmetric Aziridination of sulfinylimine 4(S).

Method A: with dimethylsulfonium ylide in DMSO..

Sodium hydride (0.87 mmol) previously washed with hexanes was added to a solution of trimethylsulfonium iodide (0.87 mmol) in dimethyl sulfoxide (5 mL). The mixture was stirred 2 h, then a solution of the sulfinylimine **4(S)** (0.29 mmol) in DMSO (10 mL) was added. The reaction was stirred for 1 hour, then poured into cold water, and the aqueous layer was extracted with ether (8x100mL). The organic layer was washed with saturated NaCl aqueous solution and dried over Na_2SO_4 . The solvent was removed under reduced pressure, and the diastereomeric aziridine ratio was determined from the crude mixture by $^1\text{HNMR}$.

Method B: with dimethyloxosulfonium ylide in toluene.

Sodium hydride (1.43 mmol) previously washed with hexanes was added to a suspension of trimethyloxosulfonium (1.43 mmol) in anhydrous toluene (5 mL). The mixture was stirred 2 h then, a solution of the N-sulfinylaldimine **4(S)** (0.5 mmol) in toluene (10 mL) was added. The reaction was stirred for 48 hours, then poured into cold water, and the aqueous layer was extracted with ethyl acetate (8x100mL). The organic layer was washed with saturated NaCl aqueous solution and dried over Na_2SO_4 . The solvent was removed under reduced pressure, and the diastereomeric aziridine ratio was determined from the crude mixture by $^1\text{HNMR}$.

(*S_S,2*R)-N-(Isopropylsulfinyl)-2-phenylaziridine, 9(*S_S,2*R**).** (Data taken from a mixture of both diastereomers **9(*S_S,2*S*)*** and **9(*S_S,2*R*)***). ¹H NMR (CDCl₃, 500 MHz) δ: 7.30-7.28 (m, 5H, Ph), 3.64 (dd, 1H, *J* = 7.0, 4.0 Hz), 2.77 (m, 1H, *J* = 6.9 Hz, CHMe₂), 2.54 (dd, 1H, *J* = 7.0 Hz), 2.23 (d, 1H, *J* = 4.0 Hz), 1.25 (d, 3H, *J* = 6.9 Hz, CHMe₂), 1.24 (d, 3H, *J* = 6.9 Hz, CHMe₂). ¹³C NMR (CDCl₃, 125 MHz) δ: 137.0, 128.6, 127.8, 126.6, 54.7, 32.0, 30.9, 15.3, 15.2. HRMS Calc. for C₁₁H₁₅NOS (M+1)⁺: 210.0952. Found: 210.0950 (0.9 ppm).

(*S_S,2*S)-N-(Isopropylsulfinyl)-2-phenylaziridine, 9(*S_S,2*S**).** (Data taken from a mixture both diastereomers **9(*S_S,2*S*)*** and **9(*S_S,2*R*)***). ¹H NMR (CDCl₃, 500 MHz) δ: 7.30-7.28 (m, 5H, Ph), 3.21 (dd, 1H, *J* = 7.0, 3.9 Hz), 2.97 (d, 1H, *J* = 7.0 Hz), 2.71 (m, 1H, *J* = 7.0 Hz, CHMe₂), 2.03 (d, 1H, *J* = 3.9 Hz), 1.37 (d, 3H, *J* = 6.9 Hz, CHMe₂), 1.35 (d, 3H, *J* = 7.0 Hz, CHMe₂), 1.24 (d, 3H, *J* = 6.9 Hz, CHMe₂).

Enantioselective allylation of N-(benzoyl)isobutylhydrazone. General method: (Kobayashi conditions) To a solution of N-(benzoyl)isobutylhydrazone **10** (20.5 mg, 0.108 mmol), the chiral ferrocenyl sulfoxide **13-15** (0.32 mmol), and 2-methyl-2-butene (27 μL, 0.054 mmol) in dichloromethane (0.7 mL) was added allyltrimethylsilane **11** (23 μL, 0.162 mmol) at -78°C. After stirred at -78°C for the time indicated in Table 2, the reaction was quenched by adding saturated aqueous NaHCO₃ (1 mL). After warmed to room temperature, saturated NaCl aqueous solution was added, and the mixture was extracted with dichloromethane (three times). The combined organic layers were dried over Na₂SO₄, filtered and concentrated in vacuo. The residue was purified by column chromatography (AcOEt: hexanes, 1:4) to afford the corresponding *N'*-(1-isopropylbut-3-enyl)benzohydrazide **12** in high chemical yields as a white solid, mp 73-74°C. The enantiomeric ratio was determined by HPLC analysis using chiralpack AD column (flow rate 1 mL/min, iPrOH:Hexane 3:97, 30°C, *t_R* = 27.9 min(**12*R***) and *t_R* = 33.2 min (**12*S***); ¹H NMR (CDCl₃, 500 MHz) δ: 7.75-7.78 (m, 2H), 7.58 (bs, 1H), 7.53-7.45 (m, 1H), 7.45-7.40 (m, 2H), 6.00-5.90 (m, 1H), 5.23-5.10 (m, 2H), 2.90 (quint, 1H, *J* = 4.4 Hz), 2.35-2.25 (m, 1H), 2.19-2.10 (m, 1H), 1.85-1.95 (m, 1H), 0.93 (d, 3H, *J* = 6.8 Hz, CHMe₂), 0.92 (d, 3H, *J* = 6.8 Hz).

X-Ray Data for Compounds 4 *S_S* and 15*S_S*

Thermal ellipsoid plots (50% ellipsoids) of 4 *S_S*

Table 1. Crystal data and structure refinement for 4 *S_S*

Identification code	(Ss)-4	
Empirical formula	C ₁₀ H ₁₃ N O S	
Formula weight	195.27	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 5.9008(2) Å	α = 90°.
	b = 9.6079(3) Å	β = 90°.
	c = 17.7589(6) Å	γ = 90°.
Volume	1006.83(6) Å ³	
Z	4	
Density (calculated)	1.288 Mg/m ³	
Absorption coefficient	0.281 mm ⁻¹	
F(000)	416	
Crystal size	0.34 x 0.30 x 0.11 mm ³	

Theta range for data collection	2.29 to 30.56°.
Index ranges	-8<=h<=8, -13<=k<=13, -25<=l<=25
Reflections collected	11848
Independent reflections	3088 [R(int) = 0.0207]
Completeness to theta = 30.56°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9698 and 0.9105
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3088 / 0 / 118
Goodness-of-fit on F ²	1.045
Final R indices [I>2sigma(I)]	R1 = 0.0240, wR2 = 0.0648
R indices (all data)	R1 = 0.0248, wR2 = 0.0657
Absolute structure parameter	0.00(5)
Largest diff. peak and hole	0.340 and -0.195 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for **4 S₈**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	4342(1)	8221(1)	1588(1)	16(1)
O(1)	2645(1)	7705(1)	2142(1)	21(1)
N(1)	4520(2)	7129(1)	837(1)	17(1)
C(1)	2916(2)	6242(1)	772(1)	16(1)
C(2)	2843(2)	5234(1)	151(1)	16(1)
C(3)	4631(2)	5122(1)	-365(1)	19(1)
C(4)	4498(2)	4169(1)	-949(1)	22(1)
C(5)	2589(2)	3319(1)	-1028(1)	22(1)
C(6)	827(2)	3410(1)	-511(1)	22(1)
C(7)	957(2)	4367(1)	79(1)	19(1)
C(8)	7140(2)	7798(1)	1962(1)	15(1)
C(9)	7350(2)	6260(1)	2153(1)	20(1)
C(10)	7526(2)	8732(1)	2645(1)	20(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **4 S₅**

S(1)-O(1)	1.4894(8)	C(3)-C(2)-C(1)	121.31(9)
S(1)-N(1)	1.7002(9)	C(4)-C(3)-C(2)	119.85(10)
S(1)-C(8)	1.8257(10)	C(4)-C(3)-H(3)	120.1
N(1)-C(1)	1.2791(13)	C(2)-C(3)-H(3)	120.1
C(1)-C(2)	1.4678(13)	C(3)-C(4)-C(5)	120.37(10)
C(1)-H(1)	0.9500	C(3)-C(4)-H(4)	119.8
C(2)-C(7)	1.3963(14)	C(5)-C(4)-H(4)	119.8
C(2)-C(3)	1.4014(14)	C(6)-C(5)-C(4)	120.03(10)
C(3)-C(4)	1.3870(14)	C(6)-C(5)-H(5)	120.0
C(3)-H(3)	0.9500	C(4)-C(5)-H(5)	120.0
C(4)-C(5)	1.3985(16)	C(5)-C(6)-C(7)	119.75(10)
C(4)-H(4)	0.9500	C(5)-C(6)-H(6)	120.1
C(5)-C(6)	1.3891(16)	C(7)-C(6)-H(6)	120.1
C(5)-H(5)	0.9500	C(2)-C(7)-C(6)	120.37(10)
C(6)-C(7)	1.3963(14)	C(2)-C(7)-H(7)	119.8
C(6)-H(6)	0.9500	C(6)-C(7)-H(7)	119.8
C(7)-H(7)	0.9500	C(9)-C(8)-C(10)	112.42(8)
C(8)-C(9)	1.5221(14)	C(9)-C(8)-S(1)	111.77(7)
C(8)-C(10)	1.5252(13)	C(10)-C(8)-S(1)	107.06(7)
C(8)-H(8)	1.0000	C(9)-C(8)-H(8)	108.5
C(9)-H(9A)	0.9800	C(10)-C(8)-H(8)	108.5
C(9)-H(9B)	0.9800	S(1)-C(8)-H(8)	108.5
C(9)-H(9C)	0.9800	C(8)-C(9)-H(9A)	109.5
C(10)-H(10A)	0.9800	C(8)-C(9)-H(9B)	109.5
C(10)-H(10B)	0.9800	H(9A)-C(9)-H(9B)	109.5
C(10)-H(10C)	0.9800	C(8)-C(9)-H(9C)	109.5
		H(9A)-C(9)-H(9C)	109.5
O(1)-S(1)-N(1)	110.74(4)	H(9B)-C(9)-H(9C)	109.5
O(1)-S(1)-C(8)	107.08(5)	C(8)-C(10)-H(10A)	109.5
N(1)-S(1)-C(8)	95.29(4)	C(8)-C(10)-H(10B)	109.4
C(1)-N(1)-S(1)	115.87(7)	H(10A)-C(10)-H(10B)	109.5
N(1)-C(1)-C(2)	121.93(9)	C(8)-C(10)-H(10C)	109.5
N(1)-C(1)-H(1)	119.0	H(10A)-C(10)-H(10C)	109.5
C(2)-C(1)-H(1)	119.0	H(10B)-C(10)-H(10C)	109.5
C(7)-C(2)-C(3)	119.62(9)		
C(7)-C(2)-C(1)	119.07(9)		

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4 S₈**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	15(1)	14(1)	18(1)	0(1)	-2(1)	1(1)
O(1)	14(1)	28(1)	21(1)	-5(1)	2(1)	0(1)
N(1)	21(1)	17(1)	14(1)	0(1)	-1(1)	0(1)
C(1)	16(1)	17(1)	16(1)	1(1)	-1(1)	1(1)
C(2)	18(1)	15(1)	15(1)	1(1)	-1(1)	1(1)
C(3)	19(1)	19(1)	17(1)	2(1)	1(1)	0(1)
C(4)	24(1)	24(1)	17(1)	1(1)	3(1)	3(1)
C(5)	29(1)	21(1)	18(1)	-3(1)	-4(1)	4(1)
C(6)	24(1)	19(1)	23(1)	0(1)	-6(1)	-2(1)
C(7)	18(1)	20(1)	20(1)	0(1)	0(1)	0(1)
C(8)	12(1)	15(1)	18(1)	0(1)	0(1)	0(1)
C(9)	19(1)	16(1)	26(1)	1(1)	-3(1)	1(1)
C(10)	16(1)	21(1)	22(1)	-4(1)	-2(1)	-1(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **4 S₈**.

	x	y	z	U(eq)
H(1)	1737	6234	1136	19
H(3)	5931	5697	-314	22
H(4)	5711	4093	-1299	26
H(5)	2497	2678	-1434	27
H(6)	-461	2823	-559	26
H(7)	-245	4428	434	23
H(8)	8301	8032	1571	18
H(9A)	8893	6063	2328	30
H(9B)	7025	5702	1704	30
H(9C)	6266	6024	2552	30

H(10A)	6435	8492	3040	29
H(10B)	7320	9707	2498	29
H(10C)	9070	8597	2834	29

Table 6. Torsion angles [°] for **4 S_S**.

O(1)-S(1)-N(1)-C(1)	14.47(9)
C(8)-S(1)-N(1)-C(1)	124.98(8)
S(1)-N(1)-C(1)-C(2)	179.90(7)
N(1)-C(1)-C(2)-C(7)	-175.03(10)
N(1)-C(1)-C(2)-C(3)	5.44(15)
C(7)-C(2)-C(3)-C(4)	1.12(15)
C(1)-C(2)-C(3)-C(4)	-179.35(9)
C(2)-C(3)-C(4)-C(5)	0.01(15)
C(3)-C(4)-C(5)-C(6)	-1.05(16)
C(4)-C(5)-C(6)-C(7)	0.95(16)
C(3)-C(2)-C(7)-C(6)	-1.22(15)
C(1)-C(2)-C(7)-C(6)	179.24(9)
C(5)-C(6)-C(7)-C(2)	0.19(15)
O(1)-S(1)-C(8)-C(9)	53.69(8)
N(1)-S(1)-C(8)-C(9)	-59.92(8)
O(1)-S(1)-C(8)-C(10)	-69.83(7)
N(1)-S(1)-C(8)-C(10)	176.56(7)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **4 S_S** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(1)-H(1)...O(1)	0.95	2.34	2.8143(12)	110.4

Thermal ellipsoid plots (50% ellipsoids) of **15 S_s**

Table 1. Crystal data and structure refinement for **15 S_s**.

Identification code	(Ss)-15	
Empirical formula	C ₁₃ H ₁₆ Fe O S	
Formula weight	276.17	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P212121	
Unit cell dimensions	a = 5.9295(6) Å	α = 90°.
	b = 12.3312(12) Å	β = 90°.
	c = 16.8830(16) Å	γ = 90°.
Volume	1234.4(2) Å ³	
Z	4	
Density (calculated)	1.486 Mg/m ³	
Absorption coefficient	1.365 mm ⁻¹	
F(000)	576	

Crystal size	0.34 x 0.31 x 0.13 mm ³
Theta range for data collection	2.05 to 29.19°.
Index ranges	-8<=h<=7, -16<=k<=16, -22<=l<=17
Reflections collected	7761
Independent reflections	2933 [R(int) = 0.0381]
Completeness to theta = 27.50°	98.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8425 and 0.6539
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2933 / 0 / 145
Goodness-of-fit on F ²	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0373, wR2 = 0.0690
R indices (all data)	R1 = 0.0550, wR2 = 0.0742
Absolute structure parameter	0.00(2)
Largest diff. peak and hole	0.223 and -0.220 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for **15 S₈**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	8418(1)	2860(1)	7097(1)	39(1)
S(1)	7668(1)	4636(1)	8530(1)	44(1)
O(1)	5175(4)	4705(2)	8398(1)	66(1)
C(1)	8544(6)	3322(2)	8247(2)	37(1)
C(2)	10758(5)	3064(2)	7969(2)	40(1)
C(3)	10739(6)	1962(2)	7721(2)	49(1)
C(4)	8536(7)	1548(2)	7836(2)	53(1)
C(5)	7160(6)	2385(2)	8161(2)	45(1)
C(6)	7134(7)	4114(3)	6461(2)	61(1)
C(7)	9230(7)	3820(3)	6161(2)	63(1)
C(8)	9146(7)	2740(4)	5913(2)	66(1)
C(9)	6967(7)	2356(3)	6068(2)	62(1)
C(10)	5715(6)	3205(3)	6402(2)	65(1)
C(11)	8052(5)	4561(2)	9598(2)	44(1)
C(12)	10571(5)	4509(3)	9782(2)	60(1)
C(13)	6720(7)	3652(3)	9970(2)	62(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **15 S₅**.

Fe(1)-C(1)	2.025(3)
Fe(1)-C(6)	2.031(3)
Fe(1)-C(5)	2.031(3)
Fe(1)-C(10)	2.032(3)
Fe(1)-C(7)	2.033(3)
Fe(1)-C(9)	2.035(3)
Fe(1)-C(2)	2.038(3)
Fe(1)-C(4)	2.044(3)
Fe(1)-C(8)	2.050(3)
Fe(1)-C(3)	2.057(3)
S(1)-O(1)	1.497(2)
S(1)-C(1)	1.767(3)
S(1)-C(11)	1.821(3)
C(1)-C(5)	1.425(4)
C(1)-C(2)	1.430(4)
C(2)-C(3)	1.422(4)
C(2)-H(2)	0.9300
C(3)-C(4)	1.415(5)
C(3)-H(3)	0.9300
C(4)-C(5)	1.426(4)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(6)-C(7)	1.390(5)
C(6)-C(10)	1.406(5)
C(6)-H(6)	0.9300
C(7)-C(8)	1.397(5)
C(7)-H(7)	0.9300
C(8)-C(9)	1.401(5)
C(8)-H(8)	0.9300
C(9)-C(10)	1.401(5)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-C(13)	1.509(4)
C(11)-C(12)	1.527(4)
C(11)-H(11)	0.9800
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600

C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(1)-Fe(1)-C(6)	107.84(13)
C(1)-Fe(1)-C(5)	41.12(11)
C(6)-Fe(1)-C(5)	123.32(15)
C(1)-Fe(1)-C(10)	121.61(14)
C(6)-Fe(1)-C(10)	40.50(14)
C(5)-Fe(1)-C(10)	106.34(14)
C(1)-Fe(1)-C(7)	124.96(14)
C(6)-Fe(1)-C(7)	40.02(14)
C(5)-Fe(1)-C(7)	160.48(15)
C(10)-Fe(1)-C(7)	67.41(15)
C(1)-Fe(1)-C(9)	156.87(15)
C(6)-Fe(1)-C(9)	67.86(14)
C(5)-Fe(1)-C(9)	120.74(14)
C(10)-Fe(1)-C(9)	40.30(14)
C(7)-Fe(1)-C(9)	67.33(15)
C(1)-Fe(1)-C(2)	41.21(12)
C(6)-Fe(1)-C(2)	122.90(14)
C(5)-Fe(1)-C(2)	69.31(13)
C(10)-Fe(1)-C(2)	158.19(14)
C(7)-Fe(1)-C(2)	109.19(14)
C(9)-Fe(1)-C(2)	160.32(14)
C(1)-Fe(1)-C(4)	68.68(11)
C(6)-Fe(1)-C(4)	159.75(16)
C(5)-Fe(1)-C(4)	40.95(12)
C(10)-Fe(1)-C(4)	123.02(15)
C(7)-Fe(1)-C(4)	158.03(16)
C(9)-Fe(1)-C(4)	107.06(14)
C(2)-Fe(1)-C(4)	68.50(13)
C(1)-Fe(1)-C(8)	161.33(15)
C(6)-Fe(1)-C(8)	67.58(15)
C(5)-Fe(1)-C(8)	156.73(15)
C(10)-Fe(1)-C(8)	67.55(15)
C(7)-Fe(1)-C(8)	40.01(14)
C(9)-Fe(1)-C(8)	40.11(14)

C(2)-Fe(1)-C(8)	124.73(14)
C(4)-Fe(1)-C(8)	122.04(15)
C(1)-Fe(1)-C(3)	68.62(11)
C(6)-Fe(1)-C(3)	158.71(15)
C(5)-Fe(1)-C(3)	68.73(12)
C(10)-Fe(1)-C(3)	159.46(15)
C(7)-Fe(1)-C(3)	123.62(15)
C(9)-Fe(1)-C(3)	123.75(13)
C(2)-Fe(1)-C(3)	40.62(11)
C(4)-Fe(1)-C(3)	40.38(13)
C(8)-Fe(1)-C(3)	108.66(13)
O(1)-S(1)-C(1)	107.60(15)
O(1)-S(1)-C(11)	105.87(14)
C(1)-S(1)-C(11)	100.61(13)
C(5)-C(1)-C(2)	108.3(2)
C(5)-C(1)-S(1)	127.0(2)
C(2)-C(1)-S(1)	124.3(2)
C(5)-C(1)-Fe(1)	69.65(15)
C(2)-C(1)-Fe(1)	69.88(15)
S(1)-C(1)-Fe(1)	120.39(14)
C(3)-C(2)-C(1)	107.6(3)
C(3)-C(2)-Fe(1)	70.39(17)
C(1)-C(2)-Fe(1)	68.91(15)
C(3)-C(2)-H(2)	126.2
C(1)-C(2)-H(2)	126.2
Fe(1)-C(2)-H(2)	126.1
C(4)-C(3)-C(2)	108.2(3)
C(4)-C(3)-Fe(1)	69.33(17)
C(2)-C(3)-Fe(1)	68.99(15)
C(4)-C(3)-H(3)	125.9
C(2)-C(3)-H(3)	125.9
Fe(1)-C(3)-H(3)	127.3
C(3)-C(4)-C(5)	108.6(3)
C(3)-C(4)-Fe(1)	70.29(17)
C(5)-C(4)-Fe(1)	69.03(15)
C(3)-C(4)-H(4)	125.7
C(5)-C(4)-H(4)	125.7
Fe(1)-C(4)-H(4)	126.5

C(1)-C(5)-C(4)	107.3(3)
C(1)-C(5)-Fe(1)	69.22(15)
C(4)-C(5)-Fe(1)	70.01(17)
C(1)-C(5)-H(5)	126.4
C(4)-C(5)-H(5)	126.3
Fe(1)-C(5)-H(5)	126.0
C(7)-C(6)-C(10)	107.5(3)
C(7)-C(6)-Fe(1)	70.1(2)
C(10)-C(6)-Fe(1)	69.79(19)
C(7)-C(6)-H(6)	126.2
C(10)-C(6)-H(6)	126.2
Fe(1)-C(6)-H(6)	125.4
C(6)-C(7)-C(8)	109.0(4)
C(6)-C(7)-Fe(1)	69.9(2)
C(8)-C(7)-Fe(1)	70.66(19)
C(6)-C(7)-H(7)	125.5
C(8)-C(7)-H(7)	125.5
Fe(1)-C(7)-H(7)	125.6
C(7)-C(8)-C(9)	107.4(4)
C(7)-C(8)-Fe(1)	69.3(2)
C(9)-C(8)-Fe(1)	69.4(2)
C(7)-C(8)-H(8)	126.3
C(9)-C(8)-H(8)	126.3
Fe(1)-C(8)-H(8)	126.6
C(8)-C(9)-C(10)	108.1(3)
C(8)-C(9)-Fe(1)	70.5(2)
C(10)-C(9)-Fe(1)	69.71(19)
C(8)-C(9)-H(9)	125.9
C(10)-C(9)-H(9)	126.0
Fe(1)-C(9)-H(9)	125.4
C(9)-C(10)-C(6)	107.9(3)
C(9)-C(10)-Fe(1)	70.0(2)
C(6)-C(10)-Fe(1)	69.71(19)
C(9)-C(10)-H(10)	126.1
C(6)-C(10)-H(10)	126.0
Fe(1)-C(10)-H(10)	125.8
C(13)-C(11)-C(12)	113.4(3)
C(13)-C(11)-S(1)	112.6(2)

C(12)-C(11)-S(1)	109.0(2)
C(13)-C(11)-H(11)	107.2
C(12)-C(11)-H(11)	107.2
S(1)-C(11)-H(11)	107.2
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.3
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.6
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.6
C(11)-C(13)-H(13B)	109.4
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **15** S_s . The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	46(1)	39(1)	32(1)	0(1)	-4(1)	2(1)
S(1)	55(1)	35(1)	41(1)	3(1)	2(1)	8(1)
O(1)	56(2)	73(2)	70(2)	-11(1)	-12(1)	27(1)
C(1)	45(2)	35(1)	30(1)	2(1)	-4(1)	0(2)
C(2)	43(2)	43(2)	34(2)	-1(1)	-7(1)	7(1)
C(3)	58(2)	48(2)	41(2)	-3(1)	-6(1)	19(2)
C(4)	81(2)	34(2)	44(2)	2(1)	-8(2)	-1(2)
C(5)	52(2)	44(2)	40(2)	7(1)	1(1)	-1(2)
C(6)	87(3)	59(2)	38(2)	10(2)	-11(2)	17(2)
C(7)	71(3)	75(3)	43(2)	20(2)	-9(2)	-12(2)
C(8)	77(3)	87(3)	35(2)	1(2)	5(2)	15(2)
C(9)	77(3)	72(2)	38(2)	-10(2)	-15(2)	-6(2)
C(10)	47(2)	105(3)	44(2)	9(2)	-9(2)	10(2)
C(11)	50(2)	42(2)	38(2)	-7(1)	6(1)	6(2)

C(12)	57(2)	72(2)	52(2)	-11(2)	-5(2)	-2(2)
C(13)	64(2)	71(2)	50(2)	8(2)	11(2)	-3(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **15** *S*₈.

	x	y	z	U(eq)
H(2)	11987	3532	7953	48
H(3)	11962	1580	7519	59
H(4)	8065	847	7718	63
H(5)	5642	2330	8292	54
H(6)	6743	4789	6665	73
H(7)	10485	4270	6129	75
H(8)	10321	2348	5687	80
H(9)	6444	1659	5968	75
H(10)	4211	3172	6556	78
H(11)	7482	5241	9822	52
H(12A)	10803	4606	10340	90
H(12B)	11337	5074	9497	90
H(12C)	11158	3817	9622	90
H(13A)	7437	2971	9857	93
H(13B)	5219	3649	9756	93
H(13C)	6651	3758	10533	93

Table 6. Torsion angles [$^\circ$] for **15** *S*₈.

O(1)-S(1)-C(1)-C(5)	-19.0(3)
C(11)-S(1)-C(1)-C(5)	91.6(2)
O(1)-S(1)-C(1)-C(2)	152.7(2)
C(11)-S(1)-C(1)-C(2)	-96.8(2)
O(1)-S(1)-C(1)-Fe(1)	67.4(2)
C(11)-S(1)-C(1)-Fe(1)	178.00(18)
C(6)-Fe(1)-C(1)-C(5)	120.6(2)
C(10)-Fe(1)-C(1)-C(5)	78.3(2)
C(7)-Fe(1)-C(1)-C(5)	161.4(2)

C(9)-Fe(1)-C(1)-C(5)	45.3(4)
C(2)-Fe(1)-C(1)-C(5)	-119.5(2)
C(4)-Fe(1)-C(1)-C(5)	-38.22(18)
C(8)-Fe(1)-C(1)-C(5)	-166.8(4)
C(3)-Fe(1)-C(1)-C(5)	-81.72(19)
C(6)-Fe(1)-C(1)-C(2)	-119.9(2)
C(5)-Fe(1)-C(1)-C(2)	119.5(2)
C(10)-Fe(1)-C(1)-C(2)	-162.2(2)
C(7)-Fe(1)-C(1)-C(2)	-79.1(2)
C(9)-Fe(1)-C(1)-C(2)	164.8(3)
C(4)-Fe(1)-C(1)-C(2)	81.29(19)
C(8)-Fe(1)-C(1)-C(2)	-47.3(5)
C(3)-Fe(1)-C(1)-C(2)	37.80(17)
C(6)-Fe(1)-C(1)-S(1)	-1.2(2)
C(5)-Fe(1)-C(1)-S(1)	-121.8(3)
C(10)-Fe(1)-C(1)-S(1)	-43.5(2)
C(7)-Fe(1)-C(1)-S(1)	39.6(3)
C(9)-Fe(1)-C(1)-S(1)	-76.5(4)
C(2)-Fe(1)-C(1)-S(1)	118.7(3)
C(4)-Fe(1)-C(1)-S(1)	-160.0(3)
C(8)-Fe(1)-C(1)-S(1)	71.4(5)
C(3)-Fe(1)-C(1)-S(1)	156.5(2)
C(5)-C(1)-C(2)-C(3)	-0.8(3)
S(1)-C(1)-C(2)-C(3)	-173.7(2)
Fe(1)-C(1)-C(2)-C(3)	-60.02(19)
C(5)-C(1)-C(2)-Fe(1)	59.26(18)
S(1)-C(1)-C(2)-Fe(1)	-113.7(2)
C(1)-Fe(1)-C(2)-C(3)	118.8(2)
C(6)-Fe(1)-C(2)-C(3)	-161.9(2)
C(5)-Fe(1)-C(2)-C(3)	81.05(19)
C(10)-Fe(1)-C(2)-C(3)	163.3(3)
C(7)-Fe(1)-C(2)-C(3)	-119.7(2)
C(9)-Fe(1)-C(2)-C(3)	-43.5(5)
C(4)-Fe(1)-C(2)-C(3)	37.02(18)
C(8)-Fe(1)-C(2)-C(3)	-77.9(2)
C(6)-Fe(1)-C(2)-C(1)	79.4(2)
C(5)-Fe(1)-C(2)-C(1)	-37.72(16)
C(10)-Fe(1)-C(2)-C(1)	44.6(4)

C(7)-Fe(1)-C(2)-C(1)	121.57(19)
C(9)-Fe(1)-C(2)-C(1)	-162.2(4)
C(4)-Fe(1)-C(2)-C(1)	-81.75(18)
C(8)-Fe(1)-C(2)-C(1)	163.36(19)
C(3)-Fe(1)-C(2)-C(1)	-118.8(2)
C(1)-C(2)-C(3)-C(4)	0.7(3)
Fe(1)-C(2)-C(3)-C(4)	-58.4(2)
C(1)-C(2)-C(3)-Fe(1)	59.09(18)
C(1)-Fe(1)-C(3)-C(4)	81.81(19)
C(6)-Fe(1)-C(3)-C(4)	166.2(3)
C(5)-Fe(1)-C(3)-C(4)	37.51(18)
C(10)-Fe(1)-C(3)-C(4)	-42.2(5)
C(7)-Fe(1)-C(3)-C(4)	-159.6(2)
C(9)-Fe(1)-C(3)-C(4)	-76.0(2)
C(2)-Fe(1)-C(3)-C(4)	120.1(3)
C(8)-Fe(1)-C(3)-C(4)	-117.9(2)
C(1)-Fe(1)-C(3)-C(2)	-38.33(17)
C(6)-Fe(1)-C(3)-C(2)	46.0(4)
C(5)-Fe(1)-C(3)-C(2)	-82.63(19)
C(10)-Fe(1)-C(3)-C(2)	-162.3(4)
C(7)-Fe(1)-C(3)-C(2)	80.3(2)
C(9)-Fe(1)-C(3)-C(2)	163.82(19)
C(4)-Fe(1)-C(3)-C(2)	-120.1(3)
C(8)-Fe(1)-C(3)-C(2)	122.0(2)
C(2)-C(3)-C(4)-C(5)	-0.4(3)
Fe(1)-C(3)-C(4)-C(5)	-58.5(2)
C(2)-C(3)-C(4)-Fe(1)	58.2(2)
C(1)-Fe(1)-C(4)-C(3)	-81.66(19)
C(6)-Fe(1)-C(4)-C(3)	-165.5(3)
C(5)-Fe(1)-C(4)-C(3)	-120.0(3)
C(10)-Fe(1)-C(4)-C(3)	163.7(2)
C(7)-Fe(1)-C(4)-C(3)	50.9(4)
C(9)-Fe(1)-C(4)-C(3)	122.4(2)
C(2)-Fe(1)-C(4)-C(3)	-37.24(17)
C(8)-Fe(1)-C(4)-C(3)	81.2(2)
C(1)-Fe(1)-C(4)-C(5)	38.38(18)
C(6)-Fe(1)-C(4)-C(5)	-45.4(4)
C(10)-Fe(1)-C(4)-C(5)	-76.3(2)

C(7)-Fe(1)-C(4)-C(5)	171.0(3)
C(9)-Fe(1)-C(4)-C(5)	-117.5(2)
C(2)-Fe(1)-C(4)-C(5)	82.8(2)
C(8)-Fe(1)-C(4)-C(5)	-158.8(2)
C(3)-Fe(1)-C(4)-C(5)	120.0(3)
C(2)-C(1)-C(5)-C(4)	0.5(3)
S(1)-C(1)-C(5)-C(4)	173.3(2)
Fe(1)-C(1)-C(5)-C(4)	59.94(19)
C(2)-C(1)-C(5)-Fe(1)	-59.39(19)
S(1)-C(1)-C(5)-Fe(1)	113.3(2)
C(3)-C(4)-C(5)-C(1)	-0.1(3)
Fe(1)-C(4)-C(5)-C(1)	-59.43(18)
C(3)-C(4)-C(5)-Fe(1)	59.3(2)
C(6)-Fe(1)-C(5)-C(1)	-78.7(2)
C(10)-Fe(1)-C(5)-C(1)	-119.6(2)
C(7)-Fe(1)-C(5)-C(1)	-51.4(5)
C(9)-Fe(1)-C(5)-C(1)	-161.03(19)
C(2)-Fe(1)-C(5)-C(1)	37.80(17)
C(4)-Fe(1)-C(5)-C(1)	118.4(3)
C(8)-Fe(1)-C(5)-C(1)	169.4(3)
C(3)-Fe(1)-C(5)-C(1)	81.44(18)
C(1)-Fe(1)-C(5)-C(4)	-118.4(3)
C(6)-Fe(1)-C(5)-C(4)	162.8(2)
C(10)-Fe(1)-C(5)-C(4)	121.9(2)
C(7)-Fe(1)-C(5)-C(4)	-169.9(4)
C(9)-Fe(1)-C(5)-C(4)	80.5(2)
C(2)-Fe(1)-C(5)-C(4)	-80.6(2)
C(8)-Fe(1)-C(5)-C(4)	50.9(4)
C(3)-Fe(1)-C(5)-C(4)	-37.00(19)
C(1)-Fe(1)-C(6)-C(7)	123.6(2)
C(5)-Fe(1)-C(6)-C(7)	166.2(2)
C(10)-Fe(1)-C(6)-C(7)	-118.3(3)
C(9)-Fe(1)-C(6)-C(7)	-80.7(2)
C(2)-Fe(1)-C(6)-C(7)	80.7(2)
C(4)-Fe(1)-C(6)-C(7)	-159.8(3)
C(8)-Fe(1)-C(6)-C(7)	-37.1(2)
C(3)-Fe(1)-C(6)-C(7)	46.8(4)
C(1)-Fe(1)-C(6)-C(10)	-118.1(2)

C(5)-Fe(1)-C(6)-C(10)	-75.4(2)
C(7)-Fe(1)-C(6)-C(10)	118.3(3)
C(9)-Fe(1)-C(6)-C(10)	37.7(2)
C(2)-Fe(1)-C(6)-C(10)	-161.0(2)
C(4)-Fe(1)-C(6)-C(10)	-41.5(5)
C(8)-Fe(1)-C(6)-C(10)	81.2(2)
C(3)-Fe(1)-C(6)-C(10)	165.1(3)
C(10)-C(6)-C(7)-C(8)	0.0(4)
Fe(1)-C(6)-C(7)-C(8)	60.1(2)
C(10)-C(6)-C(7)-Fe(1)	-60.0(2)
C(1)-Fe(1)-C(7)-C(6)	-75.4(3)
C(5)-Fe(1)-C(7)-C(6)	-36.6(5)
C(10)-Fe(1)-C(7)-C(6)	38.2(2)
C(9)-Fe(1)-C(7)-C(6)	82.1(2)
C(2)-Fe(1)-C(7)-C(6)	-118.7(2)
C(4)-Fe(1)-C(7)-C(6)	161.4(4)
C(8)-Fe(1)-C(7)-C(6)	119.7(3)
C(3)-Fe(1)-C(7)-C(6)	-161.5(2)
C(1)-Fe(1)-C(7)-C(8)	164.8(2)
C(6)-Fe(1)-C(7)-C(8)	-119.7(3)
C(5)-Fe(1)-C(7)-C(8)	-156.3(4)
C(10)-Fe(1)-C(7)-C(8)	-81.5(3)
C(9)-Fe(1)-C(7)-C(8)	-37.7(2)
C(2)-Fe(1)-C(7)-C(8)	121.6(2)
C(4)-Fe(1)-C(7)-C(8)	41.6(5)
C(3)-Fe(1)-C(7)-C(8)	78.8(3)
C(6)-C(7)-C(8)-C(9)	-0.4(4)
Fe(1)-C(7)-C(8)-C(9)	59.1(2)
C(6)-C(7)-C(8)-Fe(1)	-59.6(2)
C(1)-Fe(1)-C(8)-C(7)	-42.1(6)
C(6)-Fe(1)-C(8)-C(7)	37.2(2)
C(5)-Fe(1)-C(8)-C(7)	160.2(3)
C(10)-Fe(1)-C(8)-C(7)	81.1(3)
C(9)-Fe(1)-C(8)-C(7)	118.9(3)
C(2)-Fe(1)-C(8)-C(7)	-78.2(3)
C(4)-Fe(1)-C(8)-C(7)	-163.0(2)
C(3)-Fe(1)-C(8)-C(7)	-120.5(2)
C(1)-Fe(1)-C(8)-C(9)	-161.1(4)

C(6)-Fe(1)-C(8)-C(9)	-81.8(2)
C(5)-Fe(1)-C(8)-C(9)	41.2(5)
C(10)-Fe(1)-C(8)-C(9)	-37.8(2)
C(7)-Fe(1)-C(8)-C(9)	-118.9(3)
C(2)-Fe(1)-C(8)-C(9)	162.8(2)
C(4)-Fe(1)-C(8)-C(9)	78.1(3)
C(3)-Fe(1)-C(8)-C(9)	120.6(2)
C(7)-C(8)-C(9)-C(10)	0.7(4)
Fe(1)-C(8)-C(9)-C(10)	59.8(2)
C(7)-C(8)-C(9)-Fe(1)	-59.1(2)
C(1)-Fe(1)-C(9)-C(8)	164.7(3)
C(6)-Fe(1)-C(9)-C(8)	81.0(3)
C(5)-Fe(1)-C(9)-C(8)	-162.4(2)
C(10)-Fe(1)-C(9)-C(8)	118.9(3)
C(7)-Fe(1)-C(9)-C(8)	37.6(2)
C(2)-Fe(1)-C(9)-C(8)	-46.1(5)
C(4)-Fe(1)-C(9)-C(8)	-119.8(2)
C(3)-Fe(1)-C(9)-C(8)	-78.7(3)
C(1)-Fe(1)-C(9)-C(10)	45.8(4)
C(6)-Fe(1)-C(9)-C(10)	-37.9(2)
C(5)-Fe(1)-C(9)-C(10)	78.8(2)
C(7)-Fe(1)-C(9)-C(10)	-81.3(2)
C(2)-Fe(1)-C(9)-C(10)	-165.0(4)
C(4)-Fe(1)-C(9)-C(10)	121.3(2)
C(8)-Fe(1)-C(9)-C(10)	-118.9(3)
C(3)-Fe(1)-C(9)-C(10)	162.4(2)
C(8)-C(9)-C(10)-C(6)	-0.7(4)
Fe(1)-C(9)-C(10)-C(6)	59.6(2)
C(8)-C(9)-C(10)-Fe(1)	-60.3(2)
C(7)-C(6)-C(10)-C(9)	0.4(4)
Fe(1)-C(6)-C(10)-C(9)	-59.8(2)
C(7)-C(6)-C(10)-Fe(1)	60.2(2)
C(1)-Fe(1)-C(10)-C(9)	-160.7(2)
C(6)-Fe(1)-C(10)-C(9)	118.9(3)
C(5)-Fe(1)-C(10)-C(9)	-118.5(2)
C(7)-Fe(1)-C(10)-C(9)	81.1(2)
C(2)-Fe(1)-C(10)-C(9)	166.4(3)
C(4)-Fe(1)-C(10)-C(9)	-77.0(3)

C(8)-Fe(1)-C(10)-C(9)	37.6(2)
C(3)-Fe(1)-C(10)-C(9)	-45.7(5)
C(1)-Fe(1)-C(10)-C(6)	80.4(2)
C(5)-Fe(1)-C(10)-C(6)	122.6(2)
C(7)-Fe(1)-C(10)-C(6)	-37.8(2)
C(9)-Fe(1)-C(10)-C(6)	-118.9(3)
C(2)-Fe(1)-C(10)-C(6)	47.5(5)
C(4)-Fe(1)-C(10)-C(6)	164.1(2)
C(8)-Fe(1)-C(10)-C(6)	-81.3(2)
C(3)-Fe(1)-C(10)-C(6)	-164.6(3)
O(1)-S(1)-C(11)-C(13)	54.3(3)
C(1)-S(1)-C(11)-C(13)	-57.6(3)
O(1)-S(1)-C(11)-C(12)	-179.0(2)
C(1)-S(1)-C(11)-C(12)	69.1(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **15** S_8 [$\text{\AA}$ and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
C(2)-H(2)...O(1)#1	0.93	2.50	3.388(4)	160.8

Symmetry transformations used to generate equivalent atoms:

#1 $x+1,y,z$