Supporting Information

Poly(thiaheterohelicene): A Stiff Conjugated Helical Polymer Comprised of Fused Benzothiophene rings

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Molecular design to form helical structure through the intramolecular ring-closing.

Figure S1. Schematic representation of intramolecular ring-closing reaction to form helical structure without (a) and with (b) 2-methyl group.

Experimental Section

Preparations

1,5-Dibromo-2,4-bis(methylthio)benzene was prepared according to the previous paper reported by research group at Waseda (K. Miyatake, A. S. Hay, F. Mitsuhashi, E. Tsuchida, *Macromolecules*, **2001**, *34*, 2385-2388).

2,6-Dibromo-4-nitrotoluene (1). Bromine (42.0 g, 260 mmol) was added dropwisely to a solution of *p*-nitrotoluene (10.0 g, 36.0 mmol) and iron powder (0.80 g, 14.1 mmol) in chloroform (20 ml) at 0 °C. The mixture was refluxed at 50 °C for 24 hr. The reaction mixture was cooled to 0 °C and neutralized with a saturated aqueous sodium sulfite solution. After extraction with chloroform, the organic phase was washed with aqueous sodium carbonate solution (one time) and water (two times), dried over anhydrous sodium sulfate and concentrated. The crude product was recovered by vacuum distillation (100 °C / 1 mmHg), and then the obtained yellow solid was purified by recrystallization from hexane to yield yellow rod-like crystals (13.1 g, 44.6 mmol, 60%). Yield: 60%. ¹H NMR (CDCl₃, 500 MHz; ppm): δ 8.37 (s, 2H), 2.67 (s, 3H). ¹³C NMR (CDCl₃, 125 MHz; ppm): δ 146.2, 135.2, 126.6, 125.3, 24.2. MS (EI, m/z) 294 (M⁺), 294.93 (calcd). Anal. Calcd for C, 28.5; H, 1.7. Found: C, 28.1; H, 1.5.

4-Amino-2,6-dibromotoluene (2). **1** (21.92 g, 74.3 mmol) was dissolved in 2-methoxyethanol (200 ml) under Ar. Sodium dithionite (61.9 g, 355 mmol) and water (200 ml) were added to the solution, the heterogeneous mixture was stirred and heated at 110 °C for 3 hr. After cooling to 50 °C and addition of water (150 ml) and 10 N hydrochloric acid (150 ml), the result mixture was refluxed for further 15 min. The white suspension was poured into a saturated aqueous sodium carbonate solution (500 ml), and the mixture was stirred under basic condition for overnight (> 12 hr). The insoluble material was recovered by filtration, dissolved in chloroform and washed with water. The organic phase was dried and concentrated, the residue was purified by silica gel filtration with hexane as the first eluent (exclusion of by-product) and chloroform as the second eluent (recovery of the crude product). The obtained crude product was recrystallized from hexane and chloroform mixture to

give white needle crystals (14.8 g, 55.7 mmol). Yield: 75%. ^1H NMR (CDCl_3 , 500 MHz; ppm): δ 6.86 (s, 2H), 3.60 (s, 2H), 2.43 (s, 3H). ^{13}C NMR (CDCl_3 , 125 MHz; ppm): δ 145.8, 126.5, 125.3, 118.3, 22.4. MS (EI, m/z) 264 (M^+), 264.95 (calcd). IR (KBr, cm^{-1}): 3288, 3170 (ν_{NH_2}). Anal. Calcd for C, 31.7; H, 2.7. Found: C, 31.3; H, 2.5.

2,6-Dibromotoluene (3). 98% sulfuric acid (27 ml, 49.4 g, 500 mmol), water (50 ml) and **2** (27.3 g, 103 mmol) were stirred in a 300 ml beaker at 80°C for 1 hr. The mixture was cooled to 0 °C, a aqueous solution (50 ml) of sodium nitrite (27.6 g, 400 mmol) was added dropwisely for 1 hr. After stirring at r.t. for 3 hr, the formed white suspension was dropped slowly into 32–34 wt% aqueous phosphinic acid solution (500 mmol, 103 g as a aqueous solution) and the reaction mixture was stirred vigorously at r.t. for 12 hr. After the extraction with chloroform, washing with water, and drying, the organic solution was concentrated. The residue was vacuum distilled (83 °C / 20 mmHg) to obtain the product as a transparent liquid (21.1 g, 84.5 mmol). Yield: 82%. ^1H NMR (CDCl_3 , 500 MHz; ppm): δ 7.46 (d, $J = 8.2$ Hz, 2H), 6.86 (t, $J = 8.2$ Hz, 1H), 2.54 (s, 3H). ^{13}C NMR (CDCl_3 , 125 MHz; ppm): δ 137.4, 131.8, 128.1, 125.4, 23.7. MS (EI, m/z) 249 (M^+), 249.93 (calcd). Anal. Calcd for C, 33.6; H, 2.4. Found: C, 33.9; H, 2.2.

2-Methyl-1,3-phenylenebis(pinacol borate) (4). Magnesium turnings (1.22 g, 50 mmol) were stirred in a three-necked flask under argon at 120°C for 12 hr. After cooling to room temperature, THF (100 ml) was added and the mixture was cooled to 0°C. A THF (50 ml) solution of 2,6-dibromotoluene (4.97 g, 20 mmol) was slowly added and refluxed at 70 °C for 3 hr to afford the Grignard reagent. The solution was cooled to room temperature, 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (9.30 g, 50 mmol) was added and the mixture was heated at 70°C for 24hr. The insoluble part was filtered off, and the organic solvent was removed by evaporation. The residue was dissolved in boiled hexane (1 l) and the insoluble part was filtered off. After drying and evaporation of the filtrate, the residue was purified by silica gel (treated with triethylamine) column chromatography with a chloroform/hexane (v/v = 2/1) mixture as the eluent and recrystallized from hexane to give white cubic crystals (4.9 g, 15.5 mmol). Yield: 62%. ^1H

NMR (CDCl₃, 500 MHz; ppm): δ 7.79 (d, J = 7.5 Hz, 2H), 7.14 (t, J = 7.5 Hz, 1H), 2.74 (s, 3H), 1.34 (s, 24H). ¹³C NMR (CDCl₃, 125 MHz; ppm): δ 151.3, 141.2, 138.2, 123.9, 83.4, 24.9, 21.1. IR (KBr, cm⁻¹): 1328 ($\nu_{\text{B-O}}$). MS (EI, m/z): 343 (M⁺), 344.06 (calcd). Anal. Calcd for C₁₉H₃₀B₂O₄: C, 66.3; H, 8.8. Found: C, 66.4; H, 8.9. m. p. = 101°C.

1,3-Bis(((S)-(+)-2-methylbutylthio)benzene (5). THF (15 ml) and sodium hydride (0.60 g, 25 mmol) was stirred under argon at room temperature. A THF (10 ml) solution of 1,3-benzenedithiol (1.42 g, 10 mmol) was dropwise added to the mixture, and the solution was stirred at room temperature for 30 min until the thiorate anion was completely formed (hydrogen gas decreased). (S)-(+)-1-Iodo-2-methylbutane (4.95 g, 25 mmol) was added and then stirred at room temperature for 4 hr. To quench the sodium hydride, an excess of methanol was added to the reaction mixture. After evaporation of the organic solvent, the residue was dissolved in chloroform and washed with water. The organic phase was dried and concentrated, and the product was obtained as a transparent pale oil (2.51 g, 8.9 mmol), without further purification for characterization and the following reaction. Yield: 89%. ¹H NMR (CDCl₃, 500 MHz; ppm): δ 7.24 (s, 1H), 7.15 (t, J = 8.2 Hz, 1H), 7.08 (d, J = 8.2 Hz, 2H), 2.93 (dd, 2J = -12.5 Hz, 3J = 6.1 Hz, 2H), 2.74 (dd, 2J = -12.5 Hz, 3J = 7.3 Hz, 2H), 1.69 (m, 3J = 6.8 Hz, 3J = 7.1 Hz, 3J = 6.1 Hz, 2H), 1.53 (m, 2J = -12.8 Hz, 3J = 5.3 Hz, 3J = 6.5 Hz, 2H), 1.31 (m, 2J = -13.4 Hz, 3J = 6.1 Hz, 3J = 7.3 Hz, 2H), 1.06 (d, 3J = 6.7 Hz, 6H), 0.93 (t, 3J = 7.6 Hz, 6H). ¹³C NMR (CDCl₃, 125 MHz; ppm): δ 138.3, 134.2, 128.7, 125.9, 40.2, 35.0, 28.5, 18.9, 11.4. IR (KBr, cm⁻¹): 2931 ($\nu_{\text{aromaticC-H}}$), 855 ($\delta_{\text{aromaticC-H}}$). MS (EI, m/z): 282 (M⁺), 282.51 (calcd). Anal. Calcd for C₁₆H₂₆S₂: C, 68.0; H, 9.2. Found: C, 67.8; H, 9.4.

1,5-Dibromo-2,4-bis((S)-(+)-2-methylbutylthio)benzene (6). **5** (1.41 g, 5.0 mmol) was dissolved in chloroform (10 ml) and the solution was stirred at 0°C. Bromine (1.95 g, 12.5 mmol) was added to the solution and stirred at 0°C for 30 min. The reaction mixture was neutralized with a saturated aqueous sodium sulfite solution. The organic layer was extracted and washed with an aqueous sodium carbonate solution and water. The organic solvent was evaporated, and the residue was purified by column chromatography with the hexane and chloroform mixture (v/v = 1/1) to yield

transparent pale oil (2.03 g, 4.6 mmol). Yield: 92%. ^1H NMR (CDCl_3 , 500 MHz; ppm): δ 7.68 (s, 1H), 7.08 (s, 1H), 2.94 (dd, $^2J = -12.2$ Hz, $^3J = 5.7$ Hz, 2H), 2.72 (dd, $^2J = -12.2$ Hz, $^3J = 7.6$ Hz, 2H), 1.69 (m, $^3J = 6.2$ Hz, $^3J = 7.3$ Hz, $^3J = 5.7$ Hz, 2H), 1.56 (m, $^2J = -13.1$ Hz, $^3J = 5.2$ Hz, $^3J = 6.7$ Hz, 2H), 1.30 (m, $^2J = -13.7$ Hz, $^3J = 6.4$ Hz, $^3J = 7.4$ Hz, 2H), 1.06 (d, $^3J = 6.7$ Hz, 6H), 0.92 (t, $^3J = 7.6$ Hz, 6H). ^{13}C NMR (CDCl_3 , 125 MHz; ppm): δ 138.6, 135.9, 127.2, 120.2, 40.6, 34.2, 28.9, 19.0, 11.3. IR (KBr, cm^{-1}): 2942 ($\nu_{\text{aromatic C-H}}$), 867 ($\delta_{\text{aromatic C-H}}$). MS (EI, m/z): 440 (M^+), 440.30 (calcd). Anal. Calcd for $\text{C}_{16}\text{H}_{24}\text{Br}_2\text{S}_2$: C, 43.6; H, 5.5. Found: C, 43.3; H, 5.8.

Figure S2. ^1H -NMR spectrum of **6** in CDCl_3 .

¹H-NMR of oxidized-6: **oxidized-6** was prepared according to the same manner for the oxidation of **Tri-S**.

Figure S3. ¹H-NMR spectrum of **oxidized-6** in CD₂Cl₂.

Poly[4,6-bis((S)-(+)-2-methylbutylthio)-1,3-phenylene-*alt*-2-methyl-1,3-phenylene] (Poly-S). 4 (158.0 mg, 0.50 mmol), **6** (220.2 mg, 0.50 mmol), tetrakis(triphenylphosphine)palladium(0) (11.6 mg, 0.010 mmol) and THF (5.0 ml) were placed in a 10 ml ampoule in a glove box under argon. After the addition of a 2.0 M aqueous sodium carbonate solution (1.0 ml), the ampoule was evacuated, sealed, and heated at 80 °C for 72 hr. The reaction mixture was dropwise poured into 200 ml of methanol, and the precipitate was filtered. The precipitate was dissolved in chloroform then re-precipitated into 200 ml of hexane. The precipitate was dried in a vacuum to give a white powder (137 mg, 0.37 mmol). Yield: 74%. ¹H NMR (CD₂Cl₂, 500 MHz; ppm): δ 7.23 – 6.90 (m, 5H), 2.74 (d, 4H), 1.91 (s, 3H), 1.65 (m, 2H), 1.38 (d, 4H), 0.99 (s, 6H), 0.90 (s, 6H). ¹³C NMR (CD₂Cl₂, 125 MHz; ppm): δ 154.9, 138.3, 133.1, 132.1, 126.2, 122.0, 117.7, 114.5, 41.9, 37.4, 30.4, 21.1, 19.9, 11.5. IR (KBr, cm⁻¹): 2949 (ν_{aromaticC-H}), 864 (δ_{aromaticC-H}). GPC (CHCl₃, PSt calibration): $M_n = 1.1 \times 10^4$, $M_w = 1.3 \times 10^4$ ($M_w / M_n = 1.20$). UV-vis (CH₂Cl₂): λ_{max} = 256, 292 nm, absorption tail = 330 nm. Anal. Calcd for C₂₃H₃₀S₂: C, 74.5; H, 8.2. Found: C, 74.2; H, 7.9.

Poly[4,6-bis((S)-(+)-2-methylbutylsulfinyl)-1,3-phenylene-*alt*-2-methyl-1,3-phenylene] (Poly-SO).

A dichloromethane (4 ml) solution of **Poly-S** (22 mg, 0.060 mmol), a 30% aqueous hydrogen peroxide solution (0.25 ml) and acetic acid (0.12 ml) were stirred at 30°C for 9 hr. The organic phase was extracted with CHCl₃, and washed with water. After drying and evaporation, the residue was dissolved in 0.5 ml of CHCl₃ and precipitated into hexane. The precipitate was dried in a vacuum that produced a white powder (21 mg, 0.05 unit mmol). Yield: 86%. ¹H NMR (CD₂Cl₂, 500 MHz; ppm): δ 8.21 (s, 1H), 7.56 – 7.15 (m, 4H), 2.57 (d, 4H), 2.22 – 1.81 (m, 5H), 1.26 (s, 4H), 0.99 (s, 6H), 0.89 (s, 6H). IR (KBr, cm⁻¹): 2960 (ν_{aromatic}C-H), 1050 (ν_{S=O}), 855 (δ_{aromatic}C-H). GPC (CHCl₃, PSt calibration): $M_n = 1.1 \times 10^4$, $M_w = 1.3 \times 10^4$ ($M_w / M_n = 1.21$). UV-vis (CH₂Cl₂): λ_{max} = 250, 281nm, absorption tail = 318 nm. Anal. Calcd for C₂₃H₃₀O₂S₂: C, 68.6; H, 7.5. Found: C, 68.4; H, 7.8.

Figure S4. ¹H-NMR spectrum of **Poly-SO** in CD₂Cl₂.

Figure S5. GPC traces of **Poly-S** and **Poly-SO**: 0.5 g/L solution of CHCl₃ (as eluent, 0.35 mL/min)

Poly[phenylene-4,6-bis(2-methylbutylsulfonio)-1,3-diyl-*alt*-2-methylphenylene-4,6-bis(2-methylbutylsulfonio)-1,3-diyl triflate] (Poly-S⁺). Poly-SO (20 mg, 0.05 unit mmol) was dissolved in the mixture of chloroform and acetonitrile (v/v = 1:1) mixture (5 ml). Trifric acid (5 ml) was added to the solution and stirred at room temperature for 7 days and poured into diethylether (100 ml). The precipitate was dried in a vacuum that produced a light brown powder (33 mg, 0.05 unit mmol). Yield: 98%. ¹H NMR (CF₃SO₃D, 500 MHz; ppm): δ 8.48 (s, 1H), 7.22 (s, 1H), 7.05 (s, 1H), 2.99 (d, 4H), 2.24-1.80 (m, 5H), 1.25 (s, 4H), 0.98 (s, 6H), 0.89 (s, 6H). IR (KBr, cm⁻¹): 3002 ($\nu_{\text{aromatic C-H}}$), 1256, 792 ($\nu_{\text{C-F}}$), 1155 (δ_{SO_2}). UV-vis (DMF): λ_{max} = 269, 315 nm, absorption tail = 343 nm. Anal. Calcd for C₂₅H₃₂F₆O₆S₄: C, 44.7; H, 4.8. Found: C, 44.1; H, 4.1.

Figure S6. ¹H-NMR spectrum of Poly-S⁺ in CF₃SO₃D.

1,3-Diphenyl-4,6-bis(methylthio)benzene (Tri-S). 1,5-Dibromo-2,4-bis(methylthio)benzene (164 mg, 0.50 mmol), phenylboronic acid (122 mg, 1.0 mmol), tetrakis(triphenylphosphine)palladium(0) (11.6 mg, 0.010 mmol) and THF (2.5 ml) were placed in a 10 ml ampoule in a glove box under argon. After the addition of a 1.0 M aqueous sodium carbonate solution (1.0 ml), the ampoule was evacuated, sealed, and heated at 80°C for 24 hr. The organic was extracted with diethylether, and the ether phase was dried and concentrated. The residue was recrystallized to produce white plate-like crystals (145 mg, 0.45 mmol). Yield: 90%. ¹H NMR (CDCl₃, 500 MHz; ppm): δ 7.45 – 7.40 (m, 8H), 7.37 (d, 2H), 7.24 (s, 1H), 7.10 (s, 1H), 2.44 (s, 6H). ¹³C NMR (CDCl₃, 125 MHz; ppm): δ 140.3, 138.1, 137.1, 134.5, 131.9, 128.5, 127.9, 123.3, 16.5. IR (KBr, cm⁻¹): 2965 ($\nu_{\text{aromatic C-H}}$), 878 ($\delta_{\text{aromatic C-H}}$). MS (EI, m/z): 322 (M⁺), 322.49 (calcd). Anal. Calcd for C₂₀H₁₈S₂: C, 74.5; H, 5.6. Found: C, 74.0; H, 5.3.

1,3-Diphenyl-4,6-bis(methylsulfinyl)benzene. A dichloromethane (4 ml) solution of **Tri-S** (43 mg, 0.12 mmol), a 30% aqueous hydrogen peroxide solution (0.5 ml) and acetic acid (0.25 ml) were stirred at 30°C for 6 hr. The organic phase was extracted with chloroform, and washed with water. After drying and evaporation, the residue was purified by column chromatography using chloroform/methanol (v/v = 10/1) to produce a white powder (35 mg, 0.10 mmol). Yield: 86%. ¹H NMR (CDCl₃, 500 MHz; ppm): δ 8.94 (s, 1H), 7.49 – 7.42 (m, 10H), 7.31 (s, 1H), 2.48 (s, 6H). ¹³C NMR (CDCl₃, 125 MHz; ppm): δ 145.4, 141.9, 136.6, 132.3, 129.0, 128.9, 128.9, 120.2, 41.5. IR (KBr, cm⁻¹): 2944 ($\nu_{\text{aromatic C-H}}$), 1056 ($\nu_{\text{S=O}}$), 847 ($\delta_{\text{aromatic C-H}}$). MS (EI, m/z): 354 (M⁺), 354.49 (calcd). Anal. Calcd for C₂₀H₁₈O₂S₂: C, 67.8; H, 5.1. Found: C, 68.2; H, 5.5.

10,12-Dimethyl-10,12-thionia-indeno[2,1-*b*]fluorine Triflate (Tri-S⁺). Triflic acid (5ml) and 1,3-diphenyl-4,6-bis(methylsulfinyl)benzene (35 mg, 0.10 mmol) were stirred at room temperature for 72 hr then poured into diethylether (200 ml). The recovered white powder was recrystallized to give white plate crystals (64 mg, 0.094 mmol). Yield: 94%. ¹H NMR (CD₃CN, 500 MHz; ppm): δ 9.14 (s, 1H), 9.07 (s, 1H), 8.53 (d, *J* = 7.9 Hz, 2H), 8.35 (d, *J* = 7.9 Hz, 2H), 8.04 (t, *J* = 7.6 Hz, 2H), 7.91 (t, *J* = 7.6 Hz, 2H), 3.47 (s, 6H). IR (KBr, cm⁻¹): 2984 ($\nu_{\text{aromatic C-H}}$), 1251, 786 ($\nu_{\text{C-F}}$), 1153 (δ_{SO_2}). ESI-MS (m/z): 320 (M–2CF₃SO₃⁻), 320.47 (M–2CF₃SO₃⁻, calcd). Anal. Calcd for C₂₂H₁₆F₆O₆S₄: C, 42.7; H, 2.6. Found: C, 42.0; H, 2.5.

Materials and measurements. All other reagents were obtained from Kanto Chemical Co., Tokyo Kasei Co. and Aldrich Co., and used without further purification. The ¹H and ¹³C NMR, mass, and infrared spectra were recorded on a JEOL Lambda 500, a Shimadzu GCMS-QP5050, and a JASCO FT/IR-410 spectrometer, respectively. Molecular weights were determined by gel permeation chromatography (GPC) using a Tosoh highly sensitive GPC system HLC-8220GPC equipped with a UV-8220 at detection absorbance set at 254 nm. The measurements were made at 40 °C using the UV detector, Tosoh TSK GEL SuperHZ2000 × 2, SuperHZ3000 × 1, and SuperHZM-M × 1 with chloroform as the eluent. The elemental analysis was performed on a Perkin-Elmer PE-2400 and a Metrohm 645 Multi DOSIMAT. The UV-vis and circular dichroism (CD) spectra were measured on

a JASCO V-550 and a JASCO J-820, respectively.

X-ray Crystallographic Analysis

Structure Solution and Refinement

The structure was solved by direct method (SIR92) and expanded by Fourier techniques. Some non-hydrogen atoms were refined anisotropically, while the rest were refined isotropically. The hydrogen atoms were refined isotropically. The final cycle of full-matrix least-square refinement was based on 2509 (**Tri-S**) and 1022 (**Tri-S**⁺) observed reflections [$I > 3.00\sigma(I)$] and 506 (**Tri-S**) and 131 (**Tri-S**⁺) variable parameters, and converged with unweighted and weighted agreement factors of $R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$ and $R_w = (\Sigma w(|F_o| - |F_c|)^2 / \Sigma w F_o^2)^{1/2}$ as Table S1 and S2. All calculations were performed with the teXsan crystallographic software package from Molecular Structure Corp.

X-ray crystallographic Data

Table S1. Summary of X-ray crystallographic data of **Tri-S**

emp form	C ₂₀ H ₁₈ S ₂	absn coeff μ	3.08 cm ⁻¹
fw	322.49	$2\theta_{\max}$ (degree)	55.1
cryst syst	monoclinic	no. of refins cold	8319
space group	P2 ₁ /c (no. 14)	no. of unq reflns	8061
<i>a</i> (Å)	11.93 (1)	no. of obsd reflns	2509 [$I > 3.00\sigma(I)$]
<i>b</i> (Å)	17.39 (3)	params	506
<i>c</i> (Å)	17.15 (1)	refln / param ratio	4.96
<i>V</i> (Å ³)	3386 (6)	<i>R</i>	0.064
<i>Z</i>	8	<i>R</i> _w	0.051
density (calcd)	1.265 g/cm ³	goodness-of-fit	2.67
crystal size (mm)	0.2 × 0.2 × 0.1	max peak in dff map	0.27 e ⁻ /Å ³
radiation	MoK α (λ = 0.71069 Å)	min peak in dff map	-0.30 e ⁻ /Å ³

Table S2. Summary of X-ray crystallographic data of **Tri-S**⁺

emp form	C ₂₂ H ₁₆ F ₆ O ₆ S ₄	absn coeff μ	8.32 cm ⁻¹
fw	618.61	$2\theta_{\max}$ (degree)	55.0
cryst syst	monoclinic	no. of refins cold	1848
space group	C2/c (no. 15)	no. of unq reflns	1798
<i>a</i> (Å)	20.759 (7)	no. of obsd reflns	1022 [$I > 3.00\sigma(I)$]
<i>b</i> (Å)	8.096 (8)	params	131
<i>c</i> (Å)	8.646 (7)	refln / param ratio	7.80
<i>V</i> (Å ³)	1453 (1)	<i>R</i>	0.060
<i>Z</i>	2	<i>R</i> _w	0.047
density (calcd)	2.518 g/cm ³	goodness-of-fit	4.36
crystal size (mm)	0.2 × 0.2 × 0.2	max peak in dff map	0.27 e ⁻ /Å ³
radiation	MoK α (λ = 0.71069 Å)	min peak in dff map	-0.38 e ⁻ /Å ³

Crystallographic Information for **Tri-S**

Tri-S

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
S(1)	0.6932(3)	0.0938(2)	0.3241(2)	5.16(9)
S(2)	1.0401(2)	0.1702(2)	0.1824(2)	4.08(8)
S(3)	0.5591(2)	0.3870(2)	-0.0130(2)	4.69(8)
S(4)	0.1937(2)	0.3376(2)	0.1167(2)	4.77(8)
C(1)	0.5300(8)	0.0959(6)	0.1488(6)	3.3(3)
C(2)	0.4752(8)	0.0287(6)	0.1098(6)	3.7(3)
C(3)	0.3558(9)	0.0184(6)	0.1002(7)	4.2(3)
C(4)	0.2902(9)	0.0723(8)	0.1273(7)	4.5(3)
C(5)	0.3434(9)	0.1380(7)	0.1633(7)	4.7(3)
C(6)	0.4627(9)	0.1509(6)	0.1766(6)	4.3(3)
C(7)	0.8340(9)	0.0832(7)	0.4073(6)	5.8(3)
C(8)	0.7439(9)	0.1131(6)	0.2393(6)	3.5(3)
C(9)	0.8586(8)	0.1291(6)	0.2454(6)	3.7(3)
C(10)	0.8937(8)	0.1422(6)	0.1761(6)	3.0(3)
C(11)	1.1032(9)	0.2055(6)	0.2865(6)	5.2(3)
C(12)	0.7777(9)	0.1994(6)	-0.0393(6)	4.2(3)
C(13)	0.804(1)	0.2063(7)	-0.1152(7)	5.0(3)
C(14)	0.895(1)	0.1624(7)	-0.1276(7)	5.0(4)
C(15)	0.962(1)	0.1120(7)	-0.0668(8)	5.4(4)
C(16)	0.9307(9)	0.1031(6)	0.0045(6)	4.1(3)
C(17)	0.8416(8)	0.1477(6)	0.0193(6)	2.9(3)
C(18)	0.8100(8)	0.1368(5)	0.0969(6)	2.8(3)
C(19)	0.6935(8)	0.1226(6)	0.0909(6)	3.0(3)
C(20)	0.6571(8)	0.1118(6)	0.1608(6)	3.3(3)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(21)	0.7146(8)	0.3958(6)	0.1661(6)	3.2(3)
C(22)	0.7661(9)	0.4609(6)	0.2102(6)	3.6(3)
C(23)	0.884(1)	0.4736(7)	0.2201(7)	5.0(3)
C(24)	0.9496(9)	0.4249(8)	0.1844(7)	4.8(3)
C(25)	0.8953(10)	0.3591(7)	0.1428(6)	4.9(3)
C(26)	0.7767(8)	0.3432(6)	0.1322(6)	4.2(3)
C(27)	0.4278(8)	0.4084(6)	-0.0968(6)	4.4(3)
C(28)	0.5062(8)	0.3754(6)	0.0717(6)	3.2(3)
C(29)	0.3861(8)	0.3635(6)	0.0610(6)	3.3(3)
C(30)	0.3417(8)	0.3568(6)	0.1286(6)	3.3(3)
C(31)	0.1395(9)	0.2962(8)	0.0155(6)	7.7(4)
C(32)	0.4432(8)	0.3106(6)	0.3465(6)	3.5(3)
C(33)	0.408(1)	0.3089(7)	0.4189(6)	5.1(3)
C(34)	0.317(1)	0.3569(7)	0.4269(7)	5.3(4)
C(35)	0.2614(9)	0.4037(7)	0.3621(7)	4.7(3)
C(36)	0.2919(8)	0.4083(6)	0.2897(6)	3.9(3)
C(37)	0.3819(9)	0.3601(6)	0.2844(5)	3.2(3)
C(38)	0.4225(8)	0.3640(6)	0.2080(6)	3.1(3)
C(39)	0.5420(8)	0.3766(6)	0.2168(5)	3.3(3)
C(40)	0.5849(8)	0.3815(6)	0.1507(6)	3.0(3)

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos \gamma + 2U_{13}aa^*cc^* \cos \beta + 2U_{23}bb^*cc^* \cos \alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S(1)	0.058(2)	0.100(3)	0.051(2)	-0.014(2)	0.035(2)	-0.005(2)
S(2)	0.032(2)	0.078(2)	0.049(2)	-0.010(2)	0.018(1)	-0.002(2)
S(3)	0.042(2)	0.099(3)	0.044(2)	-0.003(2)	0.024(1)	0.002(2)
S(4)	0.031(2)	0.098(3)	0.056(2)	-0.011(2)	0.019(1)	-0.015(2)
C(1)	0.033(6)	0.051(8)	0.048(7)	0.001(6)	0.020(5)	0.002(6)
C(2)	0.031(6)	0.051(8)	0.059(8)	-0.008(6)	0.014(6)	-0.002(6)
C(3)	0.038(8)	0.057(8)	0.066(8)	-0.018(6)	0.019(6)	-0.011(7)
C(4)	0.030(7)	0.09(1)	0.055(8)	-0.007(7)	0.015(6)	0.008(7)
C(5)	0.031(7)	0.08(1)	0.082(9)	0.014(7)	0.038(6)	0.004(8)
C(6)	0.030(6)	0.061(9)	0.072(8)	-0.009(6)	0.015(6)	-0.015(7)
C(7)	0.058(8)	0.13(1)	0.036(7)	0.016(8)	0.022(6)	0.032(7)
C(8)	0.034(6)	0.062(8)	0.043(7)	-0.008(6)	0.019(5)	-0.002(6)
C(9)	0.035(7)	0.066(8)	0.040(6)	-0.005(6)	0.012(5)	-0.002(6)
C(10)	0.024(6)	0.045(8)	0.050(7)	-0.004(5)	0.017(5)	0.003(6)
C(11)	0.051(7)	0.10(1)	0.041(7)	-0.014(7)	0.007(6)	-0.015(7)
C(12)	0.050(7)	0.062(9)	0.039(7)	-0.012(6)	0.002(6)	0.001(6)
C(13)	0.078(9)	0.068(9)	0.051(8)	-0.032(7)	0.029(7)	-0.016(7)
C(14)	0.075(9)	0.057(10)	0.067(9)	-0.028(8)	0.032(8)	-0.018(7)
C(15)	0.078(10)	0.07(1)	0.076(10)	-0.018(8)	0.056(8)	-0.025(8)
C(16)	0.045(7)	0.064(9)	0.045(7)	0.000(6)	0.014(5)	-0.006(6)
C(17)	0.027(6)	0.049(8)	0.040(7)	-0.011(5)	0.019(5)	-0.011(6)
C(18)	0.034(6)	0.032(7)	0.046(7)	0.001(5)	0.020(5)	0.000(5)
C(19)	0.023(5)	0.048(7)	0.047(6)	-0.010(5)	0.016(5)	-0.011(5)
C(20)	0.023(6)	0.049(8)	0.058(7)	0.001(5)	0.019(5)	-0.004(6)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(21)	0.018(5)	0.056(8)	0.046(6)	0.000(5)	0.010(5)	0.006(6)
C(22)	0.030(6)	0.057(8)	0.044(7)	-0.010(6)	0.002(5)	0.001(6)
C(23)	0.046(8)	0.069(9)	0.067(9)	-0.013(7)	0.008(7)	-0.001(7)
C(24)	0.024(6)	0.09(1)	0.065(9)	-0.010(7)	0.003(6)	0.017(8)
C(25)	0.043(7)	0.09(1)	0.060(8)	0.011(7)	0.023(6)	0.002(7)
C(26)	0.037(7)	0.070(9)	0.060(7)	0.019(6)	0.028(6)	0.011(6)
C(27)	0.035(6)	0.086(9)	0.050(7)	0.007(6)	0.018(5)	-0.002(7)
C(28)	0.036(6)	0.054(8)	0.036(6)	-0.001(6)	0.019(5)	-0.003(5)
C(29)	0.026(6)	0.062(8)	0.038(6)	-0.002(5)	0.009(5)	-0.003(6)
C(30)	0.028(6)	0.050(8)	0.052(7)	-0.002(5)	0.015(5)	-0.005(6)
C(31)	0.031(7)	0.20(2)	0.055(8)	-0.037(8)	0.001(6)	-0.063(9)
C(32)	0.041(6)	0.055(8)	0.038(7)	-0.005(6)	0.012(5)	-0.001(6)
C(33)	0.079(9)	0.071(10)	0.041(7)	-0.016(8)	0.011(7)	0.004(7)
C(34)	0.074(10)	0.07(1)	0.069(9)	-0.026(8)	0.043(8)	-0.022(8)
C(35)	0.051(8)	0.08(1)	0.063(8)	-0.017(7)	0.034(7)	-0.024(7)
C(36)	0.035(6)	0.069(9)	0.057(7)	-0.016(6)	0.030(5)	-0.029(6)
C(37)	0.040(6)	0.053(8)	0.028(6)	-0.007(6)	0.011(5)	-0.007(5)
C(38)	0.026(6)	0.050(8)	0.043(7)	0.000(5)	0.015(5)	-0.004(6)
C(39)	0.033(6)	0.056(8)	0.036(6)	0.004(6)	0.009(5)	-0.002(5)
C(40)	0.025(6)	0.050(8)	0.044(6)	0.000(5)	0.018(5)	-0.002(5)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\text{\AA}$)

atom	atom	distance	atom	atom	distance
S(1)	C(6)	1.765(9)	S(1)	C(26)	1.809(10)
S(2)	C(17)	1.747(10)	S(2)	C(37)	1.81(1)
S(3)	C(12)	1.784(9)	S(3)	C(40)	1.817(10)
S(4)	C(5)	1.771(10)	S(4)	C(37)	1.85(1)
C(1)	C(10)	1.50(1)	C(1)	C(21)	1.39(1)
C(1)	C(25)	1.40(1)	C(2)	C(6)	1.39(1)
C(2)	C(7)	1.51(1)	C(2)	C(15)	1.38(1)
C(3)	C(10)	1.38(1)	C(3)	C(11)	1.41(1)
C(3)	H(19)	1.06	C(4)	C(11)	1.49(1)
C(4)	C(13)	1.40(1)	C(4)	C(29)	1.42(1)
C(5)	C(9)	1.37(1)	C(5)	C(11)	1.42(1)
C(6)	C(18)	1.40(1)	C(7)	C(14)	1.41(1)
C(7)	C(22)	1.39(1)	C(8)	C(15)	1.40(1)
C(8)	C(17)	1.41(1)	C(8)	C(19)	1.53(1)
C(9)	C(12)	1.40(1)	C(9)	H(16)	1.08
C(10)	C(12)	1.42(1)	C(13)	C(23)	1.39(1)
C(14)	C(32)	1.40(1)	C(15)	H(6)	0.98
C(16)	C(19)	1.39(1)	C(16)	C(35)	1.40(1)
C(17)	C(18)	1.42(1)	C(18)	H(4)	1.13
C(19)	C(20)	1.39(1)	C(20)	C(34)	1.43(1)
C(20)	H(9)	1.19	C(21)	C(28)	1.43(1)
C(22)	C(30)	1.38(1)	C(23)	C(24)	1.39(1)
C(23)	H(23)	1.01	C(24)	C(39)	1.36(1)
C(24)	H(11)	0.96	C(25)	C(31)	1.39(1)

Table 3. Bond Lengths($\text{\AA}$) (continued)

atom	atom	distance	atom	atom	distance
C(25)	H(17)	1.17	C(26)	H(1)	1.06
C(26)	H(2)	0.98	C(26)	H(3)	1.17
C(27)	C(25)	1.41(1)	C(27)	C(32)	1.40(1)
C(27)	H(21)	1.10	C(28)	C(38)	1.40(1)
C(29)	C(39)	1.39(1)	C(29)	H(12)	1.10
C(30)	H(20)	1.08	C(31)	C(38)	1.41(1)
C(31)	H(18)	1.17	C(32)	H(22)	1.17
C(33)	C(34)	1.41(1)	C(33)	C(35)	1.37(1)
C(34)	H(7)	1.17	C(35)	H(8)	1.22
C(36)	H(13)	1.30	C(36)	H(14)	1.23
C(37)	H(5)	1.00	C(39)	H(10)	1.07
C(40)	H(15)	1.19			

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(6)	S(1)	C(26)	103.7(5)	C(17)	S(2)	C(37)	103.8(5)
C(12)	S(3)	C(40)	104.8(5)	C(5)	S(4)	C(36)	101.2(5)
C(10)	C(1)	C(21)	119.4(9)	C(10)	C(1)	C(25)	120.2(10)
C(21)	C(1)	C(25)	120.3(9)	C(6)	C(2)	C(7)	122.1(9)
C(6)	C(2)	C(15)	118.9(9)	C(7)	C(2)	C(15)	119.0(9)
C(10)	C(3)	C(11)	121.8(9)	C(10)	C(3)	H(19)	125.7
C(11)	C(3)	H(19)	112.3	C(11)	C(4)	C(13)	121.7(9)
C(11)	C(4)	C(29)	119.0(9)	C(13)	C(4)	C(29)	119.4(9)
S(4)	C(5)	C(9)	124.2(8)	S(4)	C(5)	C(11)	116.1(7)
C(9)	C(5)	C(11)	119.7(9)	S(1)	C(6)	C(2)	119.1(7)
S(1)	C(6)	C(18)	121.2(8)	C(2)	C(6)	C(18)	119.6(9)
C(2)	C(7)	C(14)	117.5(9)	C(2)	C(7)	C(22)	119.1(9)
C(14)	C(7)	C(22)	123.4(9)	C(15)	C(8)	C(17)	119.1(9)
C(15)	C(8)	C(19)	119.6(9)	C(17)	C(8)	C(19)	121.3(9)
C(5)	C(9)	C(12)	121.6(9)	C(5)	C(9)	H(16)	119.6
C(12)	C(9)	H(16)	117.3	C(1)	C(10)	C(3)	118.5(9)
C(1)	C(10)	C(12)	123.0(9)	C(3)	C(10)	C(12)	118.6(9)
C(3)	C(11)	C(4)	118.3(9)	C(3)	C(11)	C(5)	118.5(9)
C(4)	C(11)	C(5)	123.1(9)	S(3)	C(12)	C(9)	122.5(8)
S(3)	C(12)	C(10)	117.6(7)	C(9)	C(12)	C(10)	119.8(9)
C(4)	C(13)	C(23)	118.2(10)	C(7)	C(14)	C(32)	117(1)
C(2)	C(15)	C(8)	122.8(9)	C(2)	C(15)	H(6)	113.7
C(8)	C(15)	H(6)	123.5	C(19)	C(16)	C(35)	116(1)
S(2)	C(17)	C(8)	119.7(8)	S(2)	C(17)	C(18)	122.5(8)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(8)	C(17)	C(18)	117.7(9)	C(6)	C(18)	C(17)	121.8(9)
C(6)	C(18)	H(4)	125.0	C(17)	C(18)	H(4)	112.1
C(8)	C(19)	C(16)	119.1(10)	C(8)	C(19)	C(20)	117.0(9)
C(16)	C(19)	C(20)	125.0(9)	C(19)	C(20)	C(34)	117.0(10)
C(19)	C(20)	H(9)	134.6	C(34)	C(20)	H(9)	108.4
C(1)	C(21)	C(28)	119(1)	C(7)	C(22)	C(30)	117(1)
C(13)	C(23)	C(24)	122(1)	C(13)	C(23)	H(23)	123.3
C(24)	C(23)	H(23)	114.1	C(23)	C(24)	C(39)	119.1(10)
C(23)	C(24)	H(11)	106.3	C(39)	C(24)	H(11)	133.8
C(1)	C(25)	C(31)	121(1)	C(1)	C(25)	H(17)	117.6
C(31)	C(25)	H(17)	117.5	S(1)	C(26)	H(1)	115.9
S(1)	C(26)	H(2)	88.7	S(1)	C(26)	H(3)	106.2
H(1)	C(26)	H(2)	120.1	H(1)	C(26)	H(3)	117.4
H(2)	C(26)	H(3)	104.2	C(30)	C(27)	C(32)	118(1)
C(30)	C(27)	H(21)	110.4	C(32)	C(27)	H(21)	123.0
C(21)	C(28)	C(38)	119(1)	C(4)	C(29)	C(39)	119.5(10)
C(4)	C(29)	H(12)	104.4	C(39)	C(29)	H(12)	135.7
C(22)	C(30)	C(27)	121(1)	C(22)	C(30)	H(20)	129.8
C(27)	C(30)	H(20)	108.1	C(25)	C(31)	C(38)	118(1)
C(25)	C(31)	H(18)	119.7	C(38)	C(31)	H(18)	113.4
C(14)	C(32)	C(27)	121(1)	C(14)	C(32)	H(22)	132.2
C(27)	C(32)	H(22)	106.4	C(34)	C(33)	C(25)	118(1)
C(20)	C(34)	C(33)	120(1)	C(20)	C(34)	H(7)	111.5
C(33)	C(34)	H(7)	126.0	C(16)	C(35)	C(33)	123(1)

Table 4. Bond Angles($^{\circ}$) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(16)	C(35)	H(8)	129.8	C(33)	C(35)	H(8)	105.6
S(4)	C(36)	H(13)	87.7	S(4)	C(36)	H(14)	97.7
H(13)	C(36)	H(14)	45.9	S(2)	C(37)	H(5)	125.9
C(28)	C(38)	C(31)	121(1)	C(24)	C(39)	C(29)	121(1)
C(24)	C(39)	H(10)	116.8	C(29)	C(39)	H(10)	121.7
S(3)	C(40)	H(15)	107.8				

Table 5. Torshion Angles ($^{\circ}$)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
S(1)	C(6)	C(2)	C(7)	-1(1)	S(1)	C(6)	C(2)	C(15)	176.5(8)
S(1)	C(6)	C(18)	C(17)	-177.8(9)	S(2)	C(17)	C(8)	C(15)	177.6(8)
S(2)	C(17)	C(8)	C(19)	-3(1)	S(2)	C(17)	C(18)	C(6)	-177.0(8)
S(3)	C(12)	C(9)	C(5)	175.2(8)	S(3)	C(12)	C(10)	C(1)	4(1)
S(3)	C(12)	C(10)	C(3)	-173.7(7)	S(4)	C(5)	C(9)	C(12)	178.5(8)
S(4)	C(5)	C(11)	C(3)	-176.6(8)	S(4)	C(5)	C(11)	C(4)	0(1)
C(1)	C(10)	C(3)	C(11)	179.9(9)	C(1)	C(10)	C(12)	C(9)	-178(1)
C(1)	C(21)	C(28)	C(38)	-1(1)	C(1)	C(25)	C(31)	C(38)	-5(1)
C(2)	C(6)	S(1)	C(26)	-160.6(8)	C(2)	C(6)	C(18)	C(17)	0(1)
C(2)	C(7)	C(14)	C(32)	176.5(9)	C(2)	C(7)	C(22)	C(30)	-177.4(9)
C(2)	C(15)	C(8)	C(17)	0(1)	C(2)	C(15)	C(8)	C(19)	-179(1)
C(3)	C(10)	C(1)	C(21)	50(1)	C(3)	C(10)	C(1)	C(25)	-126(1)
C(3)	C(10)	C(12)	C(9)	3(1)	C(3)	C(11)	C(4)	C(13)	64(1)
C(3)	C(11)	C(4)	C(29)	-114(1)	C(3)	C(11)	C(5)	C(9)	3(1)
C(4)	C(11)	C(3)	C(10)	-179.3(9)	C(4)	C(11)	C(5)	C(9)	-179(1)
C(4)	C(13)	C(23)	C(24)	0(1)	C(4)	C(29)	C(39)	C(24)	2(1)
C(5)	C(9)	C(12)	C(10)	-1(1)	C(5)	C(11)	C(3)	C(10)	-2(1)
C(5)	C(11)	C(4)	C(13)	-112(1)	C(5)	C(11)	C(4)	C(29)	68(1)
C(6)	C(2)	C(7)	C(14)	-56(1)	C(6)	C(2)	C(7)	C(22)	121(1)
C(6)	C(2)	C(15)	C(8)	1(1)	C(6)	C(18)	C(17)	C(8)	1(1)
C(7)	C(2)	C(6)	C(18)	-178.8(10)	C(7)	C(2)	C(15)	C(8)	179.4(9)
C(7)	C(14)	C(32)	C(27)	0(1)	C(7)	C(22)	C(30)	C(27)	2(1)
C(8)	C(17)	S(2)	C(37)	-157.9(9)	C(8)	C(19)	C(16)	C(35)	-178.0(9)
C(8)	C(19)	C(20)	C(34)	177.9(9)	C(9)	C(5)	S(4)	C(36)	-10(1)

Table 5. Torshion Angles ($^{\circ}$)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(9)	C(12)	S(3)	C(40)	-17(1)	C(10)	C(1)	C(21)	C(28)	-176.4(9)
C(10)	C(1)	C(25)	C(31)	180.0(10)	C(10)	C(12)	S(3)	C(40)	159.1(8)
C(11)	C(3)	C(10)	C(12)	-1(1)	C(11)	C(4)	C(13)	C(23)	-179.4(10)
C(11)	C(4)	C(29)	C(39)	177.9(10)	C(11)	C(5)	S(4)	C(36)	169.7(8)
C(11)	C(5)	C(9)	C(12)	-1(1)	C(12)	C(10)	C(1)	C(21)	-128(1)
C(12)	C(10)	C(1)	C(25)	55(1)	C(13)	C(4)	C(29)	C(39)	-1(1)
C(13)	C(23)	C(24)	C(39)	1(1)	C(14)	C(7)	C(2)	C(15)	125(1)
C(14)	C(7)	C(22)	C(30)	0(1)	C(14)	C(32)	C(27)	C(30)	3(1)
C(15)	C(2)	C(6)	C(18)	0(1)	C(15)	C(2)	C(7)	C(22)	53(1)
C(15)	C(8)	C(17)	C(18)	0(1)	C(15)	C(8)	C(19)	C(16)	125(1)
C(15)	C(8)	C(19)	C(20)	-51(1)	C(16)	C(19)	C(8)	C(17)	-53(1)
C(16)	C(19)	C(20)	C(34)	1(1)	C(16)	C(35)	C(33)	C(34)	-2(1)
C(17)	C(8)	C(19)	C(20)	130(1)	C(16)	C(6)	S(1)	C(26)	16(1)
C(18)	C(17)	S(2)	C(37)	20(1)	C(18)	C(17)	C(8)	C(19)	178(1)
C(19)	C(16)	C(35)	C(33)	2(1)	C(19)	C(20)	C(34)	C(33)	-1(1)
C(20)	C(19)	C(16)	C(35)	-1(1)	C(20)	C(34)	C(33)	C(35)	1(1)
C(21)	C(1)	C(25)	C(31)	3(1)	C(21)	C(28)	C(38)	C(31)	0(1)
C(22)	C(7)	C(14)	C(32)	-1(1)	C(22)	C(30)	C(27)	C(32)	-4(1)
C(23)	C(13)	C(4)	C(29)	0(1)	C(23)	C(24)	C(39)	C(29)	-2(1)
C(25)	C(1)	C(21)	C(28)	0(1)	C(25)	C(31)	C(38)	C(28)	3(1)

Table 6. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
S(1)	H(13)	2.78	55404	S(1)	H(7)	3.00	55404
S(1)	H(1)	3.19	66503	S(1)	H(14)	3.40	55404
S(1)	H(9)	3.44	55404	S(2)	H(22)	2.74	45501
S(2)	H(10)	3.06	1	S(2)	H(21)	3.27	45501
S(3)	H(20)	2.83	74502	S(3)	H(22)	2.88	1
S(3)	H(10)	2.98	65501	S(3)	H(11)	3.37	65501
S(4)	H(2)	2.89	4	C(1)	H(23)	2.88	65503
C(2)	H(1)	3.08	66503	C(2)	H(12)	3.56	1
C(3)	H(23)	3.20	65503	C(3)	H(7)	3.26	55404
C(3)	H(8)	3.34	64502	C(6)	H(7)	3.11	55404
C(6)	H(1)	3.20	66503	C(7)	H(1)	2.94	66503
C(8)	H(12)	3.22	1	C(8)	H(10)	3.56	1
C(9)	H(20)	3.03	74502	C(10)	H(23)	3.35	65503
C(10)	H(8)	3.36	64502	C(12)	H(20)	2.91	74502
C(12)	H(22)	3.47	1	C(13)	H(19)	3.45	65503
C(13)	C(16)	3.48(1)	64502	C(13)	H(6)	3.54	64502
C(13)	C(19)	3.59(1)	64502	C(14)	H(13)	3.19	55404
C(15)	H(12)	3.19	1	C(16)	H(21)	2.85	45501
C(17)	H(10)	3.34	1	C(18)	H(7)	3.23	55404
C(20)	H(3)	3.03	4	C(20)	H(12)	3.47	1
C(20)	H(19)	3.56	4	C(21)	H(9)	3.08	55404
C(21)	H(23)	3.18	65503	C(22)	H(1)	2.68	66503
C(22)	C(20)	3.40(1)	66503	C(22)	C(38)	3.47(1)	4
C(22)	H(11)	3.48	65502	C(22)	H(2)	3.57	66503

Table 6. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
C(23)	H(6)	3.15	64502	C(23)	H(19)	3.32	65503
C(23)	C(33)	3.59(2)	55404	C(24)	H(17)	3.30	45501
C(25)	H(23)	3.04	65503	C(25)	H(18)	3.20	75503
C(25)	H(11)	3.36	65501	C(25)	H(17)	3.48	75503
C(25)	H(11)	3.49	65503	C(26)	H(7)	3.42	55404
C(26)	H(9)	3.44	55404	C(26)	H(15)	3.48	45404
C(28)	H(6)	3.04	55404	C(28)	H(9)	3.26	55404
C(28)	H(5)	3.32	65501	C(28)	H(16)	3.42	55404
C(29)	H(2)	3.39	4	C(29)	H(9)	3.55	1
C(30)	H(18)	3.12	4	C(30)	H(15)	3.20	75502
C(30)	H(1)	3.47	66503	C(30)	C(38)	3.50(2)	4
C(31)	H(17)	3.28	75503	C(31)	H(8)	3.29	65404
C(31)	H(5)	3.38	65501	C(31)	H(11)	3.51	65503
C(31)	H(23)	3.54	65503	C(32)	H(13)	3.17	55404
C(34)	H(3)	2.82	4	C(34)	H(19)	3.06	4
C(35)	H(21)	3.00	45501	C(35)	H(18)	3.49	45504
C(36)	H(5)	3.32	65504	C(37)	H(22)	3.22	45501
C(37)	H(15)	3.30	45404	C(37)	H(10)	3.51	1
C(38)	H(5)	3.19	65501	C(38)	H(6)	3.49	55404
C(38)	H(16)	3.59	55404	C(39)	H(2)	3.47	4
C(40)	H(20)	3.28	74502	C(40)	H(10)	3.29	65501
C(40)	H(3)	3.33	65504	C(40)	H(22)	3.42	1
C(40)	H(5)	3.54	65504	H(1)	H(15)	3.38	45404
H(2)	H(9)	3.17	55404	H(2)	H(13)	3.41	55404

Table 6. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
H(2)	H(12)	3.44	55404	H(3)	H(7)	2.72	55404
H(3)	H(15)	2.74	45404	H(3)	H(9)	2.82	55404
H(3)	H(10)	3.36	55404	H(4)	H(15)	3.07	45404
H(4)	H(7)	3.35	55404	H(4)	H(14)	3.41	65502
H(5)	H(22)	3.03	45501	H(5)	H(16)	3.14	45404
H(5)	H(15)	3.16	45404	H(6)	H(23)	3.09	65502
H(6)	H(12)	3.52	1	H(7)	H(19)	2.61	4
H(8)	H(18)	2.47	45504	H(8)	H(21)	2.90	45501
H(8)	H(23)	3.29	4	H(8)	H(20)	3.50	45501
H(8)	H(17)	3.57	65502	H(9)	H(12)	2.80	1
H(10)	H(15)	3.59	45501	H(11)	H(17)	2.41	45501
H(11)	H(18)	3.16	65503	H(11)	H(20)	3.52	64502
H(11)	H(18)	3.58	45501	H(13)	H(22)	3.44	4
H(15)	H(20)	2.65	74502	H(16)	H(20)	3.04	74502
H(17)	H(18)	2.41	75503	H(17)	H(20)	3.26	74502
H(17)	H(17)	3.34	75503	H(18)	H(20)	2.94	55404
H(18)	H(21)	3.41	55404	H(19)	H(23)	2.65	65503

Crystallographic Information for **Tri-S⁺**

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
S(1)	0.60506(7)	-0.3160(2)	0.0443(2)	5.53(4)	1.0000
C(1)	0.5984(2)	0.0077(5)	0.0674(5)	3.7(1)	1.0000
C(2)	0.5455(2)	-0.0574(5)	0.1642(5)	3.7(1)	1.0000
C(3)	0.5000	0.0299(7)	0.2500	3.8(2)	0.5000
C(4)	0.6880(3)	-0.0837(7)	-0.0932(6)	5.4(1)	1.0000
C(5)	0.5000	-0.3216(7)	0.2500	4.3(2)	0.5000
C(6)	0.5440(2)	-0.2307(5)	0.1651(5)	4.0(1)	1.0000
C(7)	0.6144(2)	0.1700(6)	0.0392(5)	4.4(1)	1.0000
C(8)	0.6345(2)	-0.1167(5)	0.0004(5)	4.3(1)	1.0000
C(9)	0.7030(3)	0.0781(8)	-0.1179(7)	5.9(2)	1.0000
C(10)	0.6671(3)	0.2029(8)	-0.0547(6)	5.5(1)	1.0000
C(11)	0.5770(2)	-0.3889(5)	-0.0927(5)	5.5(1)	1.0000
C(12)	0.6488(3)	-0.4114(7)	0.1159(8)	9.4(2)	1.0000
H(1)	0.5000	0.156(6)	0.2500	4(1)	0.5000
H(2)	0.593(1)	0.262(4)	0.082(3)	2.6(8)	1.0000
H(3)	0.678(2)	0.304(5)	-0.069(5)	5(1)	1.0000
H(4)	0.734(2)	0.103(5)	-0.181(5)	5(1)	1.0000
H(5)	0.711(2)	-0.171(4)	-0.129(4)	3.8(10)	1.0000
H(6)	0.5000	-0.450(5)	0.2500	3(1)	0.5000

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos \gamma + 2U_{13}aa^*cc^* \cos \beta + 2U_{23}bb^*cc^* \cos \alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
S(1)	0.0675(9)	0.0549(8)	0.088(1)	0.0100(7)	0.0035(7)	-0.0103(8)
C(1)	0.043(3)	0.050(2)	0.048(3)	0.000(2)	-0.013(2)	-0.003(2)
C(2)	0.048(3)	0.042(2)	0.051(3)	-0.002(2)	-0.015(2)	0.001(2)
C(3)	0.050(4)	0.038(3)	0.056(4)	0.0000	-0.013(3)	0.0000
C(4)	0.060(4)	0.077(4)	0.067(4)	0.010(3)	-0.005(3)	-0.011(3)
C(5)	0.062(4)	0.032(3)	0.069(4)	0.0000	-0.017(3)	0.0000
C(6)	0.047(3)	0.047(2)	0.058(3)	0.007(2)	-0.009(2)	-0.005(2)
C(7)	0.053(3)	0.055(3)	0.059(3)	-0.004(3)	-0.008(2)	-0.001(3)
C(8)	0.054(3)	0.055(3)	0.056(3)	-0.001(2)	-0.011(2)	-0.002(2)
C(9)	0.062(4)	0.096(5)	0.067(4)	-0.011(4)	0.002(3)	0.001(4)
C(10)	0.070(4)	0.069(4)	0.071(4)	-0.016(3)	-0.009(3)	0.006(3)
C(11)	0.084(4)	0.058(3)	0.066(3)	-0.016(3)	-0.003(3)	-0.033(2)
C(12)	0.112(5)	0.100(5)	0.144(6)	0.033(4)	0.018(4)	0.001(4)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\text{\AA}$)

atom	atom	distance	atom	atom	distance
S(1)	C(4)	1.776(4)	S(1)	C(14)	1.450(4)
S(1)	C(30)	1.765(4)	S(1)	C(33)	1.347(6)
C(1)	C(4)	1.380(5)	C(1)	C(4)	1.380(5)
C(1)	H(10)	1.04(4)	C(2)	C(6)	1.367(7)
C(2)	C(31)	1.382(6)	C(2)	H(8)	0.86(4)
C(3)	C(6)	1.363(7)	C(3)	C(30)	1.394(6)
C(3)	H(5)	0.91(3)	C(4)	C(28)	1.403(5)
C(6)	H(11)	0.87(4)	C(28)	C(29)	1.474(5)
C(28)	C(32)	1.389(4)	C(29)	C(30)	1.380(5)
C(29)	C(31)	1.377(5)	C(31)	H(9)	0.95(3)
C(32)	H(1)	1.02(4)			

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(4)	S(1)	C(14)	110.4(2)	C(4)	S(1)	C(30)	90.9(2)
C(4)	S(1)	C(33)	115.7(3)	C(14)	S(1)	C(30)	109.7(2)
C(14)	S(1)	C(33)	114.8(3)	C(30)	S(1)	C(33)	112.9(3)
C(4)	C(1)	C(4)	115.5(5)	C(4)	C(1)	H(10)	122.2(3)
C(4)	C(1)	H(10)	122.2(3)	C(6)	C(2)	C(31)	121.3(5)
C(6)	C(2)	H(8)	120(3)	C(31)	C(2)	H(8)	118(3)
C(6)	C(3)	C(30)	117.1(5)	C(6)	C(3)	H(5)	125(2)
C(30)	C(3)	H(5)	117(2)	S(1)	C(4)	C(1)	124.9(3)
S(1)	C(4)	C(28)	111.7(3)	C(1)	C(4)	C(28)	123.4(4)
C(2)	C(6)	C(3)	121.6(6)	C(2)	C(6)	H(11)	118(2)
C(3)	C(6)	H(11)	119(2)	C(4)	C(28)	C(29)	112.1(4)
C(4)	C(28)	C(32)	119.4(4)	C(29)	C(28)	C(32)	128.4(4)
C(28)	C(29)	C(30)	112.2(4)	C(28)	C(29)	C(31)	128.3(4)
C(30)	C(29)	C(31)	119.6(4)	S(1)	C(30)	C(3)	125.0(4)
S(1)	C(30)	C(29)	113.0(3)	C(3)	C(30)	C(29)	122.0(4)
C(2)	C(31)	C(29)	118.5(5)	C(2)	C(31)	H(9)	116(1)
C(29)	C(31)	H(9)	124(1)	C(28)	C(32)	C(28)	118.8(5)
C(28)	C(32)	H(1)	120.6(3)	C(28)	C(32)	H(1)	120.6(3)

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
S(1)	C(4)	C(1)	C(4)	-179.2(4)	S(1)	C(4)	C(28)	C(29)	-1.8(4)
S(1)	C(4)	C(28)	C(32)	178.6(2)	S(1)	C(30)	C(3)	C(6)	178.4(4)
S(1)	C(30)	C(29)	C(28)	2.2(4)	S(1)	C(30)	C(29)	C(31)	-177.9(3)
C(1)	C(4)	S(1)	C(14)	71.0(4)	C(1)	C(4)	S(1)	C(30)	-177.6(3)
C(1)	C(4)	S(1)	C(33)	-61.5(5)	C(1)	C(4)	C(28)	C(29)	178.3(3)
C(1)	C(4)	C(28)	C(32)	-1.3(6)	C(1)	C(4)	S(1)	C(14)	71.0(4)
C(1)	C(4)	S(1)	C(30)	-177.6(3)	C(1)	C(4)	S(1)	C(33)	-61.5(5)
C(1)	C(4)	C(28)	C(29)	178.3(3)	C(1)	C(4)	C(28)	C(32)	-1.3(6)
C(2)	C(6)	C(3)	C(30)	-0.4(8)	C(2)	C(31)	C(29)	C(28)	179.1(4)
C(2)	C(31)	C(29)	C(30)	-0.8(6)	C(3)	C(6)	C(2)	C(31)	1.0(8)
C(3)	C(30)	S(1)	C(4)	178.0(4)	C(3)	C(30)	S(1)	C(14)	-69.8(5)
C(3)	C(30)	S(1)	C(33)	59.5(5)	C(3)	C(30)	C(29)	C(28)	-178.5(4)
C(3)	C(30)	C(29)	C(31)	1.4(6)	C(4)	S(1)	C(30)	C(29)	-2.7(3)
C(4)	C(1)	C(4)	C(28)	0.7(3)	C(4)	C(28)	C(29)	C(30)	-0.2(5)
C(4)	C(28)	C(29)	C(31)	179.8(4)	C(4)	C(28)	C(32)	C(28)	0.6(3)
C(6)	C(2)	C(31)	C(29)	-0.4(7)	C(6)	C(3)	C(30)	C(29)	-0.8(7)
C(14)	S(1)	C(4)	C(28)	-109.0(3)	C(14)	S(1)	C(30)	C(29)	109.4(4)
C(28)	C(4)	S(1)	C(30)	2.5(3)	C(28)	C(4)	S(1)	C(33)	118.6(4)
C(28)	C(32)	C(28)	C(29)	-178.9(4)	C(29)	C(30)	S(1)	C(33)	-121.2(4)
C(30)	C(29)	C(28)	C(32)	179.3(3)	C(31)	C(29)	C(28)	C(32)	-0.6(7)

Table 6. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
S(1)	H(9)	3.44(3)	54501	S(1)	H(8)	3.56(4)	54501
C(1)	C(14)	3.151(6)	65603	C(1)	C(14)	3.151(6)	4
C(1)	H(9)	3.50(3)	66603	C(1)	H(9)	3.50(3)	56504
C(2)	H(11)	3.30(4)	66607	C(2)	C(33)	3.335(9)	56404
C(2)	H(8)	3.39(4)	66607	C(2)	C(33)	3.473(9)	56501
C(2)	C(4)	3.543(7)	56404	C(2)	C(6)	3.564(8)	66607
C(3)	C(33)	3.393(9)	65607	C(3)	H(5)	3.48(3)	65607
C(3)	C(29)	3.541(6)	56404	C(3)	H(11)	3.58(4)	64506
C(4)	H(9)	3.57(3)	66603	C(4)	C(31)	3.594(6)	56504
C(6)	H(8)	3.11(4)	66607	C(6)	C(33)	3.359(9)	65607
C(6)	H(5)	3.47(3)	65506	C(6)	C(29)	3.563(7)	56404
C(14)	H(10)	2.48(2)	65603	C(14)	H(1)	2.83(3)	66603
C(14)	H(9)	3.01(3)	56404	C(14)	H(9)	3.22(3)	54501
C(14)	H(8)	3.26(4)	54501	C(14)	C(33)	3.335(8)	55404
C(14)	C(32)	3.590(7)	66603	C(28)	C(28)	3.546(8)	66603
C(29)	C(32)	3.448(4)	66603	C(30)	H(11)	3.46(4)	56504
C(30)	H(1)	3.562(6)	66603	C(31)	H(5)	3.52(3)	56504
C(31)	C(33)	3.527(8)	56501	C(33)	H(8)	2.86(4)	54501
C(33)	H(9)	2.90(3)	54501	C(33)	H(8)	2.93(4)	56504
C(33)	H(11)	2.95(4)	65607	C(33)	H(5)	2.99(4)	65607
C(33)	H(11)	3.53(4)	56504	H(1)	H(10)	3.18(7)	56501
H(5)	H(11)	2.70(5)	64506	H(5)	H(5)	3.05(7)	65607
H(5)	H(8)	3.47(6)	64506	H(5)	H(9)	3.60(5)	56404
H(8)	H(11)	2.94(6)	66607	H(8)	H(8)	3.34(8)	66607

Table 6. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
H(9)	H(10)	3.34(4)	56501				