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Supporting Information

Synthesis of a Stable Sulfenic Acid by Oxidation of Sterically Hindered Thiol (Thiophenetriptycene-8-thiol) and Its Characterization

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Characterization data (^{1}H and ^{13}C NMR, IR, and MS) for **2**, **4—6**, and **8—10**; structure determination summaries and tables of X-ray structure data for **8** (13 pages).

2,4,5',6-Tetramethyl-4,8-dihydro-4,8[3',2']thiophenobenzo[1,2-*b*:5,4-*b*']dithiophene-8-thiol (**2**): m.p. 170—172 °C decomp. (CCl_4-hexane). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.14 (s, 3H, bridgehead-4-Me), 2.31 (s, 9H, arom-Me), 2.94 (s, 1H, S-H), 6.63 (q-like, J = 0.8 Hz, 3H, arom-H); ^{13}C NMR ($CDCl_3$, 100.6 MHz) δ 14.8 (CH_3), 15.3 (CH_3), 50.0 (C), 51.5 (C), 120.2 (CH), 134.0 (C), 153.2 (C), 156.8 (C); MS *m/z* 360 (M^+, 100), 345 (13), 301 (89); IR (KBr) 2544 (S-H) cm^{-1}. Anal. Calcd for $C_{18}H_{16}S_4$: C, 59.96; H, 4.47; S, 35.57. Found: C, 59.83; H, 4.44; S, 35.72.

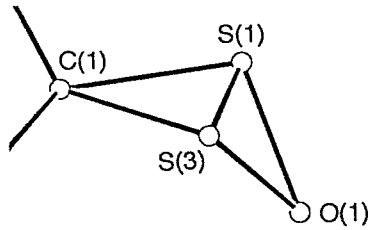
2,4,5',6-Tetramethyl-8-methylthio-4,8-dihydro-4,8[3',2']thiophenobenzo[1,2-*b*:5,4-*b*']dithiophene (**4**): colorless crystals, m.p. 167—168 °C decomp. (hexane). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.15 (s, 3H, bridgehead-4-Me), 2.33 (s, 9H, arom-Me), 2.71 (s, 3H, S-Me), 6.63 (q-like, J = 0.8 Hz, 3H, arom-H); ^{13}C NMR ($CDCl_3$, 100.6 MHz) δ 14.2 (CH_3), 14.9 (CH_3), 15.3 (CH_3), 49.9 (C), 53.4 (C), 119.7 (CH), 134.5 (C), 151.1 (C), 157.8 (C); MS *m/z* 374 (M^+, 61), 315 (100). Anal. Calcd for $C_{19}H_{18}S_4$: C, 60.92; H, 4.84. Found: C, 61.08; H, 4.85.

2,4,5',6-Tetramethyl-8-*n*-butylthio-4,8-dihydro-4,8[3',2']thiophenobenzo[1,2-*b*:5,4-*b*']dithiophene (**5**): orange crystals, m.p. 131—132 °C (hexane). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.01 (t, J = 7.3 Hz, 3H), 1.55 (sext, J = 7.5 Hz, 2H), 1.84 (quint, J = 7.5 Hz, 2H), 2.14 (s, 3H, bridgehead-4-Me), 2.33 (s, 9H, arom-Me), 3.24 (t, J = 7.5 Hz, 2H), 6.63 (s, 3H, arom-H); ^{13}C NMR ($CDCl_3$, 100.6 MHz) δ 13.7 (CH_3), 14.9 (CH_3), 15.3 (CH_3), 22.3 (CH_2), 31.0 (CH_2), 32.1 (CH_2), 49.9 (C), 56.6 (C), 119.8 (CH), 134.3 (C), 151.6 (C), 157.6 (C); MS *m/z* 416 (M^+, 100), 357 (83), 315 (94). Anal. Calcd for $C_{22}H_{24}S_4$: C, 63.41; H, 5.81. Found: C, 63.47; H, 5.79.

2,4,5',6-Tetramethyl-8-methylsulfinyl-4,8-dihydro-4,8[3',2']thiophenobenzo[1,2-*b*:5,4-*b*']dithiophene (**6**): white powder, m.p. 185—187 °C decomp. (hexane). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.19 (s, 3H, bridgehead-4-Me), 2.35 (s, 9H, arom-Me), 3.28 [s, 3H, S(O)-Me], 6.66 (q-like, J = 0.7 Hz, 3H, arom-H); ^{13}C NMR ($CDCl_3$, 100.6 MHz) δ 14.8 (CH_3), 15.1 (CH_3), 37.6 (CH_3), 50.2 (C), 71.9 (C), 119.2 (CH), 136.4 (C), 143.3 (C), 159.6 (C); MS *m/z* 390 (M^+, 100), 375 (56), 312 (98). Anal. Calcd for $C_{19}H_{18}OS_4$: C, 58.42; H, 4.65. Found: C, 58.36; H, 4.69.

2,4,5',6-trimethyl-4,8-dihydro-4,8[3',2']thiophenobenzo[1,2-*b*:5,4-*b*']dithiophene-8-sulfenic acid (**8**): colorless crystals, m.p. 78—79 °C decomp. (CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.18 (s, 3H, bridgehead-Me), 2.33 (s, 9H, arom-Me), 3.79 (s, 1H, SOH), 6.65 (s, 3H, arom-H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 14.8 (CH_3), 15.3 (CH_3), 50.2 (2×C), 119.6 (CH), 135.0 (C), 148.5 (C), 158.2 (C); MS *m/z* 376 (M^+, 25), 360 (100), 345 (68), 3219 (50), 301 (27); IR (KBr) 3456 (O-H), 766 (S-O) cm^{-1}. Anal. Calcd for $C_{18}H_{16}OS_4$: C, 57.41; H, 4.28. Found: C, 57.07; H, 4.18. *X-ray analysis:* trigonal, $P\bar{3}$, a = 20.340(3) Å, b = 20.340(3) Å, c = 10.028(2) Å, V = 3593 Å^3, Z = 8, R = 0.0709, R_w = 0.0861, GOF = 4.61. The least-square refinement was done on one whole molecule and a third part of the molecule of **8**. The sulfenic acid hydrogen did not appear by difference synthesis (F_o–F_c). In the difference synthesis, a peak appeared at the position apart from C(1) by 1.67(4) Å and assigned to another sulfur atom [S(3)] [S(3)-O(1),

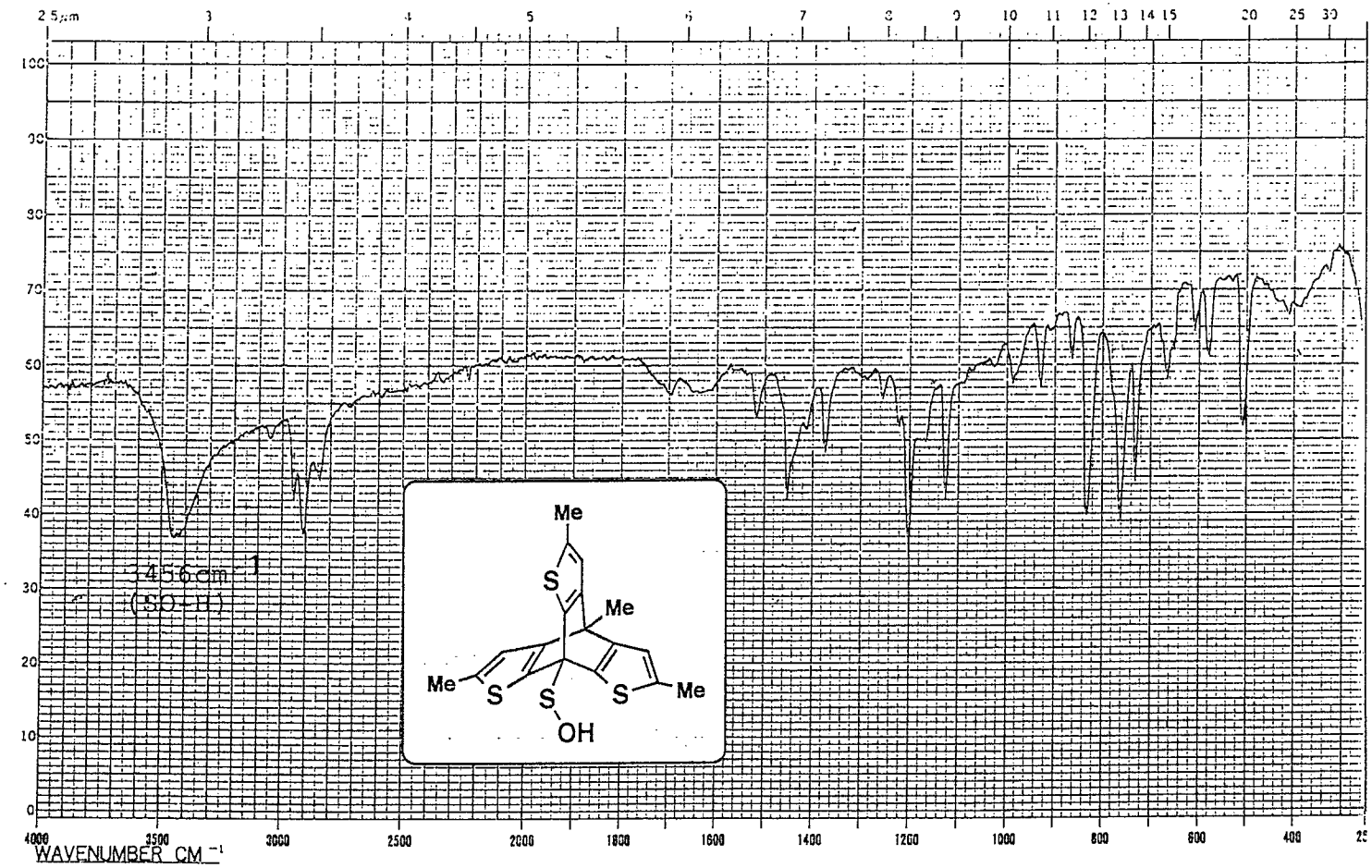
1.37(4) Å]. The ratio of occupancies of S(1) and S(3) is 0.84:0.16. This disorder seems to be ascribed to decomposition of **8** to sulfine **9** during measurement.



2,4,6-Trimethyl-8-thioxo-4-(5-methyl-3-thienyl)[2,1-*b*:4,5-*b*']dithiophenocyclohexa-1,4-diene 8-*S*-oxide (**9**): brown crystals, m.p. 169—172 °C decomp. (MeOH). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.85 (s, 3H), 2.32 (s, 3H), 2.41 (s, 3H), 2.49 (s, 3H), 6.13 (s, 1H), 6.51 (d, J = 0.8 Hz, 1H), 6.60 (s, 1H), 6.96 (d, J = 1.4 Hz, 1H); MS *m/z* 376 (M^+, 27), 360 (100), 345 (80), 329 (94). IR (KBr) 1078 (S=O) cm^{-1}. Anal. Calcd for $C_{18}H_{16}OS_4$: C, 57.41; H, 4.28. Found: C, 57.26; H, 4.30.

2,4,5',6-Tetramethyl-8-[*trans*-2-(methoxycarbonyl)ethenylsulfinyl]-4,8-dihydro-4,8[3',2']thiophenobenzo[1,2-*b*:5,4-*b*']dithiophene (**10**): pale yellow solid. ^{1}H NMR ($CDCl_3$, 200 MHz) δ 2.17 (s, 3H, bridgehead-4-Me), 2.33 (d, J = 0.8 Hz, 9H, arom-Me), 3.82 (s, 3H), 6.65 (d, J = 0.9 Hz, 3H, arom-H), 7.14 (d, J = 15 Hz, 1H), 8.18 (d, J = 15 Hz, 1H); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 14.8 (CH_3), 15.1 (CH_3), 50.1 (C), 52.5 (CH_3), 72.0 (C), 119.1 (CH), 130.5 (C), 136.7 (C), 143.4 (C), 146.5 (C), 159.3 (C), 163.7 (C=O); MS *m/z* 460 (M^+, 40), 444 (100), 385 (86), 327 (68), 312 (98). IR (KBr) 1729 (C=O), 1086 (S=O) cm^{-1}.

The IR Spectrum of Thiophenetriptycene-8-sulfenic Acid



TITLE : Thiophenetriptycene-8-sulfenic Acid

CRYSTAL :

Chemical Formula	C18 H16 O1 S4
Formula Weight	376.60
Crystal Size	0.30 * 0.34 * 0.16 mm**3
Unit-cell Dimensions :	
	a = 20.340 (3) A
	b = 20.340 (3) A
	c = 10.028 (2) A
	alpha = 90.0000000 (0) degrees
	beta = 90.0000000 (0) degrees
	gamma = 120.0000000 (0) degrees
Volume of unit cell	3593 (1) A**3
Crystal System	Trigonal
Space Group	P -3 (#147)
Z value	8
Densities: Dobs ;Dcalc	1.40; 1.39 g/cm**3

DATA COLLECTION :

Diffractometer used	Mac Science MXC3K
Radiation	Cu K-alpha (lambda= 1.54178)
Total Reflections Measured	4369
Reflection (hkl) limits	-20 < h < 20 0 < k < 23 0 < l < 11 (3 deg < 2theta < 120 deg)
Unique Reflections	3701
Internal Consistency : Rint	0.05

REFINEMENT :

Least squares refinement method	Full matrix
Absorption correction	refdelf
Function minimized	Sum[w(|Fo|-|Fc|)**2]
Weight method	Count statistics

S-Ishii

F(000)	1567
Linear absorption coefficient	47.930/cm
Reflections used in L.S.	2259
Data reduction cut-off	3.00
Maximum sin(theta)/lambda	0.576
L.S. parameters	294
L.S. matrix elements	43365
Extinction coefficient	0.0000
Residuals, R	0.0709
Residuals, Rw	0.0861
Max shift/e.s.d.	0.0751
Average shift/e.s.d.	0.0049
Sum w(Fobs-Fcal)**2	0.41807E+05
Sum (Fobs-Fcal)	0.39818E+04
Goodness of fit	4.61

FOURIER :

Fourier map type	Fo-Fc
Sim weighting	OFF
Fourier map grid	0.333 A
Maximum peak in final Fourier map	0.39 e/A**3 @(0.769 0.229 0.598)
Minimum peak in final Fourier map	-0.43 e/A**3 @(0.016 0.016 0.299)

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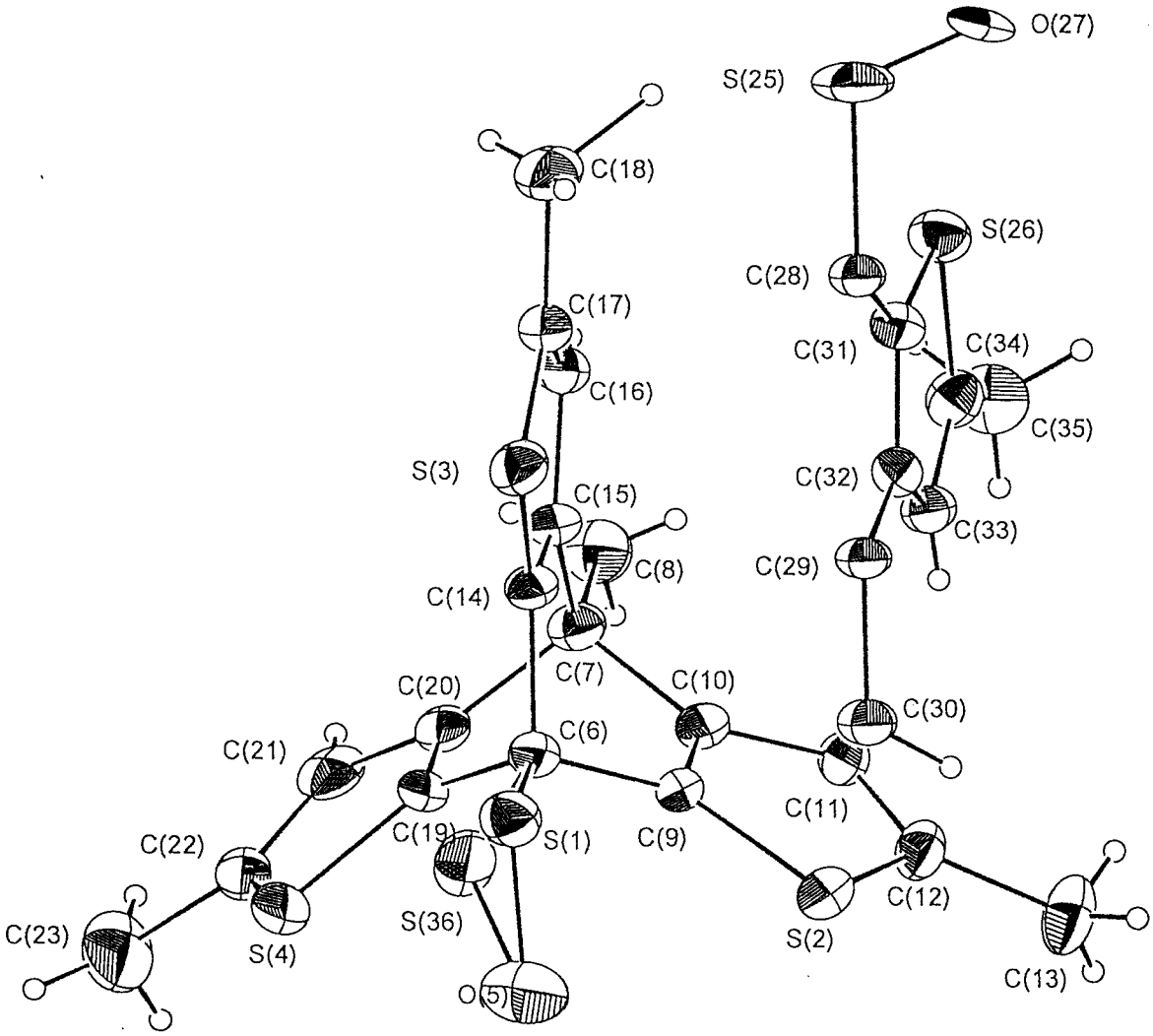
O(27)
S(25)
C(18)
S(26)
C(28)
C(17)
C(31)
C(34)
C(16)
C(35)
S(3)
C(32)
C(15)
C(33)
C(8)
C(29)
C(14)
C(7)
C(10)
C(20)
C(30)
C(6)
C(21)
C(11)
C(19)
S(1)
C(9)
C(22)
C(12)
S(36)
S(2)
C(23)
S(4)
C(13)
O(5)

Y-Ishii

FRACTIONAL ATOMIC COORDINATES & U(iso)

Atom	x/a	y/b	z/c	U(iso)
S(1)	0.8578(3)	0.3439(3)	0.7431(5)	0.087
S(2)	0.69989(11)	0.17078(12)	0.64762(22)	0.086
S(3)	0.85135(11)	0.29960(12)	1.06087(23)	0.089
S(4)	0.98438(12)	0.28078(16)	0.63011(24)	0.106
S(25)	0.6670	0.3330	1.4477(4)	0.139
S(26)	0.63067(12)	0.17272(11)	1.26709(22)	0.090
O(5)	0.8523(5)	0.3424(4)	0.5816(8)	0.156
O(27)	0.6004(10)	0.2789(11)	1.4950(16)	0.116
C(6)	0.8492(4)	0.2517(4)	0.7804(8)	0.069
C(7)	0.8317(4)	0.1201(4)	0.8676(8)	0.077
C(9)	0.7757(4)	0.1814(4)	0.7372(7)	0.066
C(10)	0.7663(4)	0.1142(4)	0.7810(7)	0.071
C(11)	0.6948(4)	0.0499(4)	0.7418(8)	0.069
C(12)	0.6534(4)	0.0740(4)	0.6676(9)	0.083
C(14)	0.8491(4)	0.2429(4)	0.9342(7)	0.068
C(15)	0.8396(4)	0.1760(4)	0.9771(7)	0.070
C(16)	0.8337(4)	0.1703(4)	1.1215(8)	0.071
C(19)	0.9099(4)	0.2338(5)	0.7354(8)	0.075
C(20)	0.9018(4)	0.1674(5)	0.7770(8)	0.082
C(28)	0.6670	0.3330	1.2687(12)	0.072
C(29)	0.6670	0.3330	1.0048(12)	0.072
C(30)	0.6670	0.3330	0.8518(14)	0.082
C(31)	0.6498(4)	0.2581(4)	1.2047(8)	0.073
C(32)	0.6517(4)	0.2587(3)	1.0683(7)	0.064
C(33)	0.6388(4)	0.1896(4)	1.0168(8)	0.077
C(8)	0.8232(5)	0.0444(5)	0.9195(10)	0.103
C(13)	0.5770(5)	0.0273(5)	0.6042(11)	0.111
C(17)	0.8392(4)	0.2325(5)	1.1756(8)	0.086
C(18)	0.8349(5)	0.2485(7)	1.3231(9)	0.139
C(21)	0.9624(5)	0.1535(5)	0.7256(9)	0.102
C(22)	1.0070(5)	0.2132(7)	0.6423(9)	0.108
C(34)	0.6264(4)	0.1367(4)	1.1085(9)	0.085
C(35)	0.6110(7)	0.0571(5)	1.0896(11)	0.117
C(23)	1.0741(6)	0.2191(8)	0.5638(13)	0.168
H(8A)	0.78280	0.02320	0.94910	0.048
H(8B)	0.81710	0.00990	0.85180	0.091
H(8C)	0.86960	0.05130	0.95260	0.089
H(11)	0.68610	0.01290	0.75690	0.002
H(13A)	0.53900	0.03660	0.60770	0.146
H(13B)	0.55320	-0.00830	0.65690	0.118
H(13C)	0.56620	-0.01160	0.54290	0.114
H(16)	0.83060	0.13620	1.14380	0.018
H(18A)	0.82460	0.28660	1.31870	0.138
H(21)	0.96160	0.11300	0.75170	0.026
H(30)	0.62470	0.29580	0.80490	0.083
H(33)	0.63470	0.18050	0.94900	0.021
H(23A)	1.06670	0.16290	0.60250	0.113
H(23B)	1.11540	0.28110	0.54030	0.134

over>

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<cont

S(36)	0.8832(14)	0.3336(17)	0.6967(30)	0.133
H(23C)	1.05400	0.18670	0.49340	0.128
H(18B)	0.78190	0.19250	1.38750	0.205
H(18C)	0.86670	0.23780	1.34720	0.140
H(35A)	0.60867	0.03713	1.00191	0.050
H(35B)	0.56337	0.02333	1.13171	0.13(4)
H(35C)	0.65087	0.05443	1.13591	0.19(6)

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ANISOTROPIC THERMAL PARAMETERS

Atom	U11	U22	U33	U12	U13	U23
S(1)	0.080(3)	0.065(2)	0.067(2)	0.027(2)	0.000(2)	0.005(2)
S(2)	0.069(1)	0.080(1)	0.058(1)	0.032(1)	-0.012(1)	-0.006(1)
S(3)	0.072(1)	0.081(1)	0.063(1)	0.036(1)	-0.009(1)	-0.015(1)
S(4)	0.071(1)	0.129(2)	0.052(1)	0.025(1)	0.008(1)	-0.009(1)
S(25)	0.144(3)	0.144	0.033(2)	0.072	0.000	0.000
S(26)	0.084(1)	0.072(1)	0.060(1)	0.039(1)	0.003(1)	0.015(1)
O(5)	0.164(7)	0.121(6)	0.087(6)	0.068(5)	0.010(5)	0.011(5)
O(27)	0.10(1)	0.14(2)	0.03(1)	0.03(1)	0.02(1)	0.02(1)
C(6)	0.058(4)	0.063(4)	0.046(5)	0.018(4)	-0.002(4)	0.008(4)
C(7)	0.072(5)	0.064(5)	0.048(5)	0.032(4)	-0.006(4)	-0.005(4)
C(9)	0.047(4)	0.069(5)	0.042(5)	0.020(4)	-0.005(3)	0.004(4)
C(10)	0.062(4)	0.066(5)	0.044(5)	0.026(4)	-0.005(4)	-0.009(4)
C(11)	0.056(4)	0.053(4)	0.060(5)	0.018(4)	-0.003(4)	-0.007(4)
C(12)	0.054(4)	0.080(5)	0.071(6)	0.030(4)	-0.010(4)	-0.023(4)
C(14)	0.062(4)	0.061(4)	0.041(5)	0.028(4)	-0.005(4)	-0.008(4)
C(15)	0.064(4)	0.066(4)	0.038(4)	0.031(4)	-0.004(4)	-0.003(4)
C(16)	0.063(4)	0.060(4)	0.049(5)	0.026(4)	0.001(4)	0.002(4)
C(19)	0.054(4)	0.087(6)	0.036(5)	0.016(4)	0.005(4)	0.000(4)
C(20)	0.064(5)	0.089(6)	0.042(5)	0.034(4)	-0.007(4)	-0.020(4)
C(28)	0.068(5)	0.068	0.036(7)	0.034	0.000	0.000
C(29)	0.067(5)	0.067	0.036(7)	0.034	0.000	0.000
C(30)	0.075(5)	0.075	0.045(8)	0.038	0.000	0.000
C(31)	0.066(4)	0.061(4)	0.049(5)	0.033(4)	0.004(4)	0.008(4)
C(32)	0.055(4)	0.048(4)	0.054(5)	0.028(3)	0.002(3)	0.004(3)
C(33)	0.065(4)	0.071(5)	0.049(5)	0.036(4)	-0.003(4)	-0.002(4)
C(8)	0.096(6)	0.071(5)	0.088(7)	0.035(5)	-0.005(5)	-0.008(5)
C(13)	0.063(5)	0.090(6)	0.129(9)	0.028(5)	-0.025(5)	-0.039(6)
C(17)	0.062(5)	0.097(6)	0.047(5)	0.034(4)	-0.001(4)	-0.003(5)
C(18)	0.098(7)	0.174(10)	0.055(6)	0.077(7)	-0.005(5)	-0.023(6)
C(21)	0.097(6)	0.091(6)	0.054(6)	0.043(5)	-0.024(5)	-0.036(5)
C(22)	0.063(5)	0.146(9)	0.046(5)	0.034(6)	0.000(4)	-0.039(6)
C(34)	0.070(5)	0.067(5)	0.073(6)	0.036(4)	-0.007(4)	-0.001(4)
C(35)	0.123(8)	0.062(5)	0.104(8)	0.046(6)	-0.001(7)	-0.003(5)
C(23)	0.100(8)	0.186(12)	0.122(10)	0.061(8)	0.018(7)	-0.056(9)
S(36)	0.08(2)	0.13(2)	0.12(2)	0.02(1)	-0.02(1)	0.08(2)

$$T=\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+U_{12}hka^*b^*+U_{23}klb^*c^*+U_{13}hla^*c^*)]$$

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INTRAMOLECULAR BOND LENGTHS (H omitted)

Minimum bond length= 1.30A		: Maximum bond length= 1.90A	
S(1)-O(5)	1.622(9)	S(1)-C(6)	1.833(9)
S(2)-C(9)	1.701(7)	S(2)-C(12)	1.716(8)
S(3)-C(14)	1.701(8)	S(3)-C(17)	1.706(9)
S(4)-C(19)	1.696(8)	S(4)-C(22)	1.656(12)
S(25)-O(27)	1.335(19)	S(25)-O(27)	1.323(18)
S(25)-O(27)	1.34(2)	S(25)-C(28)	1.795(14)
S(25)-C(28)	1.795(14)	S(25)-C(28)	1.795(14)
S(26)-C(31)	1.698(8)	S(26)-C(34)	1.735(9)
O(5)-S(36)	1.37(4)	C(6)-C(9)	1.526(10)
C(6)-C(14)	1.553(11)	C(6)-C(19)	1.520(11)
C(6)-S(36)	1.67(4)	C(7)-C(10)	1.542(11)
C(7)-C(15)	1.531(11)	C(7)-C(20)	1.553(11)
C(7)-C(8)	1.551(11)	C(9)-C(10)	1.356(11)
C(10)-C(11)	1.442(10)	C(11)-C(12)	1.385(11)
C(12)-C(13)	1.499(12)	C(14)-C(15)	1.344(10)
C(15)-C(16)	1.453(11)	C(16)-C(17)	1.330(12)
C(19)-C(20)	1.344(12)	C(20)-C(21)	1.487(12)
C(28)-C(31)	1.524(9)	C(28)-C(31)	1.530(9)
C(28)-C(31)	1.543(9)	C(29)-C(30)	1.534(19)
C(29)-C(30)	1.534(19)	C(29)-C(30)	1.534(19)
C(29)-C(32)	1.522(9)	C(29)-C(32)	1.528(9)
C(29)-C(32)	1.540(9)	C(31)-C(32)	1.368(11)
C(32)-C(33)	1.393(10)	C(33)-C(34)	1.341(12)
C(17)-C(18)	1.527(13)	C(21)-C(22)	1.377(14)
C(22)-C(23)	1.528(15)	C(34)-C(35)	1.499(12)

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INTRAMOLECULAR BOND ANGLES (H omitted)

Minimum bond length= 1.30A : Maximum bond length= 1.90A

O(5)-S(1)-C(6)	102.3(5)	C(9)-S(2)-C(12)	91.7(4)
C(14)-S(3)-C(17)	90.9(4)	C(19)-S(4)-C(22)	91.5(5)
O(27)-S(25)-O(27)	108.6(12)	O(27)-S(25)-O(27)	107.5(12)
O(27)-S(25)-C(28)	110.8(8)	O(27)-S(25)-C(28)	111.0(8)
O(27)-S(25)-C(28)	110.4(8)	O(27)-S(25)-O(27)	108.2(12)
O(27)-S(25)-C(28)	111.0(8)	O(27)-S(25)-C(28)	111.4(8)
O(27)-S(25)-C(28)	111.6(8)	O(27)-S(25)-C(28)	110.7(8)
O(27)-S(25)-C(28)	110.0(8)	O(27)-S(25)-C(28)	110.5(8)
C(28)-S(25)-C(28)	0.6(1)	C(28)-S(25)-C(28)	0.6(1)
C(28)-S(25)-C(28)	0.6(1)	C(31)-S(26)-C(34)	91.8(4)
S(1)-O(5)-S(36)	29.4(12)	S(25)-O(27)-S(25)	0.8(1)
S(25)-O(27)-S(25)	0.7(1)	S(25)-O(27)-S(25)	0.3(3)
S(1)-C(6)-C(9)	116.6(6)	S(1)-C(6)-C(14)	108.4(5)
S(1)-C(6)-C(19)	120.8(6)	S(1)-C(6)-S(36)	25.8(10)
C(9)-C(6)-C(14)	103.3(6)	C(9)-C(6)-C(19)	102.9(6)
C(9)-C(6)-S(36)	120.9(12)	C(14)-C(6)-C(19)	102.7(6)
C(14)-C(6)-S(36)	126.1(12)	C(19)-C(6)-S(36)	96.2(11)
C(10)-C(7)-C(15)	103.1(6)	C(10)-C(7)-C(20)	102.0(6)
C(10)-C(7)-C(8)	116.6(7)	C(15)-C(7)-C(20)	103.7(6)
C(15)-C(7)-C(8)	114.5(7)	C(20)-C(7)-C(8)	115.0(7)
S(2)-C(9)-C(6)	132.1(6)	S(2)-C(9)-C(10)	112.4(6)
C(6)-C(9)-C(10)	115.5(6)	C(7)-C(10)-C(9)	115.1(7)
C(7)-C(10)-C(11)	131.6(7)	C(9)-C(10)-C(11)	113.3(7)
C(10)-C(11)-C(12)	110.0(6)	S(2)-C(12)-C(11)	112.6(6)
S(2)-C(12)-C(13)	118.6(6)	C(11)-C(12)-C(13)	128.7(7)
S(3)-C(14)-C(6)	131.6(6)	S(3)-C(14)-C(15)	112.9(6)
C(6)-C(14)-C(15)	115.3(7)	C(7)-C(15)-C(14)	115.5(7)
C(7)-C(15)-C(16)	132.9(7)	C(14)-C(15)-C(16)	111.4(7)
C(15)-C(16)-C(17)	111.5(7)	S(4)-C(19)-C(6)	130.8(6)
S(4)-C(19)-C(20)	112.6(6)	C(6)-C(19)-C(20)	116.4(7)
C(7)-C(20)-C(19)	114.6(7)	C(7)-C(20)-C(21)	132.6(8)
C(19)-C(20)-C(21)	112.8(8)	S(25)-C(28)-S(25)	0.6(1)
S(25)-C(28)-S(25)	0.6(1)	S(25)-C(28)-C(31)	114.9(6)
S(25)-C(28)-C(31)	114.8(6)	S(25)-C(28)-C(31)	114.6(6)
S(25)-C(28)-S(25)	0.6(1)	S(25)-C(28)-C(31)	115.6(6)
S(25)-C(28)-C(31)	114.6(6)	S(25)-C(28)-C(31)	114.2(5)
S(25)-C(28)-C(31)	115.1(6)	S(25)-C(28)-C(31)	115.3(6)
S(25)-C(28)-C(31)	114.0(5)	C(31)-C(28)-C(31)	104.1(7)
C(31)-C(28)-C(31)	103.5(7)	C(31)-C(28)-C(31)	103.3(7)
C(30)-C(29)-C(30)	0.8(1)	C(30)-C(29)-C(30)	0.8(1)
C(30)-C(29)-C(32)	114.7(5)	C(30)-C(29)-C(32)	114.6(5)
C(30)-C(29)-C(32)	114.4(5)	C(30)-C(29)-C(30)	0.8(1)
C(30)-C(29)-C(32)	115.5(6)	C(30)-C(29)-C(32)	114.4(5)
C(30)-C(29)-C(32)	113.9(5)	C(30)-C(29)-C(32)	115.0(6)
C(30)-C(29)-C(32)	115.1(6)	C(30)-C(29)-C(32)	113.7(5)
C(32)-C(29)-C(32)	104.4(7)	C(32)-C(29)-C(32)	103.8(7)
C(32)-C(29)-C(32)	103.5(6)	C(29)-C(30)-C(29)	0.8(1)
C(29)-C(30)-C(29)	0.8(1)	C(29)-C(30)-C(29)	0.8(1)

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S(26)-C(31)-C(28)	133.4(7)	S(26)-C(31)-C(28)	133.7(7)
S(26)-C(31)-C(28)	133.5(7)	S(26)-C(31)-C(32)	111.6(6)
C(28)-C(31)-C(28)	0.4(6)	C(28)-C(31)-C(28)	0.7(1)
C(28)-C(31)-C(32)	114.9(7)	C(28)-C(31)-C(28)	0.6(3)
C(28)-C(31)-C(32)	114.6(7)	C(28)-C(31)-C(32)	114.8(7)
C(29)-C(32)-C(29)	0.3(6)	C(29)-C(32)-C(29)	0.7(1)
C(29)-C(32)-C(31)	114.7(7)	C(29)-C(32)-C(33)	133.5(8)
C(29)-C(32)-C(29)	0.6(2)	C(29)-C(32)-C(31)	114.4(7)
C(29)-C(32)-C(33)	133.8(8)	C(29)-C(32)-C(31)	114.6(7)
C(29)-C(32)-C(33)	133.6(8)	C(31)-C(32)-C(33)	111.8(7)
C(32)-C(33)-C(34)	114.8(8)	S(3)-C(17)-C(16)	113.3(7)
S(3)-C(17)-C(18)	118.9(7)	C(16)-C(17)-C(18)	127.8(9)
C(20)-C(21)-C(22)	106.6(8)	S(4)-C(22)-C(21)	116.3(7)
S(4)-C(22)-C(23)	120.3(9)	C(21)-C(22)-C(23)	123.3(10)
S(26)-C(34)-C(33)	109.9(6)	S(26)-C(34)-C(35)	120.8(7)
C(33)-C(34)-C(35)	129.3(9)	O(5)-S(36)-C(6)	124.3(21)

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