ORGANOMETALLICS
Organometallics, 1996, 15(21), 4531-4536, DOI:10.1021/om960449u

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Status of project

28-JUN-91 15:01:25

PROJECT DIRECTORY : [TEXSAN.TOKITOH.SNCS3]

TITLE : SNCS3 25-MAY-91

CELL : a= 46.252 b= 13.470 c= 18.645 alpha= 90.00 beta=105.48 gamma= 90.00

SPACEG : C2/c S.G.# 15 DENSITY : Dc= 1.166 Absorption coef.= 7.160

STORED formula		CURRENT formula		STATUS
SN	1.00	SN	1.00	O.K.
S	3.00	S	3.00	O.K.
SI	6.00	SI	6.00	O.K.
C	43.00	C	43.00	O.K.
H	82.00	H	82.00	O.K.

parameters : # of reflections= 6659 # of variables= 478 shift/error= 0.127

R-factors : R= 0.046 Rw= 0.047 Goodness of fit= 1.559 LS cycles= 1

corrections : absorption=on -type=DIF decay=off redundant=on average=off

EXPERIMENTAL

DATA COLLECTION

A yellow block crystal of $SnS_3Si_6C_{43}H_{82}$ having approximate dimensions of 0.500 X 0.400 X 0.400 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC5R diffractometer with graphite monochromated Mo Ka radiation and a 12KW rotating anode generator.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 25 carefully centered reflections in the range 37.76 < 2j < 39.42° corresponded to a monoclinic cell with dimensions:

a = 46.25 (1)Å
b = 13.470 (5)Å b = 105.48 (3)°
c = 18.645 (5)Å
V = 11195 (6)Å^3

For Z = 8 and F.W. = 982.50, the calculated density is 1.166 g/cm^3. Based on the systematic absences of:

hkl: h+k ≠ 2n
h0l: l ≠ 2n

packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

C2/c (#15)

The data were collected at a temperature of 24 ± 1°C using the w-2j scan technique to a maximum 2j value of 55.1°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.32° with a take-off angle of 6.0°. Scans of (1.10 + 0.30 tan j)° were made at a speed of 16.0°/min (in omega). The weak reflections (I < 10.0s(I)) were rescanned (maximum of 1 rescans) and the counts were accumulated to assure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 0.5 mm and the crystal to detector distance was 40 cm.

DATA REDUCTION

Of the 13654 reflections which were collected, 13488 were unique (R_{int} = 0.028). The intensities of three representative reflections which were measured after every 150 reflections remained constant throughout data collection indicating crystal and electronic stability (no decay correction was applied).

The linear absorption coefficient for Mo Ka is 7.2 cm^{-1}. An empirical absorption correction, , using the program DIFABS[3], was applied which resulted in transmission factors ranging from 0.76 to 1.17. The data were corrected for Lorentz and polarization effects.

STRUCTURE SOLUTION AND REFINEMENT

The structure was solved by direct methods[4]. The non-hydrogen atoms were refined anisotropically. The final cycle of full-matrix least-squares refinement[5] was based on 6659 observed reflections (I > 3.00s(I)) and 478 variable parameters and converged (largest parameter shift was 0.13 times its esd) with unweighted and weighted agreement factors of:

$$R = S\ ||Fo| - |Fc|| \ / \ S\ |Fo| = 0.046$$

$$R_w = [(\ S\ w\ (|Fo| - |Fc|)^2 \ / \ S\ w\ Fo^2\ )]^{1/2} = 0.047$$

The standard deviation of an observation of unit weight[6] was 1.56. The weighting scheme was based on counting statistics and included a factor (p = 0.03) to downweight the intense reflections. Plots of $S\ w\ (|Fo| - |Fc|)^2$ versus |Fo|, reflection order in data collection, sin j/l , and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.39 and -0.42 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[7]. Anomalous dispersion effects were included in Fcalc[8]; the values for Df' and Df" were those of Cromer[9]. All calculations were performed using the TEXSAN[10] crystallographic software package of Molecular Structure Corporation.

References

(1) PLUTO:
Motherwell,S. & Clegg,W.; PLUTO. Program for plotting molecular and crystal structures. Univ. of Cambridge, England (1978).

(2) ORTEP:
Johnson,C.K.; ORTEPII. Report ORNL-5138. Oak Ridge National Laboratory, Oak Ridge, Tennessee (1976).

(3) DIFABS:
Walker & Stuart, Acta Cryst. A39, 158-166, (1983).

(4) Structure Solution Methods:
MITHRIL
Gilmore,C.J.; MITHRIL - an integrated direct methods computer program. J. Appl. Cryst. 17, 42-46, Univ. of Glasgow, Scotland, (1984).
DIRDIF
Beurskens,P.T.; DIRDIF: Direct Methods for Difference Structures - an automatic procedure for phase extension and refinement of difference structure factors. Technical Report 1984/1 Crystallography Laboratory, Toernooiveld, 6525 Ed Nijmegen, Netherlands.

(5) Least-Squares:
Function minimized: $S\ w\ (|Fo| - |Fc|)^2$
where: $w = 4Fo^2/s^2(Fo^2)$
$s^2(Fo^2) = [S^2(C+R^2B) + (pFo^2)^2]/Lp^2$
S = Scan rate
C = Total Integrated Peak Count
R = Ratio of Scan Time to background counting time.
B = Total Background Count
Lp = Lorentz-polarization factor
p = p-factor

(6) Standard deviation of an observation of unit weight:

$$[S\ w(|Fo| - |Fc|)^2/(No - Nv)]^{1/2}$$

where: No = number of observations
Nv = number of variables

(7) Cromer,D.T. & Waber,J.T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(8) Ibers,J.A. & Hamilton,W.C.; Acta Crystallogr., 17, 781 (1964).

(9) D.T. Cromer, "International Tables for X-ray

Crystallography", Vol/ IV, The Kynoch Press, Birmingham, England, Table 2.3.1 (1974).

(10) TEXSAN - TEXRAY Structure Analysis Package, Molecular Structure Corporation (1985).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$SnS_3Si_6C_{43}H_{82}$
Formula Weight	982.50
Crystal Color, Habit	yellow, block
Crystal Dimensions (mm)	0.500 X 0.400 X 0.400
Crystal System	monoclinic
No. Reflections Used for Unit Cell Determination (2j range)	25 (37.8 - 39.4°)
Omega Scan Peak Width at Half-height	0.32
Lattice Parameters:	
	a = 46.25 (1)Å b = 13.470 (5)Å c = 18.645 (5)Å b = 105.48 (3)°
	V = 11195 (6)$Å^3$
Space Group	C2/c (#15)
Z value	8
D_{calc}	1.166 g/cm^3
F_{000}	4176
μ(MoKa)	7.16 cm^{-1}

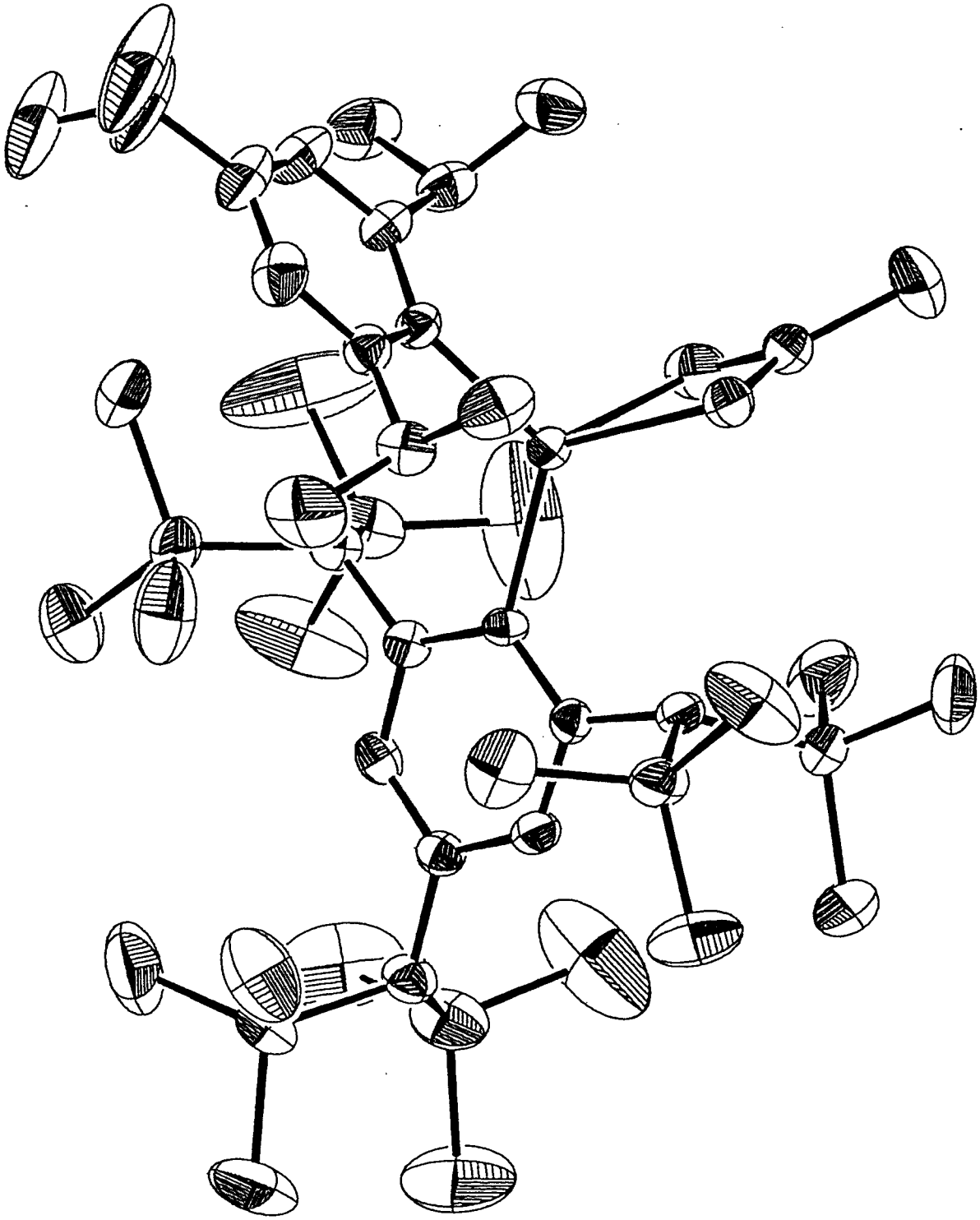
B. Intensity Measurements

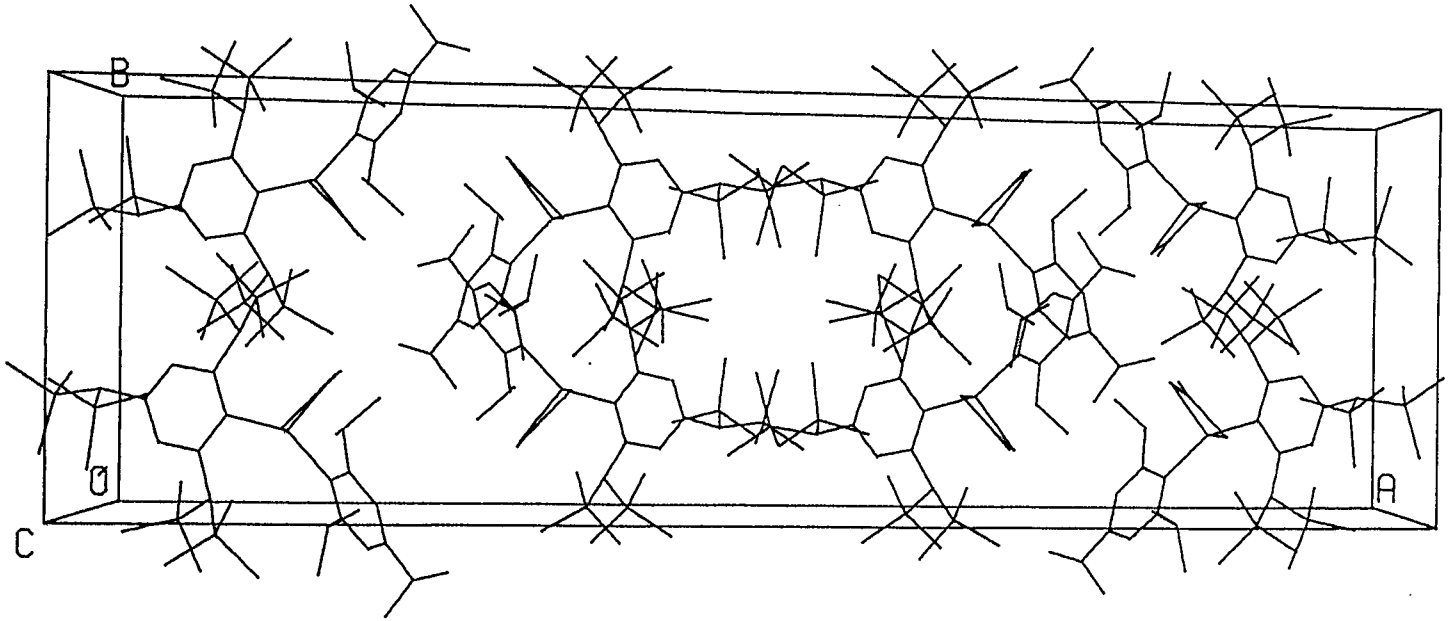
Diffractometer	Rigaku AFC5R
Radiation	MoKa (l = 0.71069 Å)
Temperature	24°C
Attenuators	Ni foil (factors: 3.7, 13.6, 49.6)
Take-off Angle	6.0°

Detector Aperture	6.0 mm horizontal 6.0 mm vertical
Crystal to Detector Distance	40 cm
Scan Type	w-2j
Scan Rate	16.0°/min (in omega) (1 rescans)
Scan Width	(1.10 + 0.30 tanj)°
$2j_{max}$	55.1°
No. of Reflections Measured	Total: 13654 Unique: 13488 (R_{int} = 0.028)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.76 - 1.17)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares
Function Minimized	$S\ w\ (\|Fo\| - \|Fc\|)^2$
Least-squares Weights	$4Fo^2/s^2(Fo^2)$
p-factor	0.03
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00s(I)) No. Variables Reflection/Parameter Ratio	6659 478 13.93
Residuals: R; R_w	0.046; 0.047
Goodness of Fit Indicator	1.56
Max Shift/Error in Final Cycle	0.13
Maximum Peak in Final Diff. Map Minimum Peak in Final Diff. Map	0.39 $e^-/Å^3$ -0.42 $e^-/Å^3$

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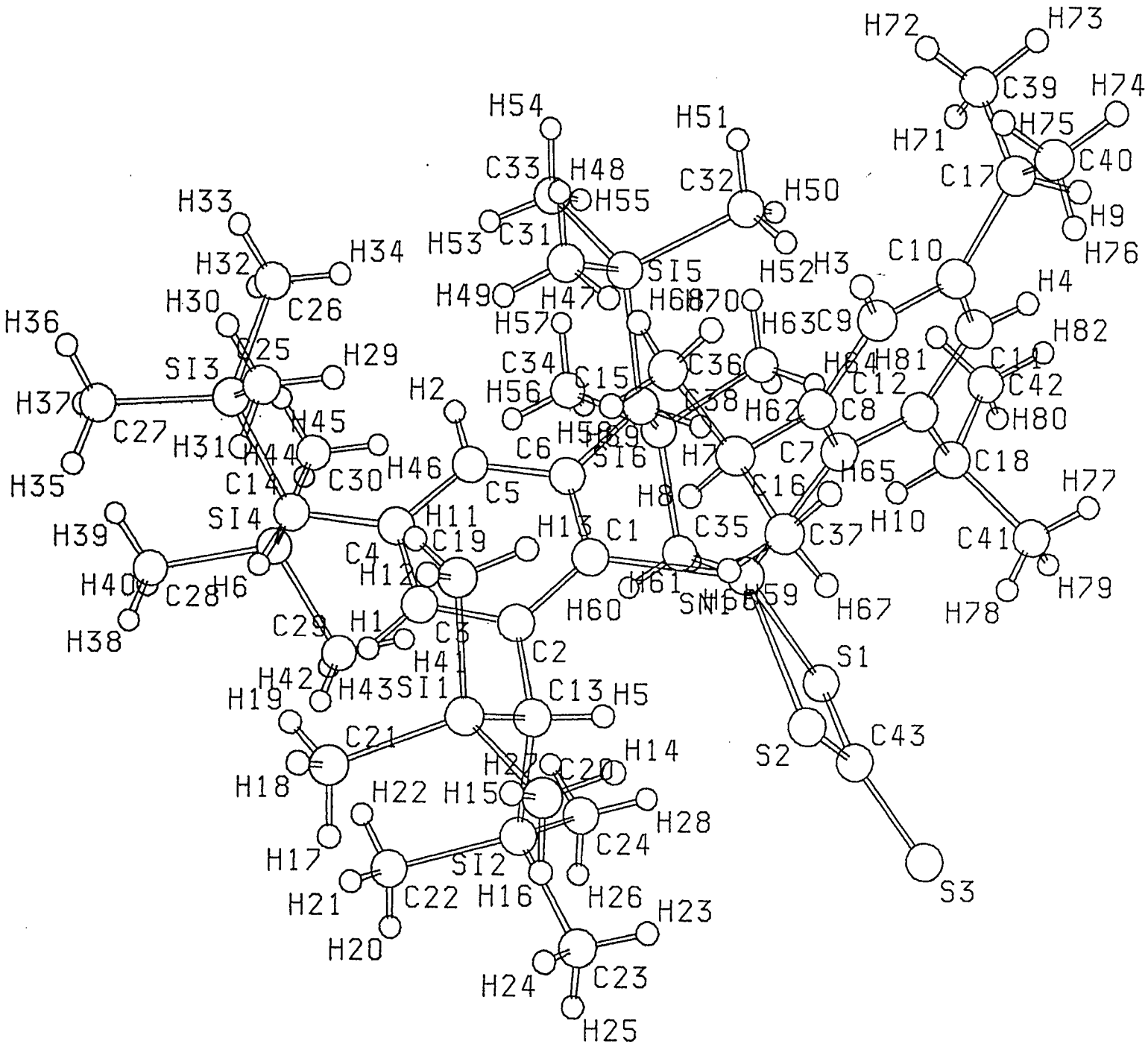
0
C
A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H55
H33
H53
C31
H34
H32
SI5
H52
H3
C10
H4
H30
C26
H49
H47
H68
H70
H57
H63
C9
H82
H36
C25
H29
SI3
C34
C15
C36
H64
H81
C11
H37
H2
H56
C38
H62
C8
C12
C42
C27
H45
H58
H69
H80
H31
H44
C6
SI6
H7
C7
H65
C18
H35
C14
C30
H46
C5
H8
C16
H77
SI4
H11
H13
C1
C35
C37
H10
C41
H39
C19
C4
H12
H61
H66
H59
H67
H79
H40
C28
H6
H60
SN1
H78
H38
C29
H1
C3
C2
S1
H4
H42
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H19
C21
C43
H14
S2
H18
H22
H15
C20
H28
C24
H17
SI2
H21
C22
H16
H26
H23
S3
H20
H24
C23
H25

Status of project

11-JUN-91 09:51:27

PROJECT DIRECTORY : [TEXSAN.TOKITOH.SNCS3]

TITLE : SNCS3 25-MAY-91

CELL : a= 46.252 b= 13.470 c= 18.645 alpha= 90.00 beta=105.48 gamma= 90.00

SPACEG : C2/c S.G.# 15 DENSITY : Dc= 2.332 Absorption coef.= 14.320

STORED formula		CURRENT formula		STATUS
SN	1.00	SN	0.50	-
S	3.00	S	1.50	-
SI	6.00	SI	3.00	-
C	43.00	C	21.50	-
H	82.00	H	41.00	-

parameters : # of reflections= 6659 # of variables= 478 shift/error= 0.127

R-factors : R= 0.046 Rw= 0.047 Goodness of fit= 1.559 LS cycles= 1

corrections : absorption=on -type=DIF decay=off redundant=on average=off

Positional parameters and B(eq) for Tb(Tip)SnCS3

atom	x	y	z	B(eq)
Sn(1)	0.339111(7)	0.29256(2)	0.07976(2)	3.37(1)
S(1)	0.34878(4)	0.2926(1)	0.21538(8)	6.62(8)
S(2)	0.30783(3)	0.1613(1)	0.1100(1)	5.86(7)
S(3)	0.30874(6)	0.1559(2)	0.2688(1)	12.3(2)
Si(1)	0.35716(4)	-0.0090(1)	-0.0364(1)	5.47(8)
Si(2)	0.39170(4)	-0.0022(1)	0.1396(1)	5.98(8)
Si(3)	0.46108(4)	0.2368(2)	-0.1078(1)	6.9(1)
Si(4)	0.49725(4)	0.2144(2)	0.0656(1)	8.1(1)
Si(5)	0.38309(4)	0.5225(1)	-0.0373(1)	6.6(1)
Si(6)	0.41664(4)	0.4987(2)	0.1396(1)	7.3(1)
C(1)	0.3798(1)	0.2569(3)	0.0491(2)	3.2(2)
C(2)	0.3888(1)	0.1597(4)	0.0406(2)	3.6(2)
C(3)	0.4155(1)	0.1442(3)	0.0207(3)	4.2(2)
C(4)	0.4339(1)	0.2212(4)	0.0111(3)	3.8(2)
C(5)	0.4248(1)	0.3166(4)	0.0212(3)	4.2(2)
C(6)	0.3980(1)	0.3383(3)	0.0401(2)	3.6(2)
C(7)	0.3071(1)	0.4009(3)	0.0210(3)	3.9(2)
C(8)	0.2921(1)	0.3791(4)	-0.0526(3)	4.4(2)
C(9)	0.2721(1)	0.4498(5)	-0.0929(3)	6.1(3)
C(10)	0.2663(1)	0.5384(5)	-0.0628(4)	6.7(3)
C(11)	0.2804(1)	0.5550(4)	0.0102(4)	6.7(3)
C(12)	0.3006(1)	0.4895(4)	0.0533(3)	4.7(2)
C(13)	0.3718(1)	0.0675(3)	0.0518(3)	4.2(2)
C(14)	0.4625(1)	0.1971(4)	-0.0109(3)	5.0(2)
C(15)	0.3908(1)	0.4455(4)	0.0518(3)	4.4(2)
C(16)	0.2955(1)	0.2816(4)	-0.0886(3)	5.1(3)
C(17)	0.2459(2)	0.6173(6)	-0.1106(6)	12.1(5)
C(18)	0.3133(1)	0.5139(4)	0.1351(3)	5.6(3)
C(19)	0.3487(2)	0.0749(5)	-0.1171(4)	9.0(4)
C(20)	0.3221(2)	-0.0714(7)	-0.0319(5)	11.6(5)
C(21)	0.3832(2)	-0.1031(6)	-0.0549(5)	10.4(5)
C(22)	0.4254(2)	-0.0738(5)	0.1325(4)	8.6(4)
C(23)	0.3643(2)	-0.0882(6)	0.1635(5)	11.2(5)
C(24)	0.4049(2)	0.0865(6)	0.2156(4)	10.2(5)
C(25)	0.4237(2)	0.2038(7)	-0.1685(4)	11.8(6)
C(26)	0.4661(2)	0.3737(7)	-0.1170(5)	12.6(6)
C(27)	0.4901(2)	0.1748(8)	-0.1424(6)	15.8(8)
C(28)	0.5289(2)	0.1452(8)	0.0470(6)	14.4(7)
C(29)	0.4908(2)	0.167(1)	0.1509(5)	22(1)
C(30)	0.5086(2)	0.3469(8)	0.0788(6)	16.7(8)
C(31)	0.3688(2)	0.4432(6)	-0.1180(4)	12.0(5)
C(32)	0.3538(2)	0.6171(6)	-0.0371(5)	12.2(6)
C(33)	0.4161(2)	0.5896(6)	-0.0508(5)	11.7(6)
C(34)	0.4545(2)	0.5262(9)	0.1359(5)	16.2(7)
C(35)	0.4180(3)	0.417(1)	0.2157(5)	21(1)
C(36)	0.4015(3)	0.6178(9)	0.1606(8)	22(1)
C(37)	0.2707(1)	0.2106(5)	-0.0843(4)	7.8(4)
C(38)	0.2966(2)	0.2901(6)	-0.1694(3)	9.6(4)
C(39)	0.2644(2)	0.7004(7)	-0.1263(6)	14.8(7)

Positional parameters and B(eq) for Tb(Tip)SnCS3

atom	x	y	z	B(eq)
C(40)	0.2217(2)	0.5973(8)	-0.1511(8)	20.2(9)
C(41)	0.2927(2)	0.4759(5)	0.1801(4)	7.6(4)
C(42)	0.3200(2)	0.6249(5)	0.1508(4)	8.4(4)
C(43)	0.3210(1)	0.2000(5)	0.2012(3)	6.9(3)
H(1)	0.4213	0.0780	0.0134	4.9
H(2)	0.4373	0.3703	0.0151	4.9
H(3)	0.2621	0.4358	-0.1436	7.2
H(4)	0.2760	0.6146	0.0325	8.0
H(5)	0.3542	0.0925	0.0623	5.0
H(6)	0.4614	0.1267	-0.0156	6.0
H(7)	0.3718	0.4423	0.0625	5.3
H(8)	0.3139	0.2532	-0.0612	6.1
H(9)	0.2391	0.6481	-0.0710	13.8
H(10)	0.3318	0.4792	0.1518	6.7
H(11)	0.3667	0.1043	-0.1217	10.8
H(12)	0.3396	0.0380	-0.1607	10.8
H(13)	0.3352	0.1250	-0.1100	10.8
H(14)	0.3086	-0.0243	-0.0225	14.0
H(15)	0.3137	-0.1046	-0.0775	14.0
H(16)	0.3268	-0.1193	0.0075	14.0
H(17)	0.3883	-0.1484	-0.0144	12.5
H(18)	0.3738	-0.1376	-0.0993	12.5
H(19)	0.4008	-0.0712	-0.0600	12.5
H(20)	0.4338	-0.1068	0.1782	10.3
H(21)	0.4195	-0.1211	0.0936	10.3
H(22)	0.4396	-0.0295	0.1221	10.3
H(23)	0.3477	-0.0512	0.1704	13.4
H(24)	0.3575	-0.1347	0.1246	13.4
H(25)	0.3737	-0.1223	0.2084	13.4
H(26)	0.4134	0.0510	0.2602	12.2
H(27)	0.4195	0.1283	0.2043	12.2
H(28)	0.3884	0.1247	0.2210	12.2
H(29)	0.4089	0.2396	-0.1525	14.1
H(30)	0.4230	0.2211	-0.2181	14.1
H(31)	0.4207	0.1348	-0.1648	14.1
H(32)	0.4851	0.3921	-0.0870	15.0
H(33)	0.4649	0.3878	-0.1680	15.0
H(34)	0.4508	0.4072	-0.1026	15.0
H(35)	0.4879	0.1042	-0.1385	18.9
H(36)	0.4871	0.1909	-0.1937	18.9
H(37)	0.5091	0.1945	-0.1147	18.9
H(38)	0.5240	0.0766	0.0437	17.3
H(39)	0.5325	0.1683	0.0032	17.3
H(40)	0.5462	0.1553	0.0882	17.3
H(41)	0.4754	0.2070	0.1619	25.8
H(42)	0.4851	0.1015	0.1445	25.8
H(43)	0.5088	0.1757	0.1894	25.8
H(44)	0.5263	0.3494	0.1206	20.2
H(45)	0.5123	0.3710	0.0368	20.2
H(46)	0.4929	0.3817	0.0927	20.2

Positional parameters and B(eq) for Tb(Tip)SnCS3

atom	x	y	z	B(eq)
H(47)	0.3506	0.4135	-0.1137	14.2
H(48)	0.3648	0.4829	-0.1614	14.2
H(49)	0.3830	0.3942	-0.1191	14.2
H(50)	0.3605	0.6594	0.0042	14.4
H(51)	0.3500	0.6544	-0.0820	14.4
H(52)	0.3359	0.5842	-0.0346	14.4
H(53)	0.4308	0.5432	-0.0555	14.0
H(54)	0.4101	0.6289	-0.0945	14.0
H(55)	0.4239	0.6313	-0.0090	14.0
H(56)	0.4636	0.4687	0.1239	19.4
H(57)	0.4536	0.5758	0.0981	19.4
H(58)	0.4655	0.5522	0.1823	19.4
H(59)	0.3981	0.4100	0.2210	25.6
H(60)	0.4255	0.3556	0.2065	25.6
H(61)	0.4303	0.4461	0.2598	25.6
H(62)	0.4135	0.6408	0.2079	26.9
H(63)	0.4015	0.6637	0.1237	26.9
H(64)	0.3815	0.6071	0.1651	26.9
H(65)	0.2522	0.2349	-0.1141	9.3
H(66)	0.2747	0.1474	-0.1019	9.3
H(67)	0.2700	0.2052	-0.0341	9.3
H(68)	0.3120	0.3349	-0.1724	11.5
H(69)	0.3007	0.2264	-0.1865	11.5
H(70)	0.2779	0.3133	-0.1989	11.5
H(71)	0.2823	0.7049	-0.0871	17.9
H(72)	0.2685	0.6895	-0.1718	17.9
H(73)	0.2532	0.7611	-0.1277	17.9
H(74)	0.2088	0.6535	-0.1543	24.1
H(75)	0.2241	0.5821	-0.1984	24.1
H(76)	0.2135	0.5427	-0.1314	24.1
H(77)	0.2737	0.5072	0.1631	9.1
H(78)	0.2906	0.4064	0.1742	9.1
H(79)	0.3012	0.4916	0.2311	9.1
H(80)	0.3296	0.6334	0.2023	10.0
H(81)	0.3329	0.6474	0.1223	10.0
H(82)	0.3018	0.6608	0.1379	10.0

Positional parameters for Tb(Tip)SnCS3

atom	x	y	z
Sn(1)	0.339111(7)	0.29256(2)	0.07976(2)
S(1)	0.34878(4)	0.2926(1)	0.21538(8)
S(2)	0.30783(3)	0.1613(1)	0.1100(1)
S(3)	0.30874(6)	0.1559(2)	0.2688(1)
Si(1)	0.35716(4)	-0.0090(1)	-0.0364(1)
Si(2)	0.39170(4)	-0.0022(1)	0.1396(1)
Si(3)	0.46108(4)	0.2368(2)	-0.1078(1)
Si(4)	0.49725(4)	0.2144(2)	0.0656(1)
Si(5)	0.38309(4)	0.5225(1)	-0.0373(1)
Si(6)	0.41664(4)	0.4987(2)	0.1396(1)
C(1)	0.3798(1)	0.2569(3)	0.0491(2)
C(2)	0.3888(1)	0.1597(4)	0.0406(2)
C(3)	0.4155(1)	0.1442(3)	0.0207(3)
C(4)	0.4339(1)	0.2212(4)	0.0111(3)
C(5)	0.4248(1)	0.3166(4)	0.0212(3)
C(6)	0.3980(1)	0.3383(3)	0.0401(2)
C(7)	0.3071(1)	0.4009(3)	0.0210(3)
C(8)	0.2921(1)	0.3791(4)	-0.0526(3)
C(9)	0.2721(1)	0.4498(5)	-0.0929(3)
C(10)	0.2663(1)	0.5384(5)	-0.0628(4)
C(11)	0.2804(1)	0.5550(4)	0.0102(4)
C(12)	0.3006(1)	0.4895(4)	0.0533(3)
C(13)	0.3718(1)	0.0675(3)	0.0518(3)
C(14)	0.4625(1)	0.1971(4)	-0.0109(3)
C(15)	0.3908(1)	0.4455(4)	0.0518(3)
C(16)	0.2955(1)	0.2816(4)	-0.0886(3)
C(17)	0.2459(2)	0.6173(6)	-0.1106(6)
C(18)	0.3133(1)	0.5139(4)	0.1351(3)
C(19)	0.3487(2)	0.0749(5)	-0.1171(4)
C(20)	0.3221(2)	-0.0714(7)	-0.0319(5)
C(21)	0.3832(2)	-0.1031(6)	-0.0549(5)
C(22)	0.4254(2)	-0.0738(5)	0.1325(4)
C(23)	0.3643(2)	-0.0882(6)	0.1635(5)
C(24)	0.4049(2)	0.0865(6)	0.2156(4)
C(25)	0.4237(2)	0.2038(7)	-0.1685(4)
C(26)	0.4661(2)	0.3737(7)	-0.1170(5)
C(27)	0.4901(2)	0.1748(8)	-0.1424(6)
C(28)	0.5289(2)	0.1452(8)	0.0470(6)
C(29)	0.4908(2)	0.167(1)	0.1509(5)
C(30)	0.5086(2)	0.3469(8)	0.0788(6)
C(31)	0.3688(2)	0.4432(6)	-0.1180(4)
C(32)	0.3538(2)	0.6171(6)	-0.0371(5)
C(33)	0.4161(2)	0.5896(6)	-0.0508(5)
C(34)	0.4545(2)	0.5262(9)	0.1359(5)
C(35)	0.4180(3)	0.417(1)	0.2157(5)
C(36)	0.4015(3)	0.6178(9)	0.1606(8)
C(37)	0.2707(1)	0.2106(5)	-0.0843(4)
C(38)	0.2966(2)	0.2901(6)	-0.1694(3)
C(39)	0.2644(2)	0.7004(7)	-0.1263(6)

Positional parameters for Tb(Tip)SnCS3

atom	x	y	z
C(40)	0.2217(2)	0.5973(8)	-0.1511(8)
C(41)	0.2927(2)	0.4759(5)	0.1801(4)
C(42)	0.3200(2)	0.6249(5)	0.1508(4)
C(43)	0.3210(1)	0.2000(5)	0.2012(3)
H(1)	0.4213	0.0780	0.0134
H(2)	0.4373	0.3703	0.0151
H(3)	0.2621	0.4358	-0.1436
H(4)	0.2760	0.6146	0.0325
H(5)	0.3542	0.0925	0.0623
H(6)	0.4614	0.1267	-0.0156
H(7)	0.3718	0.4423	0.0625
H(8)	0.3139	0.2532	-0.0612
H(9)	0.2391	0.6481	-0.0710
H(10)	0.3318	0.4792	0.1518
H(11)	0.3667	0.1043	-0.1217
H(12)	0.3396	0.0380	-0.1607
H(13)	0.3352	0.1250	-0.1100
H(14)	0.3086	-0.0243	-0.0225
H(15)	0.3137	-0.1046	-0.0775
H(16)	0.3268	-0.1193	0.0075
H(17)	0.3883	-0.1484	-0.0144
H(18)	0.3738	-0.1376	-0.0993
H(19)	0.4008	-0.0712	-0.0600
H(20)	0.4338	-0.1068	0.1782
H(21)	0.4195	-0.1211	0.0936
H(22)	0.4396	-0.0295	0.1221
H(23)	0.3477	-0.0512	0.1704
H(24)	0.3575	-0.1347	0.1246
H(25)	0.3737	-0.1223	0.2084
H(26)	0.4134	0.0510	0.2602
H(27)	0.4195	0.1283	0.2043
H(28)	0.3884	0.1247	0.2210
H(29)	0.4089	0.2396	-0.1525
H(30)	0.4230	0.2211	-0.2181
H(31)	0.4207	0.1348	-0.1648
H(32)	0.4851	0.3921	-0.0870
H(33)	0.4649	0.3878	-0.1680
H(34)	0.4508	0.4072	-0.1026
H(35)	0.4879	0.1042	-0.1385
H(36)	0.4871	0.1909	-0.1937
H(37)	0.5091	0.1945	-0.1147
H(38)	0.5240	0.0766	0.0437
H(39)	0.5325	0.1683	0.0032
H(40)	0.5462	0.1553	0.0882
H(41)	0.4754	0.2070	0.1619
H(42)	0.4851	0.1015	0.1445
H(43)	0.5088	0.1757	0.1894
H(44)	0.5263	0.3494	0.1206
H(45)	0.5123	0.3710	0.0368
H(46)	0.4929	0.3817	0.0927

Positional parameters for Tb(Tip)SnCS3

atom	x	y	z
H(47)	0.3506	0.4135	-0.1137
H(48)	0.3648	0.4829	-0.1614
H(49)	0.3830	0.3942	-0.1191
H(50)	0.3605	0.6594	0.0042
H(51)	0.3500	0.6544	-0.0820
H(52)	0.3359	0.5842	-0.0346
H(53)	0.4308	0.5432	-0.0555
H(54)	0.4101	0.6289	-0.0945
H(55)	0.4239	0.6313	-0.0090
H(56)	0.4636	0.4687	0.1239
H(57)	0.4536	0.5758	0.0981
H(58)	0.4655	0.5522	0.1823
H(59)	0.3981	0.4100	0.2210
H(60)	0.4255	0.3556	0.2065
H(61)	0.4303	0.4461	0.2598
H(62)	0.4135	0.6408	0.2079
H(63)	0.4015	0.6637	0.1237
H(64)	0.3815	0.6071	0.1651
H(65)	0.2522	0.2349	-0.1141
H(66)	0.2747	0.1474	-0.1019
H(67)	0.2700	0.2052	-0.0341
H(68)	0.3120	0.3349	-0.1724
H(69)	0.3007	0.2264	-0.1865
H(70)	0.2779	0.3133	-0.1989
H(71)	0.2823	0.7049	-0.0871
H(72)	0.2685	0.6895	-0.1718
H(73)	0.2532	0.7611	-0.1277
H(74)	0.2088	0.6535	-0.1543
H(75)	0.2241	0.5821	-0.1984
H(76)	0.2135	0.5427	-0.1314
H(77)	0.2737	0.5072	0.1631
H(78)	0.2906	0.4064	0.1742
H(79)	0.3012	0.4916	0.2311
H(80)	0.3296	0.6334	0.2023
H(81)	0.3329	0.6474	0.1223
H(82)	0.3018	0.6608	0.1379

U values for Tb(Tip)SnCS3

ATOM	U11	U22	U33	U12	U13	U23
Sn(1)	0.0424(2)	0.0424(2)	0.0428(2)	0.0008(2)	0.0103(1)	0.0006(2)
S(1)	0.091(1)	0.111(1)	0.0471(8)	0.029(1)	0.0131(8)	0.005(1)
S(2)	0.068(1)	0.0585(9)	0.109(1)	0.0037(8)	0.046(1)	0.0198(9)
S(3)	0.186(2)	0.184(2)	0.135(2)	0.055(2)	0.109(2)	0.086(2)
Si(1)	0.074(1)	0.049(1)	0.092(1)	-0.0068(8)	0.035(1)	-0.0147(9)
Si(2)	0.082(1)	0.065(1)	0.088(1)	0.024(1)	0.037(1)	0.028(1)
Si(3)	0.089(1)	0.103(2)	0.085(1)	0.004(1)	0.050(1)	0.005(1)
Si(4)	0.046(1)	0.151(2)	0.104(1)	0.001(1)	0.010(1)	-0.010(2)
Si(5)	0.086(1)	0.055(1)	0.119(2)	-0.004(1)	0.043(1)	0.016(1)
Si(6)	0.079(1)	0.090(1)	0.108(2)	-0.033(1)	0.026(1)	-0.050(1)
C(1)	0.032(3)	0.042(3)	0.045(3)	0.002(2)	0.010(2)	-0.004(2)
C(2)	0.046(3)	0.045(3)	0.043(3)	0.002(2)	0.010(2)	0.006(2)
C(3)	0.053(3)	0.043(3)	0.065(3)	0.006(2)	0.021(3)	-0.001(3)
C(4)	0.042(3)	0.056(3)	0.048(3)	-0.001(3)	0.012(2)	-0.002(3)
C(5)	0.049(3)	0.056(4)	0.054(3)	-0.018(2)	0.015(2)	-0.003(2)
C(6)	0.041(3)	0.047(3)	0.047(3)	-0.007(2)	0.006(2)	-0.005(2)
C(7)	0.043(3)	0.046(3)	0.055(3)	0.004(2)	0.009(2)	0.006(2)
C(8)	0.052(3)	0.059(3)	0.054(3)	0.002(3)	0.011(3)	0.006(3)
C(9)	0.060(4)	0.089(5)	0.068(4)	0.001(4)	-0.005(3)	0.018(4)
C(10)	0.074(5)	0.061(4)	0.108(6)	0.008(4)	0.001(4)	0.022(4)
C(11)	0.076(5)	0.049(4)	0.121(6)	0.014(3)	0.012(4)	0.003(4)
C(12)	0.058(3)	0.048(3)	0.071(4)	0.008(3)	0.011(3)	0.002(3)
C(13)	0.050(3)	0.041(3)	0.073(4)	0.005(2)	0.023(3)	0.003(3)
C(14)	0.048(3)	0.072(4)	0.074(4)	-0.003(3)	0.022(3)	-0.000(3)
C(15)	0.052(3)	0.046(3)	0.072(4)	-0.013(3)	0.020(3)	-0.014(3)
C(16)	0.058(3)	0.079(4)	0.051(3)	-0.002(3)	0.003(3)	-0.010(3)
C(17)	0.097(7)	0.102(6)	0.21(1)	0.003(5)	-0.048(6)	0.086(7)
C(18)	0.075(4)	0.052(3)	0.087(4)	0.008(3)	0.022(4)	-0.010(3)
C(19)	0.152(7)	0.094(5)	0.080(5)	-0.008(5)	0.002(5)	-0.016(4)
C(20)	0.145(8)	0.167(8)	0.155(8)	-0.100(7)	0.083(6)	-0.081(6)
C(21)	0.134(7)	0.107(6)	0.155(7)	0.033(5)	0.037(6)	-0.055(5)
C(22)	0.101(6)	0.110(6)	0.120(6)	0.050(5)	0.038(5)	0.036(5)
C(23)	0.118(6)	0.136(7)	0.187(8)	0.026(5)	0.065(6)	0.111(6)
C(24)	0.168(8)	0.127(7)	0.079(5)	0.048(6)	0.007(5)	0.020(5)
C(25)	0.160(8)	0.21(1)	0.074(5)	-0.050(7)	0.021(5)	-0.011(6)

U values for Tb(Tip)SnCS3

ATOM	U11	U22	U33	U12	U13	U23
C(26)	0.21(1)	0.140(8)	0.155(8)	-0.034(7)	0.086(8)	0.046(7)
C(27)	0.22(1)	0.26(1)	0.17(1)	0.11(1)	0.149(9)	0.047(9)
C(28)	0.058(5)	0.25(1)	0.22(1)	0.043(7)	0.009(6)	-0.03(1)
C(29)	0.106(8)	0.60(3)	0.093(7)	-0.01(1)	-0.018(6)	0.09(1)
C(30)	0.111(8)	0.22(1)	0.27(1)	-0.029(8)	-0.010(8)	-0.13(1)
C(31)	0.21(1)	0.125(7)	0.094(6)	-0.030(7)	-0.010(6)	0.028(5)
C(32)	0.165(8)	0.105(6)	0.22(1)	0.061(6)	0.108(8)	0.093(7)
C(33)	0.140(8)	0.127(7)	0.21(1)	-0.025(6)	0.099(7)	0.044(7)
C(34)	0.079(6)	0.33(1)	0.21(1)	-0.101(8)	0.048(6)	-0.15(1)
C(35)	0.39(2)	0.27(1)	0.076(6)	-0.21(1)	-0.046(8)	-0.006(8)
C(36)	0.18(1)	0.23(1)	0.37(2)	0.05(1)	-0.03(1)	-0.24(1)
C(37)	0.087(5)	0.076(4)	0.124(6)	-0.005(4)	0.011(4)	-0.024(5)
C(38)	0.138(7)	0.164(8)	0.054(4)	0.012(6)	0.011(4)	-0.028(5)
C(39)	0.102(7)	0.138(8)	0.29(1)	-0.000(6)	-0.004(7)	0.144(9)
C(40)	0.100(8)	0.17(1)	0.43(2)	-0.009(7)	-0.05(1)	0.19(1)
C(41)	0.105(5)	0.102(5)	0.092(5)	0.008(4)	0.044(4)	-0.013(4)
C(42)	0.125(6)	0.066(4)	0.132(6)	-0.002(4)	0.039(5)	-0.038(4)
C(43)	0.084(4)	0.098(5)	0.090(4)	0.045(4)	0.044(4)	0.048(4)
H(1)	0.0626					
H(2)	0.0625					
H(3)	0.0915					
H(4)	0.1016					
H(5)	0.0632					
H(6)	0.0758					
H(7)	0.0669					
H(8)	0.0777					
H(9)	0.1754					
H(10)	0.0846					
H(11)	0.1363					
H(12)	0.1363					
H(13)	0.1363					
H(14)	0.1778					
H(15)	0.1778					
H(16)	0.1778					
H(17)	0.1583					
H(18)	0.1583					

U values for Tb(Tip)SnCS3

ATOM	U11	U22	U33	U12	U13	U23
H(19)	0.1583					
H(20)	0.1303					
H(21)	0.1303					
H(22)	0.1303					
H(23)	0.1697					
H(24)	0.1697					
H(25)	0.1697					
H(26)	0.1544					
H(27)	0.1544					
H(28)	0.1544					
H(29)	0.1782					
H(30)	0.1782					
H(31)	0.1782					
H(32)	0.1899					
H(33)	0.1899					
H(34)	0.1899					
H(35)	0.2395					
H(36)	0.2395					
H(37)	0.2395					
H(38)	0.2187					
H(39)	0.2187					
H(40)	0.2187					
H(41)	0.3267					
H(42)	0.3267					
H(43)	0.3267					
H(44)	0.2554					
H(45)	0.2554					
H(46)	0.2554					
H(47)	0.1801					
H(48)	0.1801					
H(49)	0.1801					
H(50)	0.1828					
H(51)	0.1828					
H(52)	0.1828					
H(53)	0.1771					
H(54)	0.1771					

U values for Tb(Tip)SnCS3

ATOM	U11	U22	U33	U12	U13	U23
H(55)	0.1771					
H(56)	0.2455					
H(57)	0.2455					
H(58)	0.2455					
H(59)	0.3238					
H(60)	0.3238					
H(61)	0.3238					
H(62)	0.3409					
H(63)	0.3409					
H(64)	0.3409					
H(65)	0.1178					
H(66)	0.1178					
H(67)	0.1178					
H(68)	0.1454					
H(69)	0.1454					
H(70)	0.1454					
H(71)	0.2266					
H(72)	0.2266					
H(73)	0.2266					
H(74)	0.3055					
H(75)	0.3055					
H(76)	0.3055					
H(77)	0.1152					
H(78)	0.1152					
H(79)	0.1152					
H(80)	0.1264					
H(81)	0.1264					
H(82)	0.1264					

Intramolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance
SN1	S1	2.448(2)
SN1	S2	2.444(2)
SN1	C1	2.160(4)
SN1	C7	2.159(5)
S1	C43	1.758(7)
S2	C43	1.727(7)
S3	C43	1.626(6)
SI1	C13	1.906(5)
SI1	C19	1.838(7)
SI1	C20	1.848(7)
SI1	C21	1.843(7)
SI2	C13	1.898(5)
SI2	C22	1.866(6)
SI2	C23	1.858(7)
SI2	C24	1.829(8)
SI3	C14	1.868(5)
SI3	C25	1.850(9)
SI3	C26	1.873(9)
SI3	C27	1.837(8)
SI4	C14	1.857(6)
SI4	C28	1.845(8)
SI4	C29	1.81(1)
SI4	C30	1.86(1)
SI5	C15	1.910(5)
SI5	C31	1.818(8)
SI5	C32	1.862(8)
SI5	C33	1.849(7)
SI6	C15	1.891(5)
SI6	C34	1.810(8)
SI6	C35	1.79(1)
SI6	C36	1.835(9)
C1	C2	1.396(6)
C1	C6	1.420(6)
C2	C3	1.398(6)
C2	C13	1.512(6)
C3	C4	1.384(6)
C4	C5	1.382(6)
C4	C14	1.522(6)
C5	C6	1.406(6)
C6	C15	1.511(6)
C7	C8	1.394(6)
C7	C12	1.404(7)
C8	C9	1.400(7)
C8	C16	1.502(7)
C9	C10	1.376(8)
C10	C11	1.361(8)
C10	C17	1.539(9)
C11	C12	1.378(7)
C12	C18	1.518(7)
C16	C37	1.510(8)
C16	C38	1.524(8)
C17	C39	1.49(1)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances Involving the Nonhydrogen Atoms (cont

atom	atom	distance	atom	atom	distance
C17	C40	1.20(1)			
C18	C41	1.517(8)			
C18	C42	1.539(8)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances Involving the Hydrogen Atoms

atom	atom	distance	atom	atom	distance
C3	H1	0.951	C24	H27	0.945
C5	H2	0.952	C24	H28	0.949
C9	H3	0.953	C25	H29	0.946
C11	H4	0.950	C25	H30	0.946
C13	H5	0.951	C25	H31	0.945
C14	H6	0.953	C26	H32	0.939
C15	H7	0.953	C26	H33	0.957
C16	H8	0.949	C26	H34	0.940
C17	H9	0.968	C27	H35	0.961
C18	H10	0.952	C27	H36	0.954
C19	H11	0.944	C27	H37	0.933
C19	H12	0.950	C28	H38	0.949
C19	H13	0.952	C28	H39	0.930
C20	H14	0.939	C28	H40	0.958
C20	H15	0.947	C29	H41	0.963
C20	H16	0.958	C29	H42	0.916
C21	H17	0.950	C29	H43	0.950
C21	H18	0.948	C30	H44	0.967
C21	H19	0.947	C30	H45	0.906
C22	H20	0.947	C30	H46	0.955
C22	H21	0.949	C31	H47	0.958
C22	H22	0.948	C31	H48	0.947
C23	H23	0.951	C31	H49	0.933
C23	H24	0.946	C32	H50	0.942
C23	H25	0.953	C32	H51	0.951
C24	H26	0.949	C32	H52	0.950

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances Involving the Hydrogen Atoms (cont)

atom	atom	distance
C33	H53	0.945
C33	H54	0.948
C33	H55	0.950
C34	H56	0.936
C34	H57	0.963
C34	H58	0.946
C35	H59	0.959
C35	H60	0.928
C35	H61	0.951
C36	H62	0.961
C36	H63	0.925
C36	H64	0.960
C37	H65	0.949
C37	H66	0.949
C37	H67	0.949
C38	H68	0.947
C38	H69	0.952
C38	H70	0.947
C39	H71	0.947
C39	H72	0.927
C39	H73	0.964
C40	H74	0.954
C40	H75	0.941
C40	H76	0.943
C41	H77	0.948
C41	H78	0.945
C41	H79	0.951
C42	H80	0.951
C42	H81	0.948
C42	H82	0.944

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
S1	SN1	S2	73.61(7)	C14	SI4	C28	111.0(3)
S1	SN1	C1	110.0(1)	C14	SI4	C29	108.7(4)
S1	SN1	C7	115.8(1)	C14	SI4	C30	112.2(4)
S2	SN1	C1	120.7(1)	C28	SI4	C29	108.1(6)
S2	SN1	C7	103.7(1)	C28	SI4	C30	107.4(5)
C1	SN1	C7	123.0(2)	C29	SI4	C30	109.4(7)
SN1	S1	C43	85.4(2)	C15	SI5	C31	110.0(3)
SN1	S2	C43	86.2(2)	C15	SI5	C32	109.7(3)
C13	SI1	C19	108.8(3)	C15	SI5	C33	114.5(3)
C13	SI1	C20	108.7(3)	C31	SI5	C32	107.5(5)
C13	SI1	C21	115.7(3)	C31	SI5	C33	107.8(4)
C19	SI1	C20	108.6(4)	C32	SI5	C33	107.1(4)
C19	SI1	C21	106.1(4)	C15	SI6	C34	116.1(3)
C20	SI1	C21	108.7(4)	C15	SI6	C35	109.5(3)
C13	SI2	C22	114.6(3)	C15	SI6	C36	109.1(4)
C13	SI2	C23	108.1(3)	C34	SI6	C35	109.1(6)
C13	SI2	C24	109.3(3)	C34	SI6	C36	104.9(5)
C22	SI2	C23	109.3(3)	C35	SI6	C36	107.8(7)
C22	SI2	C24	106.3(4)	SN1	C1	C2	123.1(3)
C23	SI2	C24	109.2(4)	SN1	C1	C6	116.5(3)
C14	SI3	C25	108.0(3)	C2	C1	C6	120.4(4)
C14	SI3	C26	113.3(3)	C1	C2	C3	118.8(4)
C14	SI3	C27	111.6(4)	C1	C2	C13	125.0(4)
C25	SI3	C26	107.5(5)	C3	C2	C13	116.2(4)
C25	SI3	C27	109.1(5)	C2	C3	C4	122.8(4)
C26	SI3	C27	107.2(5)	C3	C4	C5	117.3(4)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
C3	C4	C14	119.0(5)	SI5	C15	SI6	118.4(3)
C5	C4	C14	123.7(4)	SI5	C15	C6	113.0(3)
C4	C5	C6	123.3(4)	SI6	C15	C6	112.0(4)
C1	C6	C5	117.4(4)	C8	C16	C37	111.0(5)
C1	C6	C15	124.0(4)	C8	C16	C38	114.3(5)
C5	C6	C15	118.5(4)	C37	C16	C38	109.0(5)
SN1	C7	C8	116.8(4)	C10	C17	C39	109.6(7)
SN1	C7	C12	123.5(4)	C10	C17	C40	122.3(9)
C8	C7	C12	119.7(5)	C39	C17	C40	122.4(9)
C7	C8	C9	117.9(5)	C12	C18	C41	110.6(5)
C7	C8	C16	122.8(5)	C12	C18	C42	113.9(5)
C9	C8	C16	119.2(5)	C41	C18	C42	110.3(5)
C8	C9	C10	123.0(6)	S1	C43	S2	114.4(3)
C9	C10	C11	117.2(6)	S1	C43	S3	122.3(4)
C9	C10	C17	121.3(7)	S2	C43	S3	123.3(5)
C11	C10	C17	121.5(7)				
C10	C11	C12	123.2(6)				
C7	C12	C11	118.9(5)				
C7	C12	C18	123.1(5)				
C11	C12	C18	117.9(5)				
SI1	C13	SI2	117.1(3)				
SI1	C13	C2	113.7(3)				
SI2	C13	C2	112.1(3)				
SI3	C14	SI4	120.6(3)				
SI3	C14	C4	113.0(4)				
SI4	C14	C4	113.7(4)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Hydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
C2	C3	H1	118.70	SI1	C19	H11	109.45
C4	C3	H1	118.50	SI1	C19	H12	109.11
C4	C5	H2	118.16	SI1	C19	H13	109.02
C6	C5	H2	118.54	H11	C19	H12	110.02
C8	C9	H3	118.24	H11	C19	H13	109.88
C10	C9	H3	118.80	H12	C19	H13	109.33
C10	C11	H4	118.26	SI1	C20	H14	109.56
C12	C11	H4	118.58	SI1	C20	H15	109.12
SI1	C13	H5	104.03	SI1	C20	H16	108.52
SI2	C13	H5	104.03	H14	C20	H15	110.76
C2	C13	H5	104.05	H14	C20	H16	109.76
SI3	C14	H6	102.05	H15	C20	H16	109.08
SI4	C14	H6	102.16	SI1	C21	H17	109.12
C4	C14	H6	101.90	SI1	C21	H18	109.25
SI5	C15	H7	103.72	SI1	C21	H19	109.26
SI6	C15	H7	104.01	H17	C21	H18	109.64
C6	C15	H7	103.80	H17	C21	H19	109.66
C8	C16	H8	107.33	H18	C21	H19	109.90
C37	C16	H8	107.37	SI2	C22	H20	109.23
C38	C16	H8	107.45	SI2	C22	H21	109.10
C10	C17	H9	97.34	SI2	C22	H22	109.15
C39	C17	H9	98.63	H20	C22	H21	109.80
C40	C17	H9	97.97	H20	C22	H22	109.86
C12	C18	H10	107.11	H21	C22	H22	109.69
C41	C18	H10	107.22	SI2	C23	H23	109.37
C42	C18	H10	107.35	SI2	C23	H24	109.63

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Hydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
SI2	C23	H25	109.28	H35	C27	H37	109.98
H23	C23	H24	109.76	H36	C27	H37	110.59
H23	C23	H25	109.17	SI4	C28	H38	108.56
H24	C23	H25	109.61	SI4	C28	H39	109.56
SI2	C24	H26	108.94	SI4	C28	H40	108.10
SI2	C24	H27	109.13	H38	C28	H39	111.24
SI2	C24	H28	108.95	H38	C28	H40	108.85
H26	C24	H27	110.03	H39	C28	H40	110.45
H26	C24	H28	109.72	SI4	C29	H41	107.01
H27	C24	H28	110.04	SI4	C29	H42	109.55
SI3	C25	H29	108.69	SI4	C29	H43	107.71
SI3	C25	H30	108.66	H41	C29	H42	111.35
SI3	C25	H31	108.75	H41	C29	H43	108.44
H29	C25	H30	110.15	H42	C29	H43	112.57
H29	C25	H31	110.31	SI4	C30	H44	106.78
H30	C25	H31	110.24	SI4	C30	H45	109.97
SI3	C26	H32	109.01	SI4	C30	H46	107.35
SI3	C26	H33	108.05	H44	C30	H45	111.86
SI3	C26	H34	108.94	H44	C30	H46	107.67
H32	C26	H33	109.77	H45	C30	H46	112.93
H32	C26	H34	111.27	SI5	C31	H47	108.08
H33	C26	H34	109.73	SI5	C31	H48	108.68
SI3	C27	H35	108.70	SI5	C31	H49	109.40
SI3	C27	H36	109.07	H47	C31	H48	109.11
SI3	C27	H37	110.26	H47	C31	H49	110.25
H35	C27	H36	108.20	H48	C31	H49	111.25

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Hydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
SI5	C32	H50	109.41	SI6	C36	H64	108.60
SI5	C32	H51	108.89	H62	C36	H63	110.66
SI5	C32	H52	108.93	H62	C36	H64	107.71
H50	C32	H51	110.09	H63	C36	H64	110.77
H50	C32	H52	110.15	C16	C37	H65	109.30
H51	C32	H52	109.34	C16	C37	H66	109.22
SI5	C33	H53	109.25	C16	C37	H67	109.22
SI5	C33	H54	109.05	H65	C37	H66	109.72
SI5	C33	H55	108.96	H65	C37	H67	109.69
H53	C33	H54	110.08	H66	C37	H67	109.67
H53	C33	H55	109.91	C16	C38	H68	109.34
H54	C33	H55	109.57	C16	C38	H69	109.07
SI6	C34	H56	109.85	C16	C38	H70	109.40
SI6	C34	H57	108.37	H68	C38	H69	109.53
SI6	C34	H58	109.34	H68	C38	H70	109.93
H56	C34	H57	109.50	H69	C38	H70	109.55
H56	C34	H58	111.03	C17	C39	H71	109.00
H57	C34	H58	108.70	C17	C39	H72	109.25
SI6	C35	H59	108.07	C17	C39	H73	108.01
SI6	C35	H60	109.76	H71	C39	H72	111.78
SI6	C35	H61	108.48	H71	C39	H73	108.49
H59	C35	H60	110.59	H72	C39	H73	110.24
H59	C35	H61	108.59	C17	C40	H74	108.67
H60	C35	H61	111.27	C17	C40	H75	108.23
SI6	C36	H62	108.53	C17	C40	H76	109.36
SI6	C36	H63	110.48	H74	C40	H75	109.89

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Hydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
H74	C40	H76	109.77				
H75	C40	H76	110.87				
C18	C41	H77	109.05				
C18	C41	H78	109.37				
C18	C41	H79	109.00				
H77	C41	H78	110.03				
H77	C41	H79	109.55				
H78	C41	H79	109.82				
C18	C42	H80	108.92				
C18	C42	H81	109.10				
C18	C42	H82	109.20				
H80	C42	H81	109.57				
H80	C42	H82	109.90				
H81	C42	H82	110.13				

Intermolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
C29	C29	3.56(2)	65502				

Contacts out to 3.60 angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Torsion or Conformation Angles

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
SN1	S1	C43	S2	5.4(3)	SI1	C13	C2	C3	-64.6(5)
SN1	S1	C43	S3	-174.1(4)	SI2	C13	SI1	C19	-164.3(3)
SN1	S2	C43	S1	-5.4(3)	SI2	C13	SI1	C20	77.6(4)
SN1	S2	C43	S3	174.1(4)	SI2	C13	SI1	C21	-45.1(4)
SN1	C1	C2	C3	-179.9(3)	SI2	C13	C2	C1	-108.5(5)
SN1	C1	C2	C13	-0.4(7)	SI2	C13	C2	C3	71.1(5)
SN1	C1	C6	C5	179.1(3)	SI3	C14	SI4	C28	-60.6(5)
SN1	C1	C6	C15	1.1(6)	SI3	C14	SI4	C29	-179.3(6)
SN1	C7	C8	C9	-177.5(4)	SI3	C14	SI4	C30	59.6(5)
SN1	C7	C8	C16	5.5(6)	SI3	C14	C4	C3	110.7(5)
SN1	C7	C12	C11	178.2(4)	SI3	C14	C4	C5	-68.2(6)
SN1	C7	C12	C18	-6.2(7)	SI4	C14	SI3	C25	178.0(4)
S1	SN1	S2	C43	3.7(2)	SI4	C14	SI3	C26	-63.0(5)
S1	SN1	C1	C2	86.6(4)	SI4	C14	SI3	C27	58.1(6)
S1	SN1	C1	C6	-91.3(3)	SI4	C14	C4	C3	-107.2(5)
S1	SN1	C7	C8	-154.8(3)	SI4	C14	C4	C5	74.0(6)
S1	SN1	C7	C12	24.6(5)	SI5	C15	SI6	C34	-60.0(6)
S2	SN1	S1	C43	-3.6(2)	SI5	C15	SI6	C35	176.0(6)
S2	SN1	C1	C2	4.3(4)	SI5	C15	SI6	C36	58.3(6)
S2	SN1	C1	C6	-173.7(3)	SI5	C15	C6	C1	-115.2(4)
S2	SN1	C7	C8	-76.6(4)	SI5	C15	C6	C5	66.8(5)
S2	SN1	C7	C12	102.8(4)	SI6	C15	SI5	C31	160.9(4)
SI1	C13	SI2	C22	58.8(4)	SI6	C15	SI5	C32	-81.1(4)
SI1	C13	SI2	C23	-63.3(4)	SI6	C15	SI5	C33	39.4(5)
SI1	C13	SI2	C24	177.9(3)	SI6	C15	C6	C1	108.1(5)
SI1	C13	C2	C1	115.8(5)	SI6	C15	C6	C5	-69.9(5)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle
C1	SN1	S1	C43	-121.0(2)
C1	SN1	S2	C43	107.5(2)
C1	SN1	C7	C8	65.2(4)
C1	SN1	C7	C12	-115.4(4)
C1	C2	C3	C4	2.0(7)
C1	C6	C5	C4	0.1(7)
C2	C1	SN1	C7	-131.4(4)
C2	C1	C6	C5	1.1(7)
C2	C1	C6	C15	-176.9(4)
C2	C3	C4	C5	-0.8(7)
C2	C3	C4	C14	-179.8(4)
C2	C13	SI1	C19	-30.9(5)
C2	C13	SI1	C20	-149.1(5)
C2	C13	SI1	C21	88.3(5)
C2	C13	SI2	C22	-75.2(4)
C2	C13	SI2	C23	162.6(4)
C2	C13	SI2	C24	43.9(5)
C3	C2	C1	C6	-2.1(7)
C3	C4	C5	C6	-0.2(7)
C4	C3	C2	C13	-177.6(5)
C4	C5	C6	C15	178.2(5)
C4	C14	SI3	C25	-42.7(5)
C4	C14	SI3	C26	76.2(5)
C4	C14	SI3	C27	-162.7(5)
C4	C14	SI4	C28	160.4(5)
C4	C14	SI4	C29	41.7(7)
C4	C14	SI4	C30	-79.4(6)
C6	C1	SN1	C7	50.7(4)
C6	C1	C2	C13	177.5(4)
C6	C5	C4	C14	178.6(4)
C6	C15	SI5	C31	27.1(5)
C6	C15	SI5	C32	145.2(4)
C6	C15	SI5	C33	-94.4(5)
C6	C15	SI6	C34	74.2(6)
C6	C15	SI6	C35	-49.9(7)
C6	C15	SI6	C36	-167.6(6)
C7	SN1	S1	C43	94.0(2)
C7	SN1	S2	C43	-109.6(2)
C7	C8	C9	C10	-1.1(9)
C7	C8	C16	C37	95.2(6)
C7	C8	C16	C38	-141.0(5)
C7	C12	C11	C10	0(1)
C7	C12	C18	C41	-89.5(6)
C7	C12	C18	C42	145.6(5)
C8	C7	C12	C11	-2.5(8)
C8	C7	C12	C18	173.1(5)
C8	C9	C10	C11	-2(1)
C8	C9	C10	C17	175.6(6)
C9	C8	C7	C12	3.2(7)
C9	C8	C16	C37	-81.8(6)
C9	C8	C16	C38	42.1(7)
C9	C10	C11	C12	3(1)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
C9	C10	C17	C39	-105(1)					
C9	C10	C17	C40	48(2)					
C10	C9	C8	C16	176.0(6)					
C10	C11	C12	C18	-176.3(6)					
C11	C10	C17	C39	72(1)					
C11	C10	C17	C40	-134(1)					
C11	C12	C18	C41	86.1(7)					
C11	C12	C18	C42	-38.8(8)					
C12	C7	C8	C16	-173.8(5)					
C12	C11	C10	C17	-174.8(7)					

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Table of Least-Squares Planes

---------- Plane number 1 ----------

Atoms Defining Plane	Distance	esd
SN1	-0.0001	0.0003
S1	0.0073	0.0016
S2	0.0060	0.0015
C43	-0.1007	0.0054

Mean deviation from plane is 0.0285 angstroms
Chi-squared: 384.8

---------- Plane number 2 ----------

Atoms Defining Plane	Distance	esd
SN1	0.0000	
S1	0.0000	
S2	0.0000	

Mean deviation from plane is 0.0000 angstroms
Chi-squared: 0.0

Dihedral angles between least-squares planes

plane	plane	angle
2	1	179.80

---------- Plane number 3 ----------

Atoms Defining Plane	Distance	esd
S1	0.0000	
S2	0.0000	
C43	0.0000	

Mean deviation from plane is 0.0000 angstroms
Chi-squared: 0.0

Dihedral angles between least-squares planes

plane	plane	angle
3	1	6.53
3	2	173.27

Table of Least-Squares Planes (continued)

---------- Plane number 4 ----------

Atoms Defining Plane	Distance	esd
S1	-0.0002	0.0016
S2	-0.0001	0.0015
C43	0.0045	0.0054
S3	-0.0004	0.0024

Mean deviation from plane is 0.0013 angstroms
Chi-squared: 0.8

Dihedral angles between least-squares planes

plane	plane	angle
4	1	6.82
4	2	172.99
4	3	0.29