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Experimental Details

Crystal data:

Chemical formula	:	C28 H60 S2 Si6
formula weight	:	629.43
Crystal system	:	monoclinic
Space group	:	P 21(No.4)
Z	:	2
a(Angs.)	:	12.747(3)
b(Angs.)	:	8.055(2)
c(Angs.)	:	19.401(1)
alpha(Deg.)	:	90.0
beta(Deg.)	:	90.437(8)
gamma(Deg.)	:	90.0
cell volume	:	1991.98 Angs.**3
Density calc.	:	1.049 g/cm**3
Radiation	:	Mo K(alpha) (0.71069 Angs.)
Range for lattice parameters	:	7.58 < theta < 18.16
Absorption coefficient	:	3.20 1/cm
Temperature	:	200 K
Crystal source	:	recrystallized from
Crystal colour	:	colourless
Crystal shape	:	rod-like
Crystal size	:	ca.0.5 x 0.3 x 0.3 mm

Data Collection

Diffractometer type	:	CAD4 Enraf-Nonius
Collection method	:	omega/2theta
Absorption correction	:	none
No. of reflections measured	:	6612
No. of independent reflections	:	5941
No. of observed reflections	:	4076
maximum theta(Deg.)	:	30.1

hmin -> hmax	:	-17 -> 17
kmin -> kmax	:	0 -> 11
lmin -> lmax	:	0 -> 27
Criterion for observed	:	I > 2sigma(I)
Rint	:	0.012(28)
Standard reflections	:	3 -1 5; -3 -1 6; -2 -1 7
Variation (%)	:	< 3.5%
Refinement: On	:	F
Treatment of hydrogens	:	Positions calculated. Us fixed at 1.5 times U of the relevant heavy atom. Not refined.
R	:	0.052
Rw	:	0.037
Weighting sheme	:	w=1/sigma**2
No. of parameters refined	:	325
No. of reflections in refmnt.	:	4075
Residual electron density	:	-0.5/+0.5
r*[1]	:	944
XABS[2]	:	not refined
Error of fit	:	2.064
Solution	:	XTAL3.2[3]
Remarks	:	

Definitions:

$$Ueq = (1/3)\,Sum(i)\,Sum(j)\; U(ij)\,a(i^*)\,a(j^*)\,a(i)\,a(j)$$

The anisotropic displacement factor in the structure factor expression is:

$$t = \exp[-2\pi^{**}2\,(Sum(i)\,Sum(j)\,Uij\; h(i)\,h(j)\,a(i^*)\,a(j^*)]$$

Literature:

[1] a)A.C.Larson; Crystallographic Computing. F.R.Ahmed, S.R. Hall, C.P.Huber, eds., Munksgaard. Copenhagen: 291-294, (1970). b)W.H.Zachariasen; Acta Cryst. 23, 558-564(1967).

[2] H.D.Flack; Acta Cryst. A39, 876-881(1983)

[3] S.R.Hall, H.D.Flack and J.M. Stewart; Eds. XTAL3.2 Reference Manual.

Universities of Western Australia, Geneva and Maryland.
Lamb: Perth (1992).

[4] G.M.Sheldrick in Crystallographic Computing 3, Eds. G.M.Sheldrick, C.Krueger, and R.Goodard; Oxford University Press, 1985, p.175-189.

monoclinic, space group P 21 (No.4)
a=12.747(3)
b=8.055(2)
c=19.401(1)
beta=90.437(8)

Coordinates to Plot the Molecule

ATOM	SI1	.70744	-.33031	.28355
ATOM	SI2	.63757	-.08389	.23788
ATOM	SI3	.47974	-.12121	.17590
ATOM	SI4	.39109	.13187	.16229
ATOM	SI5	.23615	.09949	.09710
ATOM	SI6	.14287	.35024	.08753
ATOM	S1	-.03922	.30666	.35511
ATOM	S2	.40725	-.45449	.49545
ATOM	C1	.11243	.44760	.17307
ATOM	C2	.05103	.33921	.22343
ATOM	C3	.03994	.41764	.29409
ATOM	C4	.05157	.15723	.38473
ATOM	C5	.02677	.02393	.44065
ATOM	C6	.10316	.01110	.34348
ATOM	C7	.15899	.17982	.42020
ATOM	C8	.14236	-.01058	.41915
ATOM	C9	.21692	-.14046	.44141
ATOM	C10	.21923	-.32542	.41900
ATOM	C11	.24518	-.20103	.51485
ATOM	C12	.33556	-.13502	.42765
ATOM	C13	.31651	-.30098	.46637
ATOM	C14	.46763	-.51313	.41572
ATOM	C15	.54992	-.39517	.38812
ATOM	C16	.60886	-.46438	.32565
ATOM	C17	.80883	-.26949	.34918
ATOM	C18	.76937	-.45461	.21317
ATOM	C19	.62023	.06929	.31020
ATOM	C20	.73963	.00291	.17828
ATOM	C21	.39003	-.27032	.22002
ATOM	C22	.51172	-.20835	.08920
ATOM	C23	.35739	.21439	.25004
ATOM	C24	.48032	.28710	.11908
ATOM	C25	.14900	-.06297	.13555
ATOM	C26	.26807	.03413	.00684
ATOM	C27	.22100	.50275	.03502
ATOM	C28	.01579	.30930	.04147
ATOM	H16A	.55338	-.49778	.28928
ATOM	H16B	.64364	-.57208	.34088
ATOM	H15A	.60134	-.36829	.42557
ATOM	H15B	.51409	-.28669	.37365
ATOM	H14A	.41055	-.52500	.37835
ATOM	H14B	.50189	-.62568	.42047
ATOM	H12H	.37910	-.04529	.45133
ATOM	H12B	.36080	-.13742	.37724
ATOM	H10A	.22966	-.35607	.36684
ATOM	H10B	.15974	-.40567	.43394
ATOM	H11A	.18921	-.25887	.54314
ATOM	H11B	.27970	-.11572	.54774
ATOM	H7A	.16240	.23470	.46665

ATOM H7B	.21958	.22577	.39171
ATOM H5A	-.02917	-.06410	.42851
ATOM H5B	.01113	.06224	.48897
ATOM H6A	.15596	.03665	.30439
ATOM H6B	.05545	-.08107	.32217
ATOM H3A	.00843	.53222	.28668
ATOM H3B	.11280	.43486	.31456
ATOM H2A	.09045	.22777	.22993
ATOM H2B	-.01964	.31217	.20439
ATOM H1A	.07187	.55515	.16537
ATOM H1B	.18244	.48353	.19630
ATOM H18A	.80651	-.55721	.23116
ATOM H18B	.71770	-.49037	.17678
ATOM H18C	.82507	-.38244	.18972
ATOM H17A	.77539	-.20935	.38817
ATOM H17B	.84485	-.37194	.36744
ATOM H17C	.86290	-.19609	.32743
ATOM H19A	.56864	.02215	.34658
ATOM H19B	.68712	.09341	.33495
ATOM H19C	.58830	.17482	.29258
ATOM H20A	.80698	.02814	.20267
ATOM H20B	.75488	-.07678	.13904
ATOM H20C	.71063	.10911	.15737
ATOM H21A	.42630	-.38201	.22724
ATOM H21B	.37344	-.22741	.26890
ATOM H21C	.32308	-.28873	.19574
ATOM H22A	.55836	-.12744	.06307
ATOM H22B	.54912	-.31608	.09324
ATOM H22C	.44531	-.22333	.06160
ATOM H23A	.31268	.13583	.27654
ATOM H23B	.42459	.23442	.27863
ATOM H23C	.32056	.32459	.24608
ATOM H24A	.54629	.30931	.14471
ATOM H24B	.50081	.24786	.07005
ATOM H24C	.44349	.39959	.11088
ATOM H25A	.18458	-.17621	.13705
ATOM H25B	.12739	-.03526	.18417
ATOM H25C	.08016	-.08153	.10833
ATOM H26A	.31564	.12056	-.01546
ATOM H26B	.30906	-.07401	.00774
ATOM H26C	.20448	.02050	-.02158
ATOM H27A	.29266	.52594	.05759
ATOM H27B	.23623	.45865	-.01291
ATOM H27C	.18414	.61204	.03001
ATOM H28A	.02728	.26520	-.00661
ATOM H28B	-.02942	.22802	.06698
ATOM H28C	-.02662	.41688	.03636

Fractional Atomic Coordinates and Isotropic Displacement Parameters (U)

Equivalent isotropic displacement parameters (Ueq) are given for anisotropically refined atoms (flagged with *).

	x/a	y/b	z/c		U,Ueq
SI1	0.7074(1)	0.66969	0.28356(7)	*	0.0396(5)
SI2	0.6376(1)	0.9161(2)	0.23789(7)	*	0.0419(5)
SI3	0.4797(1)	0.8788(2)	0.17591(6)	*	0.0363(4)
SI4	0.3911(1)	1.1319(2)	0.16230(7)	*	0.0350(4)
SI5	0.2361(1)	1.0995(2)	0.09710(7)	*	0.0368(5)
SI6	0.1429(1)	1.3502(2)	0.08753(7)	*	0.0418(5)
S1	-0.0392(1)	1.3067(3)	0.35511(8)	*	0.0666(6)

S2	0.4072(1)	0.5455(2)	0.49545(7)	*	0.0516(5)
C1	0.1124(3)	1.4476(6)	0.1731(2)	*	0.042(2)
C2	0.0510(3)	1.3392(6)	0.2234(2)	*	0.043(2)
C3	0.0399(4)	1.4176(7)	0.2941(3)	*	0.054(2)
C4	0.0516(3)	1.1572(7)	0.3847(2)	*	0.049(2)
C5	0.0268(3)	1.0239(8)	0.4406(2)	*	0.058(2)
C6	0.1032(3)	1.0111(7)	0.3435(2)	*	0.049(2)
C7	0.1590(4)	1.1798(7)	0.4202(3)	*	0.052(2)
C8	0.1424(3)	0.9894(7)	0.4191(2)	*	0.041(2)
C9	0.2169(3)	0.8595(6)	0.4414(2)	*	0.037(2)
C10	0.2192(4)	0.6746(7)	0.4190(3)	*	0.053(2)
C11	0.2452(3)	0.7990(8)	0.5149(2)	*	0.053(2)
C12	0.3356(3)	0.8650(7)	0.4277(2)	*	0.045(2)
C13	0.3165(3)	0.6990(7)	0.4664(2)	*	0.042(2)
C14	0.4676(3)	0.4869(6)	0.4157(2)	*	0.045(2)
C15	0.5499(3)	0.6048(6)	0.3881(2)	*	0.042(2)
C16	0.6089(3)	0.5356(6)	0.3256(2)	*	0.040(2)
C17	0.8088(4)	0.7305(7)	0.3492(3)	*	0.059(2)
C18	0.7694(4)	0.5454(7)	0.2132(3)	*	0.061(2)
C19	0.6202(4)	1.0693(7)	0.3102(3)	*	0.068(2)
C20	0.7396(4)	1.0029(9)	0.1783(3)	*	0.082(3)
C21	0.3900(4)	0.7297(7)	0.2200(3)	*	0.051(2)
C22	0.5117(4)	0.7917(7)	0.0892(3)	*	0.059(2)
C23	0.3574(4)	1.2144(7)	0.2500(2)	*	0.047(2)
C24	0.4803(4)	1.2871(7)	0.1191(3)	*	0.056(2)
C25	0.1490(3)	0.9370(6)	0.1355(2)	*	0.047(2)
C26	0.2681(4)	1.0341(7)	0.0068(2)	*	0.055(2)
C27	0.2210(4)	1.5027(7)	0.0350(2)	*	0.059(2)
C28	0.0158(4)	1.3093(8)	0.0415(3)	*	0.070(2)
H16A	0.5534	0.5022	0.2893		0.060
H16B	0.6436	0.4279	0.3409		0.060
H15A	0.6013	0.6317	0.4256		0.063
H15B	0.5141	0.7133	0.3737		0.063
H14A	0.4106	0.4750	0.3784		0.066
H14B	0.5019	0.3743	0.4205		0.066
H12H	0.3791	0.9547	0.4513		0.065
H12B	0.3608	0.8626	0.3772		0.065
H10A	0.2297	0.6439	0.3668		0.078
H10B	0.1597	0.5943	0.4339		0.078
H11A	0.1892	0.7411	0.5431		0.078
H11B	0.2797	0.8843	0.5477		0.078
H7A	0.1624	1.2347	0.4667		0.078
H7B	0.2196	1.2258	0.3917		0.078
H5A	-0.0292	0.9359	0.4285		0.084
H5B	0.0111	1.0622	0.4890		0.084
H6A	0.1560	1.0366	0.3044		0.070
H6B	0.0555	0.9189	0.3222		0.070
H3A	0.0084	1.5322	0.2867		0.080
H3B	0.1128	1.4349	0.3146		0.080
H2A	0.0904	1.2278	0.2299		0.065
H2B	-0.0196	1.3122	0.2044		0.065
H1A	0.0719	1.5552	0.1654		0.062
H1B	0.1824	1.4835	0.1963		0.062
H18A	0.8065	0.4428	0.2312		0.090
H18B	0.7177	0.5096	0.1768		0.090
H18C	0.8251	0.6176	0.1897		0.090
H17A	0.7754	0.7907	0.3882		0.087
H17B	0.8449	0.6281	0.3674		0.087
H17C	0.8629	0.8039	0.3274		0.087
H19A	0.5686	1.0222	0.3466		0.099
H19B	0.6871	1.0934	0.3350		0.099
H19C	0.5883	1.1748	0.2926		0.099
H20A	0.8070	1.0281	0.2027		0.123
H20B	0.7549	0.9232	0.1390		0.123

H20C	0.7106	1.1091	0.1574	0.123
H21A	0.4263	0.6180	0.2272	0.075
H21B	0.3734	0.7726	0.2689	0.075
H21C	0.3231	0.7113	0.1957	0.075
H22A	0.5584	0.8726	0.0631	0.090
H22B	0.5491	0.6839	0.0932	0.090
H22C	0.4453	0.7767	0.0616	0.090
H23A	0.3127	1.1358	0.2765	0.070
H23B	0.4246	1.2344	0.2786	0.070
H23C	0.3206	1.3246	0.2461	0.070
H24A	0.5463	1.3093	0.1447	0.082
H24B	0.5008	1.2479	0.0701	0.082
H24C	0.4435	1.3996	0.1109	0.082
H25A	0.1846	0.8238	0.1371	0.069
H25B	0.1274	0.9647	0.1842	0.069
H25C	0.0802	0.9185	0.1083	0.069
H26A	0.3156	1.1206	-0.0155	0.080
H26B	0.3091	0.9260	0.0077	0.080
H26C	0.2045	1.0205	-0.0216	0.080
H27A	0.2927	1.5259	0.0576	0.087
H27B	0.2362	1.4587	-0.0129	0.087
H27C	0.1841	1.6120	0.0300	0.087
H28A	0.0273	1.2652	-0.0066	0.102
H28B	-0.0294	1.2280	0.0670	0.102
H28C	-0.0266	1.4169	0.0364	0.102

Non-H fractional coordinates and isotropic displacement parameters (U)

Equivalent isotropic displacement parameters (Ueq)
are given for anisotropically refined atoms (flagged with *).

	x/a	y/b	z/c		U,Ueq
SI1	0.7074(1)	0.66969	0.28356(7)	*	0.0396(5)
SI2	0.6376(1)	0.9161(2)	0.23789(7)	*	0.0419(5)
SI3	0.4797(1)	0.8788(2)	0.17591(6)	*	0.0363(4)
SI4	0.3911(1)	1.1319(2)	0.16230(7)	*	0.0350(4)
SI5	0.2361(1)	1.0995(2)	0.09710(7)	*	0.0368(5)
SI6	0.1429(1)	1.3502(2)	0.08753(7)	*	0.0418(5)
S1	-0.0392(1)	1.3067(3)	0.35511(8)	*	0.0666(6)
S2	0.4072(1)	0.5455(2)	0.49545(7)	*	0.0516(5)
C1	0.1124(3)	1.4476(6)	0.1731(2)	*	0.042(2)
C2	0.0510(3)	1.3392(6)	0.2234(2)	*	0.043(2)
C3	0.0399(4)	1.4176(7)	0.2941(3)	*	0.054(2)
C4	0.0516(3)	1.1572(7)	0.3847(2)	*	0.049(2)
C5	0.0268(3)	1.0239(8)	0.4406(2)	*	0.058(2)
C6	0.1032(3)	1.0111(7)	0.3435(2)	*	0.049(2)
C7	0.1590(4)	1.1798(7)	0.4202(3)	*	0.052(2)
C8	0.1424(3)	0.9894(7)	0.4191(2)	*	0.041(2)
C9	0.2169(3)	0.8595(6)	0.4414(2)	*	0.037(2)
C10	0.2192(4)	0.6746(7)	0.4190(3)	*	0.053(2)
C11	0.2452(3)	0.7990(8)	0.5149(2)	*	0.053(2)
C12	0.3356(3)	0.8650(7)	0.4277(2)	*	0.045(2)
C13	0.3165(3)	0.6990(7)	0.4664(2)	*	0.042(2)
C14	0.4676(3)	0.4869(6)	0.4157(2)	*	0.045(2)
C15	0.5499(3)	0.6048(6)	0.3881(2)	*	0.042(2)
C16	0.6089(3)	0.5356(6)	0.3256(2)	*	0.040(2)
C17	0.8088(4)	0.7305(7)	0.3492(3)	*	0.059(2)
C18	0.7694(4)	0.5454(7)	0.2132(3)	*	0.061(2)
C19	0.6202(4)	1.0693(7)	0.3102(3)	*	0.068(2)
C20	0.7396(4)	1.0029(9)	0.1783(3)	*	0.082(3)

C21	0.3900(4)	0.7297(7)	0.2200(3)	* 0.051(2)
C22	0.5117(4)	0.7917(7)	0.0892(3)	* 0.059(2)
C23	0.3574(4)	1.2144(7)	0.2500(2)	* 0.047(2)
C24	0.4803(4)	1.2871(7)	0.1191(3)	* 0.056(2)
C25	0.1490(3)	0.9370(6)	0.1355(2)	* 0.047(2)
C26	0.2681(4)	1.0341(7)	0.0068(2)	* 0.055(2)
C27	0.2210(4)	1.5027(7)	0.0350(2)	* 0.059(2)
C28	0.0158(4)	1.3093(8)	0.0415(3)	* 0.070(2)

Hydrogen Positional and Isotropic Displacement Parameters

	x/a	y/b	z/c	U
H16A	0.5534	0.5022	0.2893	0.060
H16B	0.6436	0.4279	0.3409	0.060
H15A	0.6013	0.6317	0.4256	0.063
H15B	0.5141	0.7133	0.3737	0.063
H14A	0.4106	0.4750	0.3784	0.066
H14B	0.5019	0.3743	0.4205	0.066
H12H	0.3791	0.9547	0.4513	0.065
H12B	0.3608	0.8626	0.3772	0.065
H10A	0.2297	0.6439	0.3668	0.078
H10B	0.1597	0.5943	0.4339	0.078
H11A	0.1892	0.7411	0.5431	0.078
H11B	0.2797	0.8843	0.5477	0.078
H7A	0.1624	1.2347	0.4667	0.078
H7B	0.2196	1.2258	0.3917	0.078
H5A	-0.0292	0.9359	0.4285	0.084
H5B	0.0111	1.0622	0.4890	0.084
H6A	0.1560	1.0366	0.3044	0.070
H6B	0.0555	0.9189	0.3222	0.070
H3A	0.0084	1.5322	0.2867	0.080
H3B	0.1128	1.4349	0.3146	0.080
H2A	0.0904	1.2278	0.2299	0.065
H2B	-0.0196	1.3122	0.2044	0.065
H1A	0.0719	1.5552	0.1654	0.062
H1B	0.1824	1.4835	0.1963	0.062
H18A	0.8065	0.4428	0.2312	0.090
H18B	0.7177	0.5096	0.1768	0.090
H18C	0.8251	0.6176	0.1897	0.090
H17A	0.7754	0.7907	0.3882	0.087
H17B	0.8449	0.6281	0.3674	0.087
H17C	0.8629	0.8039	0.3274	0.087
H19A	0.5686	1.0222	0.3466	0.099
H19B	0.6871	1.0934	0.3350	0.099
H19C	0.5883	1.1748	0.2926	0.099
H20A	0.8070	1.0281	0.2027	0.123
H20B	0.7549	0.9232	0.1390	0.123
H20C	0.7106	1.1091	0.1574	0.123
H21A	0.4263	0.6180	0.2272	0.075
H21B	0.3734	0.7726	0.2689	0.075
H21C	0.3231	0.7113	0.1957	0.075
H22A	0.5584	0.8726	0.0631	0.090
H22B	0.5491	0.6839	0.0932	0.090
H22C	0.4453	0.7767	0.0616	0.090
H23A	0.3127	1.1358	0.2765	0.070
H23B	0.4246	1.2344	0.2786	0.070
H23C	0.3206	1.3246	0.2461	0.070
H24A	0.5463	1.3093	0.1447	0.082
H24B	0.5008	1.2479	0.0701	0.082
H24C	0.4435	1.3996	0.1109	0.082

H25A	0.1846	0.8238	0.1371	0.069
H25B	0.1274	0.9647	0.1842	0.069
H25C	0.0802	0.9185	0.1083	0.069
H26A	0.3156	1.1206	-0.0155	0.080
H26B	0.3091	0.9260	0.0077	0.080
H26C	0.2045	1.0205	-0.0216	0.080
H27A	0.2927	1.5259	0.0576	0.087
H27B	0.2362	1.4587	-0.0129	0.087
H27C	0.1841	1.6120	0.0300	0.087
H28A	0.0273	1.2652	-0.0066	0.102
H28B	-0.0294	1.2280	0.0670	0.102
H28C	-0.0266	1.4169	0.0364	0.102

Atomic Displacement Parameters

	U11	U22	U33	U12	U13	U23
SI1	.0361(7)	.0388(9)	.0439(8)	.0094(7)	-.0029(6)	.0025(7)
SI2	.0407(8)	.0373(9)	.0476(8)	-.0015(7)	-.0049(6)	.0055(8)
SI3	.0405(7)	.0318(8)	.0365(8)	.0046(7)	-.0024(6)	-.0024(7)
SI4	.0365(7)	.0298(8)	.0387(7)	.0010(6)	-.0028(6)	-.0001(6)
SI5	.0402(7)	.0313(9)	.0389(8)	-.0005(6)	-.0057(6)	.0004(7)
SI6	.0441(8)	.0376(9)	.0435(8)	.0044(7)	-.0061(6)	.0051(8)
S1	.0519(8)	.084(1)	.064(1)	.0302(9)	.0219(7)	.0216(9)
S2	.0544(8)	.0554(9)	.0452(8)	.0097(8)	.0030(6)	.0135(7)
C1	.047(3)	.031(3)	.049(3)	.004(2)	.003(2)	.005(3)
C2	.039(2)	.041(3)	.049(3)	.004(2)	.005(2)	-.001(3)
C3	.054(3)	.050(4)	.058(3)	.011(3)	.011(3)	.007(3)
C4	.036(3)	.064(4)	.047(3)	.011(3)	.008(2)	.008(3)
C5	.039(3)	.083(4)	.053(3)	.010(3)	.011(2)	.011(4)
C6	.047(3)	.058(4)	.041(3)	.010(3)	.000(2)	-.003(3)
C7	.052(3)	.045(3)	.060(4)	.003(3)	.001(3)	-.011(3)
C8	.034(3)	.049(3)	.040(3)	.000(2)	.005(2)	-.003(3)
C9	.034(2)	.040(3)	.037(3)	-.000(2)	.001(2)	-.004(3)
C10	.050(3)	.049(4)	.059(4)	-.003(3)	-.011(3)	-.004(3)
C11	.052(3)	.072(4)	.036(3)	.020(3)	.001(2)	-.002(3)
C12	.037(3)	.047(3)	.051(3)	.004(3)	.001(2)	.005(3)
C13	.040(3)	.053(3)	.035(3)	-.001(3)	-.001(2)	.000(3)
C14	.049(3)	.035(3)	.051(3)	.006(2)	.002(2)	-.000(3)
C15	.049(3)	.033(3)	.045(3)	.007(2)	.001(2)	.001(2)
C16	.050(3)	.029(3)	.041(3)	.011(2)	-.009(2)	-.003(2)
C17	.044(3)	.060(4)	.072(4)	.009(3)	-.012(3)	.000(3)
C18	.056(3)	.061(4)	.067(4)	.018(3)	.007(3)	-.008(3)
C19	.079(4)	.039(4)	.085(4)	.013(3)	-.032(3)	-.016(3)
C20	.056(3)	.092(5)	.098(5)	-.009(4)	.005(3)	.036(4)
C21	.051(3)	.042(3)	.060(4)	-.010(3)	-.011(3)	.008(3)
C22	.065(4)	.063(4)	.049(3)	.020(3)	.003(3)	-.014(3)
C23	.046(3)	.047(4)	.048(3)	.006(3)	-.000(2)	-.014(3)
C24	.054(3)	.049(4)	.065(4)	-.012(3)	-.006(3)	.006(3)
C25	.049(3)	.037(3)	.054(3)	-.006(3)	.000(2)	.003(3)
C26	.057(3)	.061(4)	.047(3)	-.003(3)	-.002(3)	-.005(3)
C27	.080(4)	.046(4)	.051(3)	.016(3)	.015(3)	.015(3)
C28	.064(3)	.064(4)	.081(4)	.015(3)	-.028(3)	.004(4)
H16A	.060	.060	.060	.000	.000	.000
H16B	.060	.060	.060	.000	.000	.000
H15A	.063	.063	.063	.000	.000	.000
H15B	.063	.063	.063	.000	.000	.000
H14A	.066	.066	.066	.000	.001	.000
H14B	.066	.066	.066	.000	.001	.000
H12H	.065	.065	.065	.000	.000	.000
H12B	.065	.065	.065	.000	.000	.000

H10A	.078	.078	.078	.000	.001	.000
H10B	.078	.078	.078	.000	.001	.000
H11A	.078	.078	.078	.000	.001	.000
H11B	.078	.078	.078	.000	.001	.000
H7A	.078	.078	.078	.000	.001	.000
H7B	.078	.078	.078	.000	.001	.000
H5A	.084	.084	.084	.000	.001	.000
H5B	.084	.084	.084	.000	.001	.000
H6A	.070	.070	.070	.000	.001	.000
H6B	.070	.070	.070	.000	.001	.000
H3A	.080	.080	.080	.000	.001	.000
H3B	.080	.080	.080	.000	.001	.000
H2A	.065	.065	.065	.000	.000	.000
H2B	.065	.065	.065	.000	.000	.000
H1A	.062	.062	.062	.000	.000	.000
H1B	.062	.062	.062	.000	.000	.000
H18A	.090	.090	.090	.000	.001	.000
H18B	.090	.090	.090	.000	.001	.000
H18C	.090	.090	.090	.000	.001	.000
H17A	.087	.087	.087	.000	.001	.000
H17B	.087	.087	.087	.000	.001	.000
H17C	.087	.087	.087	.000	.001	.000
H19A	.099	.099	.099	.000	.001	.000
H19B	.099	.099	.099	.000	.001	.000
H19C	.099	.099	.099	.000	.001	.000
H20A	.123	.123	.123	.000	.001	.000
H20B	.123	.123	.123	.000	.001	.000
H20C	.123	.123	.123	.000	.001	.000
H21A	.075	.075	.075	.000	.001	.000
H21B	.075	.075	.075	.000	.001	.000
H21C	.075	.075	.075	.000	.001	.000
H22A	.090	.090	.090	.000	.001	.000
H22B	.090	.090	.090	.000	.001	.000
H22C	.090	.090	.090	.000	.001	.000
H23A	.070	.070	.070	.000	.001	.000
H23B	.070	.070	.070	.000	.001	.000
H23C	.070	.070	.070	.000	.001	.000
H24A	.082	.082	.082	.000	.001	.000
H24B	.082	.082	.082	.000	.001	.000
H24C	.082	.082	.082	.000	.001	.000
H25A	.069	.069	.069	.000	.001	.000
H25B	.069	.069	.069	.000	.001	.000
H25C	.069	.069	.069	.000	.001	.000
H26A	.080	.080	.080	.000	.001	.000
H26B	.080	.080	.080	.000	.001	.000
H26C	.080	.080	.080	.000	.001	.000
H27A	.087	.087	.087	.000	.001	.000
H27B	.087	.087	.087	.000	.001	.000
H27C	.087	.087	.087	.000	.001	.000
H28A	.102	.102	.102	.000	.001	.000
H28B	.102	.102	.102	.000	.001	.000
H28C	.102	.102	.102	.000	.001	.000

Bond Distances (Angstroms)

SI1-C16	1.851(5)	SI1-C17	1.873(5)	SI1-C18	1.873(5)
SI1-SI2	2.347(2)	SI2-C20	1.882(6)	SI2-C19	1.883(6)
SI2-SI3	2.355(2)	SI3-C21	1.870(5)	SI3-C22	1.870(5)
SI3-SI4	2.345(3)	SI4-C23	1.880(5)	SI4-C24	1.891(5)
SI4-SI5	2.352(2)	SI5-C25	1.875(5)	SI5-C26	1.876(5)
SI5-SI6	2.350(3)	SI6-C28	1.873(5)	SI6-C1	1.879(5)
SI6-C27	1.885(6)	S1-C4	1.763(5)	S1-C3	1.799(5)
S2-C13	1.782(5)	S2-C14	1.796(5)	C1-H1A	1.019(5)

C1-H1B	1.038(4)	C1-C2	1.530(7)	C2-H2B	.995(4)
C2-H2A	1.036(5)	C2-C3	1.517(7)	C3-H3A	1.016(6)
C3-H3B	1.017(5)	C4-C7	1.539(7)	C4-C5	1.560(8)
C4-C6	1.570(7)	C5-H5B	1.008(5)	C5-H5A	1.032(5)
C5-C8	1.559(6)	C6-H6A	1.038(5)	C6-H6B	1.043(5)
C6-C8	1.557(6)	C7-H7A	1.005(5)	C7-H7B	1.023(5)
C7-C8	1.548(8)	C8-C9	1.476(7)	C9-C12	1.538(6)
C9-C11	1.546(6)	C9-C10	1.552(8)	C10-H10B	1.039(5)
C10-H10A	1.051(5)	C10-C13	1.550(6)	C11-H11A	1.016(5)
C11-H11B	1.034(5)	C11-C13	1.540(7)	C12-H12H	1.019(5)
C12-H12B	1.032(4)	C12-C13	1.553(7)	C14-H14B	1.010(5)
C14-H14A	1.028(5)	C14-C15	1.516(7)	C15-H15A	.999(4)
C15-H15B	1.024(5)	C15-C16	1.536(6)	C16-H16B	1.017(5)
C16-H16A	1.031(4)	C17-H17A	.997(5)	C17-H17C	1.004(5)
C17-H17B	1.007(5)	C18-H18B	1.004(5)	C18-H18A	1.013(6)
C18-H18C	1.027(5)	C19-H19B	.994(5)	C19-H19C	1.002(5)
C19-H19A	1.040(5)	C20-H20A	.998(5)	C20-H20C	1.015(7)
C20-H20B	1.016(6)	C21-H21C	.983(5)	C21-H21A	1.021(5)
C21-H21B	1.033(5)	C22-H22B	.993(6)	C22-H22C	1.005(5)
C22-H22A	1.020(5)	C23-H23A	.997(5)	C23-H23C	1.007(5)
C23-H23B	1.030(5)	C24-H24A	.990(5)	C24-H24C	1.032(5)
C24-H24B	1.038(5)	C25-H25B	1.010(5)	C25-H25A	1.019(5)
C25-H25C	1.032(4)	C26-H26C	.983(5)	C26-H26B	1.016(6)
C26-H26A	1.022(5)	C27-H27C	1.002(6)	C27-H27B	1.015(5)
C27-H27A	1.027(5)	C28-H28B	1.005(6)	C28-H28A	1.010(5)
C28-H28C	1.026(6)				

Bond Angles (degrees)

C16-SI1-C17	108.7(2)	C16-SI1-C18	107.5(2)
C16-SI1-SI2	113.8(2)	C17-SI1-C18	110.1(2)
C17-SI1-SI2	107.1(2)	C18-SI1-SI2	109.7(2)
C20-SI2-C19	107.5(3)	C20-SI2-SI1	106.5(2)
C20-SI2-SI3	109.0(2)	C19-SI2-SI1	108.6(2)
C19-SI2-SI3	111.1(2)	SI1-SI2-SI3	113.90(9)
C21-SI3-C22	108.0(2)	C21-SI3-SI4	108.3(2)
C21-SI3-SI2	111.8(2)	C22-SI3-SI4	109.5(2)
C22-SI3-SI2	108.4(2)	SI4-SI3-SI2	110.83(9)
C23-SI4-C24	108.1(2)	C23-SI4-SI3	108.6(2)
C23-SI4-SI5	109.2(2)	C24-SI4-SI3	109.5(2)
C24-SI4-SI5	109.9(2)	SI3-SI4-SI5	111.48(9)
C25-SI5-C26	108.0(2)	C25-SI5-SI6	109.3(2)
C25-SI5-SI4	111.2(2)	C26-SI5-SI6	106.3(2)
C26-SI5-SI4	110.2(2)	SI6-SI5-SI4	111.68(9)
C28-SI6-C1	108.1(2)	C28-SI6-C27	108.4(2)
C28-SI6-SI5	108.8(2)	C1-SI6-C27	108.6(2)
C1-SI6-SI5	113.4(2)	C27-SI6-SI5	109.5(2)
C4-S1-C3	100.6(2)	C13-S2-C14	101.0(2)
H1A-C1-H1B	105.1(4)	H1A-C1-C2	108.5(4)
H1A-C1-SI6	109.5(3)	H1B-C1-C2	108.9(4)
H1B-C1-SI6	108.5(3)	C2-C1-SI6	115.8(3)
H2B-C2-H2A	107.0(5)	H2B-C2-C3	109.6(4)
H2B-C2-C1	110.7(4)	H2A-C2-C3	107.4(4)
H2A-C2-C1	108.8(4)	C3-C2-C1	113.0(4)
H3A-C3-H3B	106.9(5)	H3A-C3-C2	106.8(4)
H3A-C3-S1	108.7(4)	H3B-C3-C2	108.6(4)
H3B-C3-S1	109.0(4)	C2-C3-S1	116.4(4)
C7-C4-C5	87.4(4)	C7-C4-C6	86.7(3)
C7-C4-S1	130.1(4)	C5-C4-C6	85.8(4)
C5-C4-S1	124.1(3)	C6-C4-S1	128.5(3)
H5B-C5-H5A	106.3(4)	H5B-C5-C8	119.8(4)
H5B-C5-C4	118.6(6)	H5A-C5-C8	118.0(5)
H5A-C5-C4	117.2(4)	C8-C5-C4	74.9(3)

H6A-C6-H6B	103.3(4)	H6A-C6-C8	120.4(4)
H6A-C6-C4	120.0(5)	H6B-C6-C8	118.4(5)
H6B-C6-C4	119.4(4)	C8-C6-C4	74.7(3)
H7A-C7-H7B	107.3(5)	H7A-C7-C4	119.1(4)
H7A-C7-C8	116.9(5)	H7B-C7-C4	118.3(4)
H7B-C7-C8	117.1(5)	C4-C7-C8	75.9(4)
C9-C8-C7	127.6(4)	C9-C8-C6	123.8(4)
C9-C8-C5	131.0(4)	C7-C8-C6	86.8(4)
C7-C8-C5	87.1(4)	C6-C8-C5	86.3(3)
C8-C9-C12	124.1(4)	C8-C9-C11	129.7(4)
C8-C9-C10	127.7(4)	C12-C9-C11	86.9(3)
C12-C9-C10	87.6(4)	C11-C9-C10	87.2(4)
H10B-C10-H10A	102.7(5)	H10B-C10-C13	119.7(5)
H10B-C10-C9	120.2(4)	H10A-C10-C13	119.6(4)
H10A-C10-C9	119.9(5)	C13-C10-C9	74.3(3)
H11A-C11-H11B	105.6(4)	H11A-C11-C13	120.7(5)
H11A-C11-C9	118.9(4)	H11B-C11-C13	118.3(4)
H11B-C11-C9	117.0(5)	C13-C11-C9	74.7(3)
H12H-C12-H12B	105.5(4)	H12H-C12-C9	118.4(4)
H12H-C12-C13	118.6(4)	H12B-C12-C9	118.5(4)
H12B-C12-C13	119.5(5)	C9-C12-C13	74.6(3)
C11-C13-C10	87.4(3)	C11-C13-C12	86.6(4)
C11-C13-S2	123.6(3)	C10-C13-C12	87.1(4)
C10-C13-S2	127.9(4)	C12-C13-S2	130.3(3)
H14B-C14-H14A	106.5(4)	H14B-C14-C15	107.1(4)
H14B-C14-S2	110.2(4)	H14A-C14-C15	107.3(4)
H14A-C14-S2	109.0(3)	C15-C14-S2	116.2(3)
H15A-C15-H15B	107.7(4)	H15A-C15-C14	109.3(4)
H15A-C15-C16	109.3(4)	H15B-C15-C14	108.9(4)
H15B-C15-C16	108.2(4)	C14-C15-C16	113.3(4)
H16B-C16-H16A	105.8(4)	H16B-C16-C15	107.2(4)
H16B-C16-SI1	109.3(3)	H16A-C16-C15	107.3(4)
H16A-C16-SI1	108.3(3)	C15-C16-SI1	118.3(3)
H17A-C17-H17C	109.4(5)	H17A-C17-H17B	109.1(5)
H17A-C17-SI1	110.3(3)	H17C-C17-H17B	108.5(4)
H17C-C17-SI1	109.9(4)	H17B-C17-SI1	109.6(4)
H18B-C18-H18A	108.1(5)	H18B-C18-H18C	107.7(5)
H18B-C18-SI1	112.8(4)	H18A-C18-H18C	107.0(4)
H18A-C18-SI1	112.5(4)	H18C-C18-SI1	108.5(4)
H19B-C19-H19C	110.1(5)	H19B-C19-H19A	106.7(5)
H19B-C19-SI2	112.5(4)	H19C-C19-H19A	106.5(5)
H19C-C19-SI2	110.6(4)	H19A-C19-SI2	110.2(4)
H20A-C20-H20C	109.1(6)	H20A-C20-H20B	108.4(5)
H20A-C20-SI2	112.4(4)	H20C-C20-H20B	107.7(5)
H20C-C20-SI2	107.9(4)	H20B-C20-SI2	111.3(5)
H21C-C21-H21A	108.9(5)	H21C-C21-H21B	107.9(4)
H21C-C21-SI3	114.2(4)	H21A-C21-H21B	105.3(4)
H21A-C21-SI3	110.5(3)	H21B-C21-SI3	109.6(4)
H22B-C22-H22C	109.8(5)	H22B-C22-H22A	108.4(5)
H22B-C22-SI3	111.4(4)	H22C-C22-H22A	107.7(5)
H22C-C22-SI3	109.6(4)	H22A-C22-SI3	109.8(4)
H23A-C23-H23C	109.3(4)	H23A-C23-H23B	107.3(4)
H23A-C23-SI4	112.2(4)	H23C-C23-H23B	106.8(5)
H23C-C23-SI4	110.6(4)	H23B-C23-SI4	110.4(3)
H24A-C24-H24C	107.6(5)	H24A-C24-H24B	107.3(4)
H24A-C24-SI4	114.1(4)	H24C-C24-H24B	104.1(5)
H24C-C24-SI4	112.0(3)	H24B-C24-SI4	111.2(4)
H25B-C25-H25A	107.2(4)	H25B-C25-H25C	105.9(4)
H25B-C25-SI5	112.6(4)	H25A-C25-H25C	105.2(4)
H25A-C25-SI5	111.8(3)	H25C-C25-SI5	113.7(4)
H26C-C26-H26B	109.6(5)	H26C-C26-H26A	109.1(5)
H26C-C26-SI5	111.8(4)	H26B-C26-H26A	106.5(4)
H26B-C26-SI5	109.9(4)	H26A-C26-SI5	109.7(4)
H27C-C27-H27B	108.1(5)	H27C-C27-H27A	107.2(5)

H27C-C27-SI6	112.1(4)	H27B-C27-H27A	106.2(5)
H27B-C27-SI6	111.9(4)	H27A-C27-SI6	111.1(4)
H28B-C28-H28A	108.3(5)	H28B-C28-H28C	107.1(5)
H28B-C28-SI6	112.1(4)	H28A-C28-H28C	106.7(5)
H28A-C28-SI6	111.8(4)	H28C-C28-SI6	110.5(4)

Dihedral Angles (degrees)

C16-SI1-SI2-SI3	-44.9(2)	C16-SI1-SI2-C19	79.4(2)
C16-SI1-SI2-C20	-165.1(3)	C17-SI1-SI2-SI3	-165.0(2)
C17-SI1-SI2-C19	-40.6(2)	C17-SI1-SI2-C20	74.8(3)
C18-SI1-SI2-SI3	75.6(2)	C18-SI1-SI2-C19	-160.1(2)
C18-SI1-SI2-C20	-44.6(3)	SI2-SI1-C16-C15	-61.3(4)
SI2-SI1-C16-H16A	61.0(4)	SI2-SI1-C16-H16B	175.8(3)
C17-SI1-C16-C15	57.8(4)	C17-SI1-C16-H16A	-179.8(3)
C17-SI1-C16-H16B	-65.1(4)	C18-SI1-C16-C15	176.9(3)
C18-SI1-C16-H16A	-60.7(4)	C18-SI1-C16-H16B	54.0(4)
SI2-SI1-C17-H17A	64.3(4)	SI2-SI1-C17-H17B	-175.6(3)
SI2-SI1-C17-H17C	-56.4(4)	C16-SI1-C17-H17A	-59.0(5)
C16-SI1-C17-H17B	61.1(4)	C16-SI1-C17-H17C	-179.7(4)
C18-SI1-C17-H17A	-176.5(4)	C18-SI1-C17-H17B	-56.4(4)
C18-SI1-C17-H17C	62.8(5)	SI2-SI1-C18-H18A	174.7(3)
SI2-SI1-C18-H18B	-62.6(5)	SI2-SI1-C18-H18C	56.6(4)
C16-SI1-C18-H18A	-61.1(4)	C16-SI1-C18-H18B	61.6(5)
C16-SI1-C18-H18C	-179.2(3)	C17-SI1-C18-H18A	57.1(5)
C17-SI1-C18-H18B	179.8(4)	C17-SI1-C18-H18C	-61.0(4)
SI1-SI2-SI3-SI4	162.53(7)	SI1-SI2-SI3-C21	41.6(2)
SI1-SI2-SI3-C22	-77.3(2)	C19-SI2-SI3-SI4	39.5(2)
C19-SI2-SI3-C21	-81.4(3)	C19-SI2-SI3-C22	159.7(3)
C20-SI2-SI3-SI4	-78.7(2)	C20-SI2-SI3-C21	160.4(3)
C20-SI2-SI3-C22	41.4(3)	SI1-SI2-C19-H19A	-60.7(4)
SI1-SI2-C19-H19B	58.2(4)	SI1-SI2-C19-H19C	-178.2(3)
SI3-SI2-C19-H19A	65.3(4)	SI3-SI2-C19-H19B	-175.8(3)
SI3-SI2-C19-H19C	-52.2(4)	C20-SI2-C19-H19A	-175.6(4)
C20-SI2-C19-H19B	-56.6(5)	C20-SI2-C19-H19C	67.0(5)
SI1-SI2-C20-H20A	-60.4(5)	SI1-SI2-C20-H20B	61.3(4)
SI1-SI2-C20-H20C	179.3(4)	SI3-SI2-C20-H20A	176.3(4)
SI3-SI2-C20-H20B	-62.0(5)	SI3-SI2-C20-H20C	56.0(5)
C19-SI2-C20-H20A	55.8(6)	C19-SI2-C20-H20B	177.6(4)
C19-SI2-C20-H20C	-64.5(5)	SI2-SI3-SI4-SI5	177.96(7)
SI2-SI3-SI4-C23	-61.7(2)	SI2-SI3-SI4-C24	56.1(2)
C21-SI3-SI4-SI5	-59.1(2)	C21-SI3-SI4-C23	61.3(2)
C21-SI3-SI4-C24	179.1(2)	C22-SI3-SI4-SI5	58.4(2)
C22-SI3-SI4-C23	178.8(2)	C22-SI3-SI4-C24	-63.4(3)
SI2-SI3-C21-H21A	-57.1(4)	SI2-SI3-C21-H21B	58.6(4)
SI2-SI3-C21-H21C	179.7(3)	SI4-SI3-C21-H21A	-179.5(3)
SI4-SI3-C21-H21B	-63.8(4)	SI4-SI3-C21-H21C	57.3(4)
C22-SI3-C21-H21A	62.1(4)	C22-SI3-C21-H21B	177.8(3)
C22-SI3-C21-H21C	-61.1(5)	SI2-SI3-C22-H22A	-60.9(4)
SI2-SI3-C22-H22B	59.2(4)	SI2-SI3-C22-H22C	-179.0(4)
SI4-SI3-C22-H22A	60.1(4)	SI4-SI3-C22-H22B	-179.7(3)
SI4-SI3-C22-H22C	-58.0(5)	C21-SI3-C22-H22A	177.8(4)
C21-SI3-C22-H22B	-62.0(4)	C21-SI3-C22-H22C	59.7(5)
SI3-SI4-SI5-SI6	177.38(7)	SI3-SI4-SI5-C25	55.0(2)
SI3-SI4-SI5-C26	-64.7(2)	C23-SI4-SI5-SI6	57.4(2)
C23-SI4-SI5-C25	-65.0(3)	C23-SI4-SI5-C26	175.3(3)
C24-SI4-SI5-SI6	-61.0(2)	C24-SI4-SI5-C25	176.6(2)
C24-SI4-SI5-C26	56.9(3)	SI3-SI4-C23-H23A	-58.9(4)
SI3-SI4-C23-H23B	60.8(4)	SI3-SI4-C23-H23C	178.7(3)
SI5-SI4-C23-H23A	62.9(4)	SI5-SI4-C23-H23B	-177.4(3)
SI5-SI4-C23-H23C	-59.5(4)	C24-SI4-C23-H23A	-177.6(3)
C24-SI4-C23-H23B	-57.9(4)	C24-SI4-C23-H23C	60.0(4)
SI3-SI4-C24-H24A	-59.0(4)	SI3-SI4-C24-H24B	62.4(4)

SI3-SI4-C24-H24C	178.4(3)	SI5-SI4-C24-H24A	178.2(4)
SI5-SI4-C24-H24B	-60.3(4)	SI5-SI4-C24-H24C	55.6(4)
C23-SI4-C24-H24A	59.1(5)	C23-SI4-C24-H24B	-179.5(3)
C23-SI4-C24-H24C	-63.5(4)	SI4-SI5-SI6-C1	-55.0(2)
SI4-SI5-SI6-C27	66.5(2)	SI4-SI5-SI6-C28	-175.3(2)
C25-SI5-SI6-C1	68.5(2)	C25-SI5-SI6-C27	-170.1(2)
C25-SI5-SI6-C28	-51.9(2)	C26-SI5-SI6-C1	-175.2(2)
C26-SI5-SI6-C27	-53.8(2)	C26-SI5-SI6-C28	64.4(3)
SI4-SI5-C25-H25A	-60.8(4)	SI4-SI5-C25-H25B	59.9(4)
SI4-SI5-C25-H25C	-179.7(3)	SI6-SI5-C25-H25A	175.4(3)
SI6-SI5-C25-H25B	-63.8(4)	SI6-SI5-C25-H25C	56.6(4)
C26-SI5-C25-H25A	60.2(4)	C26-SI5-C25-H25B	-179.0(3)
C26-SI5-C25-H25C	-58.7(4)	SI4-SI5-C26-H26A	-58.4(4)
SI4-SI5-C26-H26B	58.5(4)	SI4-SI5-C26-H26C	-179.6(4)
SI6-SI5-C26-H26A	62.8(4)	SI6-SI5-C26-H26B	179.7(3)
SI6-SI5-C26-H26C	-58.4(5)	C25-SI5-C26-H26A	-180.0(3)
C25-SI5-C26-H26B	-63.1(4)	C25-SI5-C26-H26C	58.8(5)
SI5-SI6-C1-C2	-56.8(3)	SI5-SI6-C1-H1A	-179.8(3)
SI5-SI6-C1-H1B	66.1(4)	C27-SI6-C1-C2	-178.7(3)
C27-SI6-C1-H1A	58.3(4)	C27-SI6-C1-H1B	-55.9(4)
C28-SI6-C1-C2	63.9(4)	C28-SI6-C1-H1A	-59.1(4)
C28-SI6-C1-H1B	-173.3(3)	SI5-SI6-C27-H27A	-59.6(4)
SI5-SI6-C27-H27B	58.8(4)	SI5-SI6-C27-H27C	-179.5(3)
C1-SI6-C27-H27A	64.7(4)	C1-SI6-C27-H27B	-176.9(4)
C1-SI6-C27-H27C	-55.3(4)	C28-SI6-C27-H27A	-178.1(4)
C28-SI6-C27-H27B	-59.6(5)	C28-SI6-C27-H27C	62.0(4)
SI5-SI6-C28-H28A	-61.0(5)	SI5-SI6-C28-H28B	60.8(5)
SI5-SI6-C28-H28C	-179.8(3)	C1-SI6-C28-H28A	175.5(4)
C1-SI6-C28-H28B	-62.7(5)	C1-SI6-C28-H28C	56.7(5)
C27-SI6-C28-H28A	57.9(5)	C27-SI6-C28-H28B	179.7(4)
C27-SI6-C28-H28C	-60.8(4)	C4-S1-C3-C2	81.1(4)
C4-S1-C3-H3A	-158.3(4)	C4-S1-C3-H3B	-42.1(5)
C3-S1-C4-C5	179.2(4)	C3-S1-C4-C6	-65.7(5)
C3-S1-C4-C7	59.2(5)	C14-S2-C13-C10	66.0(4)
C14-S2-C13-C11	-177.3(4)	C14-S2-C13-C12	-59.2(5)
C13-S2-C14-C15	78.1(4)	C13-S2-C14-H14A	-43.3(4)
C13-S2-C14-H14B	-159.8(3)	SI6-C1-C2-C3	173.5(3)
SI6-C1-C2-H2A	54.2(5)	SI6-C1-C2-H2B	-63.1(5)
H1A-C1-C2-C3	-63.0(5)	H1A-C1-C2-H2A	177.8(4)
H1A-C1-C2-H2B	60.4(5)	H1B-C1-C2-C3	50.9(5)
H1B-C1-C2-H2A	-68.3(5)	H1B-C1-C2-H2B	174.3(4)
C1-C2-C3-S1	175.6(3)	C1-C2-C3-H3A	54.0(5)
C1-C2-C3-H3B	-61.0(6)	H2A-C2-C3-S1	-64.4(4)
H2A-C2-C3-H3A	174.0(4)	H2A-C2-C3-H3B	59.0(6)
H2B-C2-C3-S1	51.6(5)	H2B-C2-C3-H3A	-70.1(5)
H2B-C2-C3-H3B	175.0(5)	S1-C4-C5-C8	179.0(4)
S1-C4-C5-H5A	64.9(7)	S1-C4-C5-H5B	-64.9(6)
C6-C4-C5-C8	44.3(3)	C6-C4-C5-H5A	-69.8(5)
C6-C4-C5-H5B	160.4(4)	C7-C4-C5-C8	-42.6(3)
C7-C4-C5-H5A	-156.6(5)	C7-C4-C5-H5B	73.5(5)
S1-C4-C6-C8	-175.7(4)	S1-C4-C6-H6A	67.7(6)
S1-C4-C6-H6B	-61.3(7)	C5-C4-C6-C8	-44.4(3)
C5-C4-C6-H6A	-161.0(4)	C5-C4-C6-H6B	69.9(5)
C7-C4-C6-C8	43.2(3)	C7-C4-C6-H6A	-73.4(5)
C7-C4-C6-H6B	157.6(5)	S1-C4-C7-C8	176.8(4)
S1-C4-C7-H7A	63.6(7)	S1-C4-C7-H7B	-69.8(7)
C5-C4-C7-C8	42.7(3)	C5-C4-C7-H7A	-70.5(6)
C5-C4-C7-H7B	156.1(5)	C6-C4-C7-C8	-43.2(3)
C6-C4-C7-H7A	-156.4(5)	C6-C4-C7-H7B	70.2(6)
C4-C5-C8-C6	-44.7(4)	C4-C5-C8-C7	42.2(3)
C4-C5-C8-C9	-177.8(5)	H5A-C5-C8-C6	68.4(5)
H5A-C5-C8-C7	155.4(5)	H5A-C5-C8-C9	-64.6(7)
H5B-C5-C8-C6	-159.4(6)	H5B-C5-C8-C7	-72.4(6)
H5B-C5-C8-C9	67.6(8)	C4-C6-C8-C5	44.4(4)

C4-C6-C8-C7	-42.9(3)	C4-C6-C8-C9	-177.2(5)
H6A-C6-C8-C5	160.6(6)	H6A-C6-C8-C7	73.3(6)
H6A-C6-C8-C9	-61.0(7)	H6B-C6-C8-C5	-71.0(5)
H6B-C6-C8-C7	-158.3(5)	H6B-C6-C8-C9	67.4(6)
C4-C7-C8-C5	-42.8(3)	C4-C7-C8-C6	43.7(3)
C4-C7-C8-C9	175.0(5)	H7A-C7-C8-C5	73.0(5)
H7A-C7-C8-C6	159.4(5)	H7A-C7-C8-C9	-69.2(6)
H7B-C7-C8-C5	-157.6(5)	H7B-C7-C8-C6	-71.2(5)
H7B-C7-C8-C9	60.2(7)	C5-C8-C9-C10	76.9(7)
C5-C8-C9-C11	-47.2(8)	C5-C8-C9-C12	-165.7(5)
C6-C8-C9-C10	-41.7(7)	C6-C8-C9-C11	-165.8(5)
C6-C8-C9-C12	75.7(6)	C7-C8-C9-C10	-157.3(5)
C7-C8-C9-C11	78.6(7)	C7-C8-C9-C12	-39.9(7)
C8-C9-C10-C13	176.3(5)	C8-C9-C10-H10A	60.9(6)
C8-C9-C10-H10B	-68.1(7)	C11-C9-C10-C13	-43.3(3)
C11-C9-C10-H10A	-158.8(4)	C11-C9-C10-H10B	72.3(5)
C12-C9-C10-C13	43.7(3)	C12-C9-C10-H10A	-71.8(5)
C12-C9-C10-H10B	159.3(5)	C8-C9-C11-C13	-177.4(5)
C8-C9-C11-H11A	65.6(8)	C8-C9-C11-H11B	-63.1(6)
C10-C9-C11-C13	43.6(3)	C10-C9-C11-H11A	-73.4(6)
C10-C9-C11-H11B	157.9(4)	C12-C9-C11-C13	-44.2(3)
C12-C9-C11-H11A	-161.1(6)	C12-C9-C11-H11B	70.2(5)
C8-C9-C12-C13	-178.9(5)	C8-C9-C12-H12H	66.5(6)
C8-C9-C12-H12B	-63.3(7)	C10-C9-C12-C13	-43.5(3)
C10-C9-C12-H12H	-158.1(5)	C10-C9-C12-H12B	72.1(5)
C11-C9-C12-C13	43.8(3)	C11-C9-C12-H12H	-70.8(5)
C11-C9-C12-H12B	159.4(5)	C9-C10-C13-S2	175.4(4)
C9-C10-C13-C11	43.5(3)	C9-C10-C13-C12	-43.2(3)
H10A-C10-C13-S2	-68.8(7)	H10A-C10-C13-C11	159.3(5)
H10A-C10-C13-C12	72.6(6)	H10B-C10-C13-S2	59.2(6)
H10B-C10-C13-C11	-72.7(6)	H10B-C10-C13-C12	-159.4(5)
C9-C11-C13-S2	-178.7(4)	C9-C11-C13-C10	-43.6(3)
C9-C11-C13-C12	43.7(3)	H11A-C11-C13-S2	-63.9(6)
H11A-C11-C13-C10	71.2(5)	H11A-C11-C13-C12	158.5(4)
H11B-C11-C13-S2	68.5(7)	H11B-C11-C13-C10	-156.4(5)
H11B-C11-C13-C12	-69.1(5)	C9-C12-C13-S2	-176.6(4)
C9-C12-C13-C10	43.6(3)	C9-C12-C13-C11	-44.0(3)
H12H-C12-C13-S2	-62.4(6)	H12H-C12-C13-C10	157.9(4)
H12H-C12-C13-C11	70.3(5)	H12B-C12-C13-S2	69.0(6)
H12B-C12-C13-C10	-70.8(5)	H12B-C12-C13-C11	-158.4(4)
S2-C14-C15-C16	172.0(3)	S2-C14-C15-H15A	49.8(5)
S2-C14-C15-H15B	-67.6(5)	H14A-C14-C15-C16	-65.8(5)
H14A-C14-C15-H15A	172.1(4)	H14A-C14-C15-H15B	54.7(5)
H14B-C14-C15-C16	48.3(5)	H14B-C14-C15-H15A	-73.9(5)
H14B-C14-C15-H15B	168.8(4)	C14-C15-C16-SI1	177.1(3)
C14-C15-C16-H16A	54.2(5)	C14-C15-C16-H16B	-59.0(5)
H15A-C15-C16-SI1	-60.7(5)	H15A-C15-C16-H16A	176.4(4)
H15A-C15-C16-H16B	63.2(5)	H15B-C15-C16-SI1	56.3(5)
H15B-C15-C16-H16A	-66.6(5)	H15B-C15-C16-H16B	-179.8(4)