

Supporting Information for

Reaction of Optically Active ζ -Aminoallenylstannanes with Aldehydes Formed in situ from the Lewis-acid Catalyzed Rearrangement of Epoxides

*Cristóbal de los Ríos, Louis S. Hegedus**

Department of Chemistry, Colorado State University, Fort Collins, CO 80523

Table of Contents

	Table of Contents		S1
	Experimental Details		S2
	¹ H NMR spectrum	6b	S3
	¹³ C NMR spectrum	6b	S4
	¹ H NMR spectrum	6d	S5
	¹³ C NMR spectrum	6d	S6
Table 1	Crystal Data	6f	S7
Table 2	Atomic Coordinates	6f	S8
“	“	6f	S9
“	“	6f	S10
Table 3	Bond Lengths and Angles	6f	S11
“	“	6f	S12
“	“	6f	S13
Table 4	Anisotropic Displacement	6f	S14
“	“	6f	S15
“	“	6f	S16
Table 5	Hydrogen Coordinates	6f	S17
“	“	6f	S18
	ORTEP	6f	S19
	“	6f	S20
	“	6f	S21

Experimental Details

Methylene chloride was distilled under a nitrogen atmosphere over calcium hydride. Boron trifluoride etherate was purchased from Aldrich and then distilled under a nitrogen atmosphere over calcium hydride. Oxiranes **6a**, **6g** and **6h** were purchased from Aldrich; oxirane **6b** was purchased from Lancaster. Oxiranes **6c**, **6e**, **6f**,¹ **6f'**, **6i**² and **6j**³ were prepared following the procedure described by Ley *et al.*⁴ using *m*-CPBA in CH₂Cl₂ as oxidant. Oxirane **6d** was prepared following the procedure described by Michnick *et al.*⁵ NMR spectra were run in CDCl₃, and recorded at 25 °C in 5mm tubes, at 300 MHz (¹H) or at 100.1 MHz (¹³C). Proton chemical shifts are given in ppm relative to CDCl₃ (7.26 ppm) and carbon shifts are relative to CDCl₃ (77.0 ppm). Column chromatography was performed with Sorben 32-63 σ m, 60Å silica gel standard grade using flash column techniques. All reactions were carried out under a nitrogen atmosphere. Diastereomeric excess was determined by analysis of the crude ¹H NMR spectra.

References

- (1) Fujisawa, T.; Takemura, I.; Ukaji, Y. *Tetrahedron Lett.* **1990**, *31*, 5479.
- (2) Fringuelli, F.; Germani, R.; Pizzo, F.; Savalli, G. *Tetrahedron Lett.* **1989**, *30*, 1427-1428.
- (3) For the synthesis of 1-phenylcyclopentene, see: Mazzocchi, P.H.; Kim, C.H. *J. Med. Chem.* **1982**, *25*, 1473-1476.
- (4) Ley, S.V.; Mitchell, C.; Pears, D.; Ramarao, C.; Yu, J.-Q.; Zhou, W. *Org. Lett.* **2003**, *5*, 4665-4668 and references therein.
- (5) Michnick, T.J.; Matteson, D.S. *Synlett* **1991**, *9*, 631-632.

STANDARD 1H OBSERVE

Solvent: CDCl3
Ambient temperature
File: cr273423
INOVA-500 "1sh"

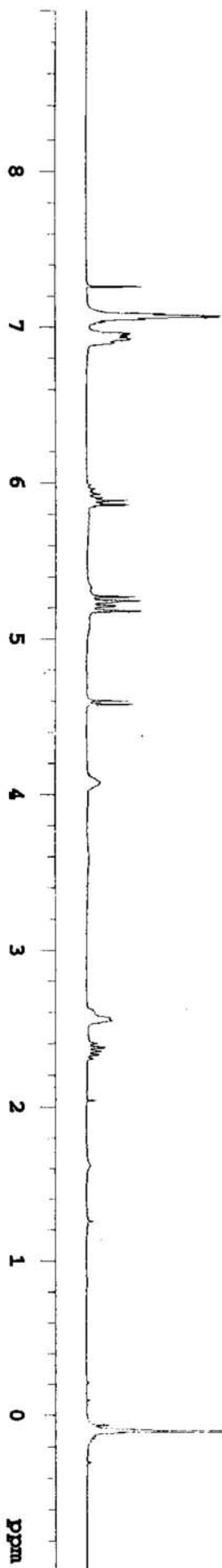
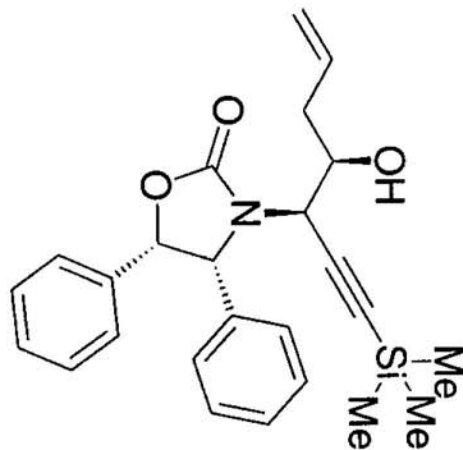
PULSE SEQUENCE

Relax. delay 1.000 sec
Pulse 38.9 degrees
Acq. time 2.732 sec
Width 6000.6 Hz
24 repetitions

OBSERVE H1, 300.1149292 MHz

DATA PROCESSING

Gauss apodization 0.824 sec
FT size 65536
Total time 1 minutes



13C OBSERVE

Pulse Sequence: zgpg30

Solvent: CDCl3

Ambient temperature

INOVA-300 "elfin"

Relax. delay 1.100 sec

Pulse 42.4 degrees

Acq. time 0.800 sec

Width 20000.0 Hz

3072 repetitions

OBSERVE C13, 75.4639595 MHz

DECOUPLE H1, 300.1164227 MHz

Power 32 dB

continuously on

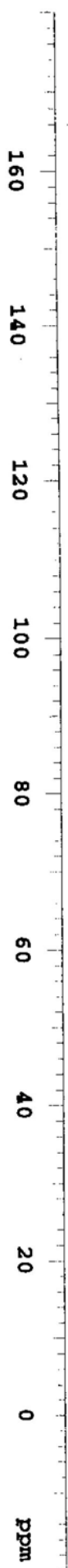
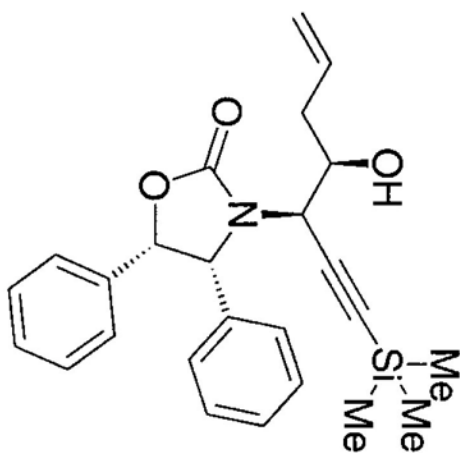
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 32768

Total time 530 hr, 13 min, 56 sec



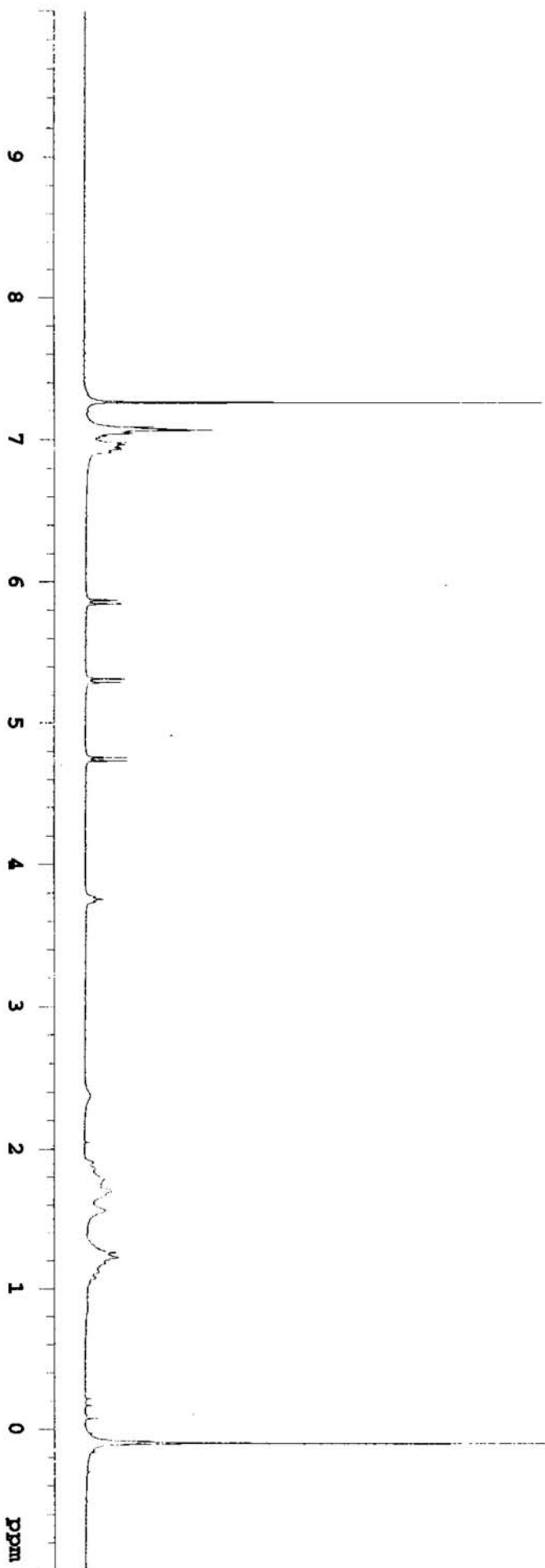
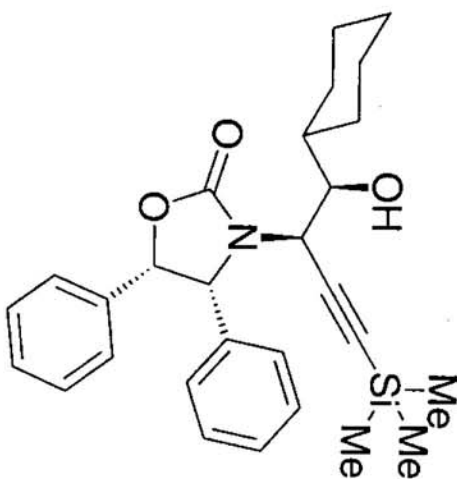
STANDARD 1H OBSERVE

Solvent: CDCl3
 Ambient temperature
 File: cr242f9
 INOVA-500 "1sh"

PULSE SEQUENCE

Relax. delay 0.000 sec
 Pulse 28.7 degrees
 Acq. time 2.667 sec
 Width 6000.0 Hz
 56 repetitions

OBSERVE H1, 300.1592102 MHz
 DATA PROCESSING
 Gauss apodization 0.896 sec
 FT size 32768
 Total time 2 minutes



13C OBSERVE

Pulse Sequence: zgpg30

Solvent: CDCl3

Ambient temperature

INNOVA-300 "elfin"

Relax. delay 1.100 sec

Pulse 42.4 degrees

Acq. time 0.800 sec

Width 20000.0 Hz

2432 repetitions

OBSERVE C13, 75.4639595 MHz

DECOUPLE H1, 300.1164227 MHz

Power 32 dB

continuously on

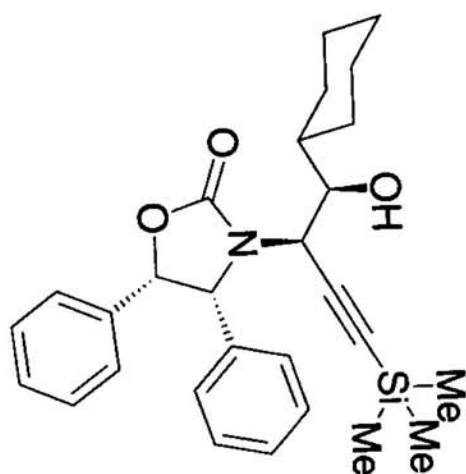
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 32768

Total time 530 hr, 13 min, 56 sec



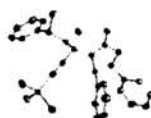


Table 1. Crystal data and structure refinement for lsh156.

Identification code	lsh156, CR258	
Empirical formula	C ₃₀ H ₃₃ N O ₃ Si	
Formula weight	483.66	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 11.699(8) Å	α = 90°.
	b = 17.054(10) Å	β = 107.790(16)°.
	c = 14.580(9) Å	γ = 90°.
Volume	2770(3) Å ³	
Z	4	
Density (calculated)	1.160 Mg/m ³	
Absorption coefficient	0.114 mm ⁻¹	
F(000)	1032	
Crystal size	0.44 x 0.21 x 0.07 mm ³	
Theta range for data collection	1.47 to 26.51°.	
Index ranges	-14 ≤ h ≤ 14, -21 ≤ k ≤ 20, -18 ≤ l ≤ 18	
Reflections collected	23589	
Independent reflections	10692 [R(int) = 0.0906]	
Completeness to theta = 26.51°	97.9 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9920 and 0.9514	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	10692 / 1 / 642	
Goodness-of-fit on F ²	0.963	
Final R indices [I > 2σ(I)]	R1 = 0.0550, wR2 = 0.1067	
R indices (all data)	R1 = 0.1066, wR2 = 0.1275	
Absolute structure parameter	-0.10(12)	
Extinction coefficient	0.0238(11)	
Largest diff. peak and hole	0.314 and -0.276 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for lsh156. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{\dagger} tensor.

	x	y	z	$U(\text{eq})$
Si(1)	6189(1)	237(1)	9395(1)	28(1)
Si(2)	6346(1)	3037(1)	5044(1)	30(1)
O(1)	2108(2)	1973(1)	10875(2)	27(1)
O(2)	1571(2)	3071(1)	8947(2)	29(1)
O(3)	301(2)	2080(1)	8315(2)	28(1)
O(4)	11175(2)	4501(2)	7844(2)	35(1)
O(5)	9107(2)	5750(1)	8639(2)	32(1)
O(6)	9088(2)	4758(1)	9663(2)	29(1)
N(1)	2209(2)	1786(2)	9044(2)	22(1)
N(2)	8930(2)	4455(2)	8155(2)	26(1)
C(1)	3471(3)	1493(2)	13013(3)	32(1)
C(2)	3518(4)	1064(2)	13831(3)	39(1)
C(3)	4452(4)	544(2)	14197(3)	40(1)
C(4)	5315(4)	457(2)	13735(3)	39(1)
C(5)	5255(3)	885(2)	12912(3)	33(1)
C(6)	4326(3)	1412(2)	12535(3)	28(1)
C(7)	4279(3)	1865(2)	11634(3)	28(1)
C(8)	4308(4)	2752(2)	11804(3)	36(1)
C(9)	3173(3)	1627(2)	10796(2)	23(1)
C(10)	3335(3)	1866(2)	9810(2)	23(1)
C(11)	4294(3)	1383(2)	9633(3)	25(1)
C(12)	5060(3)	945(2)	9545(3)	27(1)
C(13)	6116(3)	-616(2)	10152(3)	37(1)
C(14)	7713(3)	681(2)	9822(3)	43(1)
C(15)	5765(4)	-12(3)	8103(3)	45(1)
C(16)	1405(3)	2378(2)	8804(2)	24(1)
C(17)	338(3)	1240(2)	8480(3)	25(1)
C(18)	-554(3)	816(2)	7686(3)	25(1)
C(19)	-1074(3)	1151(2)	6786(3)	33(1)
C(20)	-1865(3)	707(2)	6072(3)	36(1)
C(21)	-2122(3)	-60(2)	6229(3)	35(1)

C(22)	-1604(3)	-386(2)	7126(3)	35(1)
C(23)	-832(3)	46(2)	7856(3)	31(1)
C(24)	1674(3)	1029(2)	8646(2)	23(1)
C(25)	2009(3)	805(2)	7751(3)	24(1)
C(26)	2304(4)	1349(2)	7158(3)	38(1)
C(27)	2570(4)	1117(3)	6335(3)	50(1)
C(28)	2542(4)	323(3)	6091(3)	42(1)
C(29)	2252(3)	-211(2)	6682(3)	37(1)
C(30)	1986(3)	18(2)	7501(3)	31(1)
C(31)	12270(4)	3867(3)	6154(3)	41(1)
C(32)	12913(4)	3345(3)	5763(3)	49(1)
C(33)	12369(4)	2962(3)	4922(3)	49(1)
C(34)	11173(4)	3080(3)	4473(3)	52(1)
C(35)	10520(4)	3606(3)	4847(3)	46(1)
C(36)	11058(3)	4014(2)	5703(3)	33(1)
C(37)	10331(3)	4568(2)	6102(3)	33(1)
C(38)	10833(4)	5409(2)	6207(3)	50(1)
C(39)	10208(3)	4258(2)	7061(3)	28(1)
C(40)	8988(3)	4567(2)	7176(3)	26(1)
C(41)	8022(3)	4140(2)	6475(3)	27(1)
C(42)	7356(3)	3721(2)	5884(3)	29(1)
C(43)	7214(4)	2568(2)	4312(3)	38(1)
C(44)	5850(3)	2294(2)	5773(3)	36(1)
C(45)	5057(3)	3609(2)	4279(3)	41(1)
C(46)	9050(3)	5051(2)	8779(3)	27(1)
C(47)	9313(3)	3905(2)	9644(3)	28(1)
C(48)	8866(3)	3484(2)	10371(3)	31(1)
C(49)	7776(3)	3644(2)	10530(3)	37(1)
C(50)	7385(4)	3191(3)	11173(3)	40(1)
C(51)	8084(4)	2576(3)	11651(3)	50(1)
C(52)	9170(4)	2413(3)	11500(3)	50(1)
C(53)	9562(4)	2868(2)	10863(3)	41(1)
C(54)	8720(3)	3711(2)	8568(3)	25(1)
C(55)	7408(3)	3493(2)	8330(3)	26(1)
C(56)	6505(3)	4050(2)	8126(3)	31(1)
C(57)	5332(3)	3827(2)	8024(3)	35(1)

C(58)	5042(4)	3053(3)	8120(3)	40(1)
C(59)	5938(4)	2491(2)	8290(3)	40(1)
C(60)	7115(3)	2710(2)	8390(3)	32(1)

Table 3. Bond lengths [Å] and angles [°] for lsh156.

Si(1)-C(13)	1.842(4)	C(11)-C(12)	1.204(5)
Si(1)-C(15)	1.845(4)	C(17)-C(18)	1.487(5)
Si(1)-C(12)	1.851(4)	C(17)-C(24)	1.549(5)
Si(1)-C(14)	1.860(4)	C(18)-C(19)	1.389(5)
Si(2)-C(42)	1.836(4)	C(18)-C(23)	1.393(5)
Si(2)-C(45)	1.855(4)	C(19)-C(20)	1.388(5)
Si(2)-C(44)	1.858(4)	C(20)-C(21)	1.376(5)
Si(2)-C(43)	1.864(4)	C(21)-C(22)	1.379(6)
O(1)-C(9)	1.414(4)	C(22)-C(23)	1.381(5)
O(2)-C(16)	1.205(4)	C(24)-C(25)	1.522(5)
O(3)-C(16)	1.369(4)	C(25)-C(26)	1.382(5)
O(3)-C(17)	1.451(4)	C(25)-C(30)	1.389(5)
O(4)-C(39)	1.403(4)	C(26)-C(27)	1.386(6)
O(5)-C(46)	1.213(4)	C(27)-C(28)	1.397(6)
O(6)-C(46)	1.370(5)	C(28)-C(29)	1.366(5)
O(6)-C(47)	1.479(4)	C(29)-C(30)	1.379(5)
N(1)-C(16)	1.352(4)	C(31)-C(36)	1.392(5)
N(1)-C(10)	1.450(4)	C(31)-C(32)	1.393(6)
N(1)-C(24)	1.473(4)	C(32)-C(33)	1.363(6)
N(2)-C(46)	1.343(4)	C(33)-C(34)	1.366(6)
N(2)-C(54)	1.458(4)	C(34)-C(35)	1.394(6)
N(2)-C(40)	1.461(4)	C(35)-C(36)	1.398(6)
C(1)-C(2)	1.386(5)	C(36)-C(37)	1.502(5)
C(1)-C(6)	1.389(5)	C(37)-C(39)	1.541(5)
C(2)-C(3)	1.382(6)	C(37)-C(38)	1.541(6)
C(3)-C(4)	1.382(6)	C(39)-C(40)	1.578(5)
C(4)-C(5)	1.387(5)	C(40)-C(41)	1.466(5)
C(5)-C(6)	1.388(5)	C(41)-C(42)	1.204(5)
C(6)-C(7)	1.510(5)	C(47)-C(48)	1.501(5)
C(7)-C(8)	1.531(5)	C(47)-C(54)	1.546(5)
C(7)-C(9)	1.537(5)	C(48)-C(53)	1.388(5)
C(9)-C(10)	1.560(5)	C(48)-C(49)	1.390(5)
C(10)-C(11)	1.477(5)	C(49)-C(50)	1.395(5)

C(50)-C(51)	1.380(6)	C(55)-C(60)	1.389(5)
C(51)-C(52)	1.383(6)	C(56)-C(57)	1.388(5)
C(52)-C(53)	1.390(6)	C(57)-C(58)	1.380(5)
C(54)-C(55)	1.513(5)	C(58)-C(59)	1.386(6)
C(55)-C(56)	1.383(5)	C(59)-C(60)	1.390(5)
C(13)-Si(1)-C(15)	112.5(2)	C(8)-C(7)-C(9)	111.2(3)
C(13)-Si(1)-C(12)	106.25(18)	O(1)-C(9)-C(7)	112.0(3)
C(15)-Si(1)-C(12)	106.94(18)	O(1)-C(9)-C(10)	108.9(3)
C(13)-Si(1)-C(14)	109.60(19)	C(7)-C(9)-C(10)	110.7(3)
C(15)-Si(1)-C(14)	111.5(2)	N(1)-C(10)-C(11)	111.9(3)
C(12)-Si(1)-C(14)	109.89(18)	N(1)-C(10)-C(9)	110.3(3)
C(42)-Si(2)-C(45)	107.84(18)	C(11)-C(10)-C(9)	109.2(3)
C(42)-Si(2)-C(44)	107.52(18)	C(12)-C(11)-C(10)	174.4(4)
C(45)-Si(2)-C(44)	111.36(19)	C(11)-C(12)-Si(1)	177.5(3)
C(42)-Si(2)-C(43)	107.62(18)	O(2)-C(16)-N(1)	128.8(3)
C(45)-Si(2)-C(43)	111.5(2)	O(2)-C(16)-O(3)	122.1(3)
C(44)-Si(2)-C(43)	110.79(19)	N(1)-C(16)-O(3)	109.1(3)
C(16)-O(3)-C(17)	107.8(3)	O(3)-C(17)-C(18)	111.9(3)
C(46)-O(6)-C(47)	107.3(3)	O(3)-C(17)-C(24)	103.4(3)
C(16)-N(1)-C(10)	121.6(3)	C(18)-C(17)-C(24)	116.3(3)
C(16)-N(1)-C(24)	112.0(3)	C(19)-C(18)-C(23)	119.8(3)
C(10)-N(1)-C(24)	124.3(3)	C(19)-C(18)-C(17)	122.4(3)
C(46)-N(2)-C(54)	112.0(3)	C(23)-C(18)-C(17)	117.7(3)
C(46)-N(2)-C(40)	122.4(3)	C(20)-C(19)-C(18)	118.9(4)
C(54)-N(2)-C(40)	125.5(3)	C(21)-C(20)-C(19)	121.5(4)
C(2)-C(1)-C(6)	122.3(4)	C(20)-C(21)-C(22)	119.1(4)
C(3)-C(2)-C(1)	119.3(4)	C(21)-C(22)-C(23)	120.7(4)
C(4)-C(3)-C(2)	119.3(4)	C(22)-C(23)-C(18)	119.9(4)
C(3)-C(4)-C(5)	120.9(4)	N(1)-C(24)-C(25)	111.5(3)
C(4)-C(5)-C(6)	120.7(4)	N(1)-C(24)-C(17)	98.4(3)
C(5)-C(6)-C(1)	117.5(4)	C(25)-C(24)-C(17)	115.9(3)
C(5)-C(6)-C(7)	119.5(3)	C(26)-C(25)-C(30)	118.2(3)
C(1)-C(6)-C(7)	123.0(3)	C(26)-C(25)-C(24)	123.2(3)
C(6)-C(7)-C(8)	111.8(3)	C(30)-C(25)-C(24)	118.6(3)
C(6)-C(7)-C(9)	110.8(3)	C(25)-C(26)-C(27)	121.0(4)

C(26)-C(27)-C(28)	120.2(4)	N(2)-C(46)-O(6)	109.1(3)
C(29)-C(28)-C(27)	118.5(4)	O(6)-C(47)-C(48)	110.8(3)
C(28)-C(29)-C(30)	121.4(4)	O(6)-C(47)-C(54)	101.7(3)
C(29)-C(30)-C(25)	120.7(4)	C(48)-C(47)-C(54)	118.0(3)
C(36)-C(31)-C(32)	121.4(4)	C(53)-C(48)-C(49)	119.0(4)
C(33)-C(32)-C(31)	120.8(4)	C(53)-C(48)-C(47)	116.9(3)
C(32)-C(33)-C(34)	119.3(4)	C(49)-C(48)-C(47)	124.0(3)
C(33)-C(34)-C(35)	120.7(4)	C(48)-C(49)-C(50)	120.6(4)
C(34)-C(35)-C(36)	121.2(4)	C(51)-C(50)-C(49)	119.7(4)
C(31)-C(36)-C(35)	116.6(4)	C(50)-C(51)-C(52)	120.2(4)
C(31)-C(36)-C(37)	123.1(4)	C(51)-C(52)-C(53)	120.0(4)
C(35)-C(36)-C(37)	120.3(4)	C(48)-C(53)-C(52)	120.5(4)
C(36)-C(37)-C(39)	110.9(3)	N(2)-C(54)-C(55)	114.0(3)
C(36)-C(37)-C(38)	112.4(3)	N(2)-C(54)-C(47)	98.8(3)
C(39)-C(37)-C(38)	111.5(3)	C(55)-C(54)-C(47)	113.2(3)
O(4)-C(39)-C(37)	111.2(3)	C(56)-C(55)-C(60)	119.1(3)
O(4)-C(39)-C(40)	110.2(3)	C(56)-C(55)-C(54)	122.4(3)
C(37)-C(39)-C(40)	108.7(3)	C(60)-C(55)-C(54)	118.3(3)
N(2)-C(40)-C(41)	111.1(3)	C(55)-C(56)-C(57)	120.1(4)
N(2)-C(40)-C(39)	112.0(3)	C(58)-C(57)-C(56)	121.1(4)
C(41)-C(40)-C(39)	106.8(3)	C(57)-C(58)-C(59)	118.9(4)
C(42)-C(41)-C(40)	170.7(4)	C(58)-C(59)-C(60)	120.3(4)
C(41)-C(42)-Si(2)	176.5(3)	C(55)-C(60)-C(59)	120.5(4)
O(5)-C(46)-N(2)	128.9(4)		
O(5)-C(46)-O(6)	122.0(3)		

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for lsh156. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si(1)	23(1)	28(1)	33(1)	1(1)	8(1)	5(1)
Si(2)	29(1)	28(1)	31(1)	-4(1)	7(1)	-2(1)
O(1)	24(1)	25(1)	35(2)	5(1)	14(1)	4(1)
O(2)	30(1)	18(1)	34(2)	0(1)	5(1)	3(1)
O(3)	22(1)	23(1)	34(2)	-5(1)	3(1)	2(1)
O(4)	29(2)	34(2)	38(2)	3(1)	3(1)	-1(1)
O(5)	29(2)	24(2)	44(2)	-8(1)	11(1)	-3(1)
O(6)	30(2)	26(1)	30(2)	-10(1)	9(1)	-1(1)
N(1)	21(2)	17(2)	25(2)	-4(1)	3(1)	2(1)
N(2)	27(2)	21(2)	28(2)	-5(1)	6(1)	2(1)
C(1)	35(2)	32(2)	28(2)	-1(2)	7(2)	-1(2)
C(2)	44(3)	41(3)	31(2)	-5(2)	12(2)	-11(2)
C(3)	57(3)	28(2)	29(2)	4(2)	5(2)	-2(2)
C(4)	47(3)	25(2)	37(3)	0(2)	-1(2)	3(2)
C(5)	32(2)	30(2)	31(2)	-6(2)	2(2)	-2(2)
C(6)	31(2)	25(2)	23(2)	-4(2)	2(2)	-1(2)
C(7)	25(2)	29(2)	29(2)	2(2)	6(2)	-2(2)
C(8)	49(3)	28(2)	29(2)	-3(2)	9(2)	-13(2)
C(9)	18(2)	20(2)	33(2)	0(2)	11(2)	3(2)
C(10)	21(2)	18(2)	29(2)	-1(2)	5(2)	0(2)
C(11)	22(2)	26(2)	26(2)	1(2)	6(2)	-3(2)
C(12)	22(2)	27(2)	32(2)	-1(2)	8(2)	-6(2)
C(13)	31(2)	32(2)	48(3)	5(2)	10(2)	5(2)
C(14)	24(2)	48(3)	56(3)	1(2)	12(2)	3(2)
C(15)	43(3)	51(3)	42(3)	-4(2)	15(2)	12(2)
C(16)	20(2)	30(2)	23(2)	-2(2)	6(2)	6(2)
C(17)	26(2)	23(2)	27(2)	-2(2)	9(2)	1(2)
C(18)	23(2)	26(2)	28(2)	-6(2)	9(2)	0(2)
C(19)	33(2)	26(2)	35(2)	-5(2)	4(2)	0(2)
C(20)	30(2)	39(3)	31(2)	-6(2)	-1(2)	5(2)
C(21)	28(2)	40(3)	36(3)	-15(2)	10(2)	-6(2)

C(22)	34(2)	32(2)	38(3)	-5(2)	13(2)	-9(2)
C(23)	27(2)	36(2)	27(2)	0(2)	7(2)	-1(2)
C(24)	23(2)	19(2)	24(2)	1(2)	2(2)	1(2)
C(25)	17(2)	26(2)	29(2)	-1(2)	6(2)	1(2)
C(26)	56(3)	28(2)	36(3)	-3(2)	21(2)	-3(2)
C(27)	71(3)	41(3)	44(3)	2(2)	29(2)	-5(2)
C(28)	49(3)	47(3)	36(2)	-13(2)	20(2)	-5(2)
C(29)	40(2)	30(2)	42(3)	-13(2)	15(2)	1(2)
C(30)	35(2)	22(2)	38(2)	-1(2)	13(2)	-3(2)
C(31)	33(2)	58(3)	30(2)	1(2)	9(2)	10(2)
C(32)	41(3)	64(3)	45(3)	9(3)	19(2)	24(2)
C(33)	62(3)	41(3)	49(3)	4(2)	27(3)	8(2)
C(34)	55(3)	50(3)	55(3)	-15(3)	24(3)	-13(3)
C(35)	31(2)	59(3)	46(3)	1(2)	8(2)	-1(2)
C(36)	25(2)	35(2)	41(3)	4(2)	13(2)	1(2)
C(37)	27(2)	38(2)	35(2)	11(2)	11(2)	5(2)
C(38)	59(3)	34(2)	68(3)	14(2)	34(3)	8(2)
C(39)	24(2)	25(2)	34(2)	-6(2)	4(2)	-3(2)
C(40)	29(2)	20(2)	31(2)	-1(2)	10(2)	-1(2)
C(41)	24(2)	24(2)	33(2)	-2(2)	9(2)	6(2)
C(42)	25(2)	29(2)	34(2)	-3(2)	9(2)	0(2)
C(43)	48(3)	34(2)	34(2)	-5(2)	15(2)	-5(2)
C(44)	35(2)	33(2)	37(2)	-3(2)	7(2)	-3(2)
C(45)	36(2)	45(3)	35(2)	-2(2)	0(2)	1(2)
C(46)	18(2)	29(2)	34(2)	-8(2)	6(2)	0(2)
C(47)	25(2)	28(2)	30(2)	-3(2)	7(2)	9(2)
C(48)	30(2)	31(2)	30(2)	-5(2)	8(2)	5(2)
C(49)	32(2)	41(3)	34(2)	-1(2)	6(2)	6(2)
C(50)	37(2)	50(3)	35(2)	-3(2)	15(2)	-4(2)
C(51)	70(4)	41(3)	41(3)	3(2)	22(3)	-5(2)
C(52)	65(3)	41(3)	45(3)	6(2)	20(3)	13(2)
C(53)	41(3)	43(3)	40(3)	-2(2)	13(2)	11(2)
C(54)	25(2)	21(2)	30(2)	0(2)	9(2)	5(2)
C(55)	28(2)	23(2)	24(2)	-1(2)	7(2)	3(2)
C(56)	27(2)	29(2)	32(2)	-1(2)	3(2)	1(2)
C(57)	27(2)	49(3)	27(2)	0(2)	6(2)	-2(2)

C(58)	36(2)	51(3)	35(2)	0(2)	15(2)	-15(2)
C(59)	50(3)	33(3)	36(3)	2(2)	11(2)	-12(2)
C(60)	35(2)	31(2)	27(2)	1(2)	5(2)	0(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for lsh156.

	x	y	z	U(eq)
H(1)	1698	1632	11046	40
H(4)	11336	4151	8269	53
H(1A)	2833	1855	12770	39
H(2)	2914	1128	14137	47
H(3)	4500	248	14760	48
H(4A)	5958	100	13985	47
H(5)	5855	815	12604	39
H(7)	5009	1724	11449	34
H(8A)	3586	2911	11962	54
H(8B)	4337	3025	11219	54
H(8C)	5022	2887	12339	54
H(9)	3085	1045	10807	27
H(10)	3588	2428	9848	27
H(13A)	6302	-449	10825	56
H(13B)	6701	-1011	10098	56
H(13C)	5308	-841	9936	56
H(14A)	7908	809	10508	64
H(14B)	7729	1160	9455	64
H(14C)	8303	307	9728	64
H(15A)	6292	-428	8003	68
H(15B)	5847	454	7734	68
H(15C)	4930	-194	7885	68
H(17)	143	1139	9092	30
H(19)	-890	1675	6662	39
H(20)	-2238	937	5460	43
H(21)	-2649	-360	5727	42
H(22)	-1781	-914	7242	41
H(23)	-490	-181	8475	37
H(24)	1931	609	9145	28
H(26)	2325	1890	7316	46

H(27)	2772	1498	5935	59
H(28)	2720	159	5527	51
H(29)	2235	-753	6526	44
H(30)	1784	-366	7897	37
H(31)	12668	4127	6741	49
H(32)	13739	3256	6087	59
H(33)	12817	2617	4651	58
H(34)	10783	2800	3899	62
H(35)	9694	3689	4515	56
H(37)	9506	4587	5631	40
H(38A)	11686	5401	6580	75
H(38B)	10393	5734	6541	75
H(38C)	10738	5629	5567	75
H(39)	10189	3672	7041	34
H(40)	8908	5139	7017	32
H(43A)	7412	2962	3895	57
H(43B)	6730	2152	3914	57
H(43C)	7956	2343	4741	57
H(44A)	6553	2028	6203	54
H(44B)	5330	1909	5344	54
H(44C)	5404	2554	6158	54
H(45A)	4665	3888	4690	62
H(45B)	4480	3253	3848	62
H(45C)	5344	3990	3896	62
H(47)	10197	3818	9807	33
H(49)	7294	4066	10199	44
H(50)	6642	3305	11281	48
H(51)	7818	2264	12086	59
H(52)	9649	1990	11831	60
H(53)	10311	2756	10765	50
H(54)	9172	3282	8365	30
H(56)	6688	4585	8057	37
H(57)	4718	4213	7886	42
H(58)	4241	2908	8071	48
H(59)	5748	1954	8338	48
H(60)	7723	2321	8499	38

