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Isopropyl 2,5-anhydro-3,4-di-*O*-*tert*-butyldiphenylsilyl-L-ribonate

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Key indicators

Single-crystal X-ray study
T = 190 K
Mean σ(C–C) = 0.003 Å
R factor = 0.050
wR factor = 0.096
Data-to-parameter ratio = 20.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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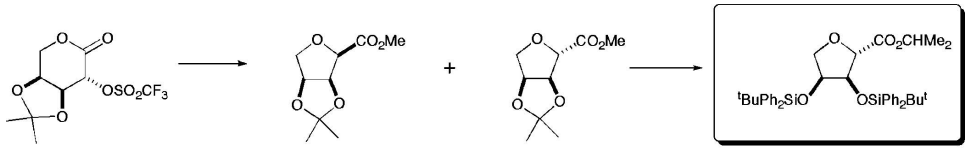
Determination of the crystal structure of the title compound, $C_{40}H_{50}O_5Si_2$, firmly established its relative configuration and hence that of some related tetrahydrofuran carboxylates. The material crystallizes with $Z' = 2$. Except for the chiral centres, the two independent molecules are related by a pseudo-centre of symmetry.

Comment

The reaction of methanol with lactones containing 2-*O*-trifluoromethanesulfonates (trifluoromethanesulfonates) in the presence of either acid (Wheatley *et al.*, 1993) or base (Choi *et al.*, 1992) provides a general synthesis of methyl tetrahydrofuran-2-carboxylates. Such materials have been exploited in the preparation of sugar amino acids (SAAs) for use as peptidomimetics (Chakraborty *et al.*, 2004; Grotenberg *et al.*, 2004; Smith *et al.*, 2003). Many THF SAA scaffolds are predisposed to form secondary structures in short oligomers (Claridge *et al.*, 2005; Long *et al.*, 1999, 2002; Hungerford *et al.*, 2000). There are only limited reports of γ-peptides based on cyclic templates (Curran *et al.*, 1996; Crisma *et al.*, 2001). In a programme directed towards the synthesis of γ-THF SAAs, it was found that reaction of the δ-lactone trifluoromethanesulfonate (1) (Stewart *et al.*, 2002) with methanol in the presence of sodium carbonate gave a mixture of the THF carboxylates (2) and (3). In order to ensure the correct assignment of the stereochemistry at C-2 in the epimers, (3) was converted to the crystalline disilyl ether (4), the structure of which is reported in this paper (Fig. 1).



(1) (2) (3) (4)

The structure of (4) contains two molecules in the asymmetric unit ($Z' = 2$). Except for the 1,4-anhydroribonate units (which are chiral and therefore cannot be related by an improper operator), the molecules are related by a pseudo-centre of symmetry at $(\frac{1}{2},\frac{1}{5},\frac{3}{4})$. The absolute configuration of the material was known unambiguously from the synthesis; the Flack (1983) parameter is in agreement with this assignment.

The structure consists of molecular layers (Fig. 2) lying parallel to the *bc* plane, and characterized by a hydrophilic and a hydrophobic surface. The hydrophobic surface of one layer faces the equivalent surface of the adjacent layer (Fig. 3).

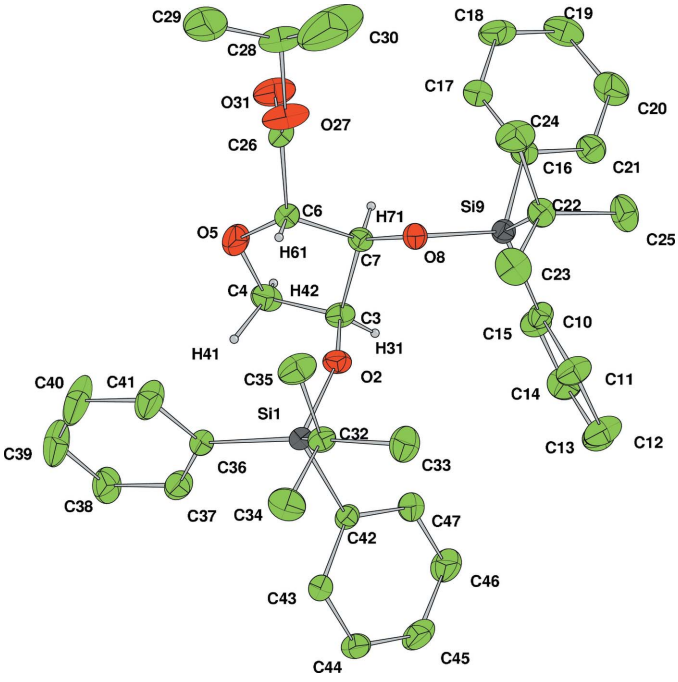


Figure 1
The structure of one molecule of the title compound with displacement ellipsoids drawn at the 50% probability level. All H atoms, except for H31, H41, H61 and H71, have been omitted for clarity. The H atoms are drawn with an arbitary radius.

Experimental

Epimer (3) was converted to the corresponding disilyl ether by standard procedures (Sanjayan *et al.*, 2003) and was crystallized from ethyl acetate–hexane (1:4).

Crystal data

$C_{40}H_{50}O_5Si_2$
M_r = 667.01
Monoclinic, $P2_1$
a = 17.2952 (2) Å
b = 10.7468 (2) Å
c = 20.4914 (4) Å
β = 100.7864 (5)°
V = 3741.40 (11) Å^3
Z = 4
D_x = 1.184 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8312 reflections
θ = 5–30°
μ = 0.14 mm^{-1}
T = 190 K
Prism, colourless
0.40 × 0.20 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (*DENZO*/*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.70, T_{max} = 0.97
27685 measured reflections
17372 independent reflections
17372 reflections with $I > -3\sigma(I)$
R_{int} = 0.027
θ_{max} = 30.0°
$h = -24 \rightarrow 24$
$k = -15 \rightarrow 15$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.096
S = 0.97
17372 reflections
848 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F^2) + (0.02P)^2 + 2.21P]$ where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}
Absolute structure: Flack (1983), 17372 Friedel pairs
Flack parameter: 0.05 (7)

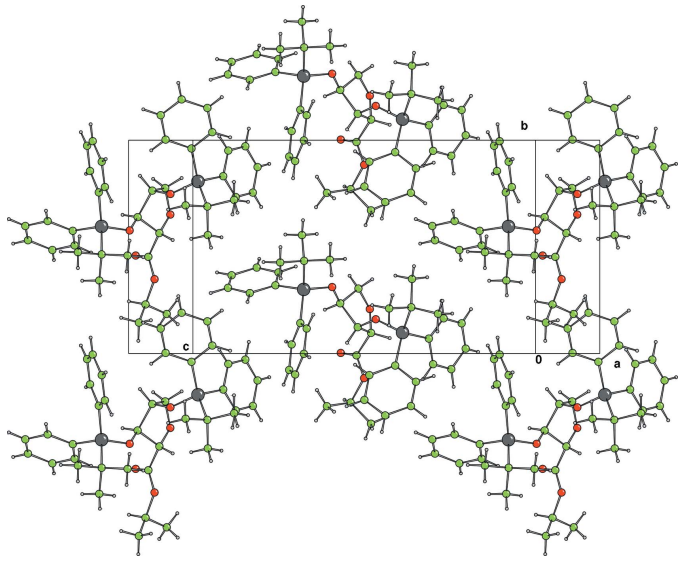


Figure 2
The crystal structure projected on to the *bc* plane.

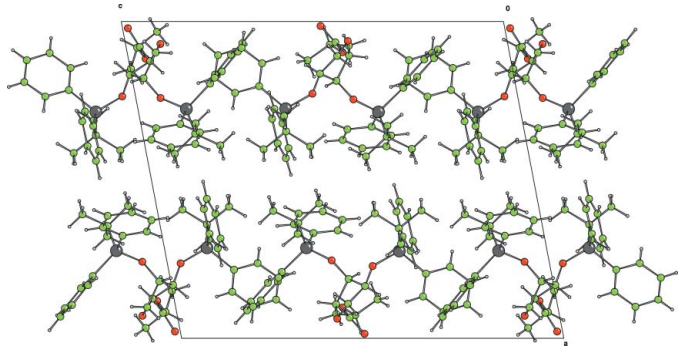


Figure 3
The crystal structure projected along the *b* axis, showing two hydrophobic faces opposing each other. By symmetry, pairs of hydrophilic faces also oppose each other.

The H atoms were all located in a difference map, but those attached to C atoms were repositioned geometrically. The H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C—H = 0.93–98 Å) and displacement parameters [U_{iso}(H) = 1.2–1.5U_{eq}(parent atom)], after which they were refined with riding constraints. The pseudo-centre of inversion did not lead to any refinement problems.

Data collection: *COLLECT* (Nonius, 2001); cell refinement: *DENZO*/*SCALEPACK*; data reduction: *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS*.

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$h = -24 \rightarrow 24$
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Refinement

Refinement on F^2
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$wR(F^2) = 0.096$
$S = 0.97$
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848 parameters
370 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F^2) + (0.02P)^2 + 2.21P]$ where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.70$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}
Absolute structure: Flack (1983), 17372 Friedel pairs
Absolute structure parameter: 0.05 (7)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Si101	0.27529 (3)	0.30044 (6)	0.61323 (3)	0.0217
O102	0.22809 (7)	0.31163 (14)	0.53577 (7)	0.0246

C103	0.16486 (10)	0.23538 (18)	0.50601 (11)	0.0217
C104	0.10903 (11)	0.3046 (2)	0.45241 (11)	0.0282
O105	0.06189 (8)	0.20842 (15)	0.41694 (9)	0.0345
C106	0.10724 (10)	0.0968 (2)	0.42112 (11)	0.0256
C107	0.18749 (10)	0.12338 (18)	0.46664 (10)	0.0200
O108	0.24611 (7)	0.16056 (13)	0.43144 (8)	0.0238
Si109	0.28559 (3)	0.09829 (6)	0.37194 (3)	0.0200
C110	0.33216 (10)	−0.05648 (19)	0.39734 (11)	0.0243
C111	0.34049 (12)	−0.1010 (2)	0.46209 (13)	0.0336
C112	0.37400 (13)	−0.2174 (2)	0.47959 (14)	0.0422
C113	0.40042 (13)	−0.2900 (2)	0.43265 (16)	0.0409
C114	0.39413 (12)	−0.2468 (2)	0.36844 (14)	0.0372
C115	0.35986 (11)	−0.1320 (2)	0.35080 (13)	0.0306
C116	0.20935 (10)	0.06992 (19)	0.29509 (11)	0.0249
C117	0.17521 (14)	0.1650 (2)	0.25346 (14)	0.0449
C118	0.11585 (17)	0.1416 (3)	0.19988 (16)	0.0666
C119	0.08840 (14)	0.0229 (3)	0.18565 (15)	0.0565
C120	0.12005 (12)	−0.0733 (3)	0.22609 (13)	0.0408
C121	0.17941 (11)	−0.0500 (2)	0.27999 (12)	0.0307
C122	0.36373 (11)	0.2169 (2)	0.36274 (12)	0.0264
C123	0.42608 (13)	0.2113 (3)	0.42695 (14)	0.0388
C124	0.32958 (14)	0.3495 (2)	0.35564 (15)	0.0405
C125	0.29827 (17)	0.5551 (2)	0.62102 (18)	0.0505
C148	0.40210 (14)	0.1865 (2)	0.30316 (14)	0.0395
C126	0.06575 (10)	−0.00860 (19)	0.45023 (11)	0.0280
O127	0.09712 (9)	−0.11542 (14)	0.43647 (9)	0.0392
C128	0.07317 (14)	−0.2296 (2)	0.46593 (14)	0.0414
C129	0.1227 (2)	−0.2470 (5)	0.5320 (3)	0.1084
C130	0.0765 (4)	−0.3287 (3)	0.4166 (3)	0.1335
O131	0.01441 (10)	0.00282 (16)	0.48086 (11)	0.0526
C132	0.34696 (12)	0.4345 (2)	0.62344 (13)	0.0310
C133	0.39454 (14)	0.4398 (2)	0.56774 (14)	0.0414
C134	0.40334 (15)	0.4268 (3)	0.69109 (14)	0.0448
C136	0.20439 (11)	0.31981 (19)	0.67144 (11)	0.0254
C137	0.22535 (12)	0.2833 (2)	0.73774 (12)	0.0314
C138	0.17757 (14)	0.3079 (2)	0.78365 (13)	0.0383
C139	0.10643 (14)	0.3670 (2)	0.76361 (15)	0.0452
C140	0.08355 (14)	0.4029 (2)	0.69816 (15)	0.0460
C141	0.13198 (13)	0.3803 (2)	0.65244 (14)	0.0376
C142	0.32126 (11)	0.1427 (2)	0.62873 (11)	0.0255
C143	0.39989 (12)	0.1172 (2)	0.62551 (13)	0.0377
C144	0.43137 (13)	−0.0014 (2)	0.63734 (13)	0.0429
C145	0.38510 (14)	−0.0979 (2)	0.65155 (12)	0.0380
C146	0.30716 (13)	−0.0770 (2)	0.65378 (11)	0.0338
C147	0.27602 (12)	0.0428 (2)	0.64295 (11)	0.0299
H1031	0.1376	0.2056	0.5394	0.0312*
H1041	0.1397	0.3480	0.4233	0.0397*
H1042	0.0772	0.3644	0.4692	0.0400*

H1061	0.1140	0.0722	0.3764	0.0355*
H1071	0.2038	0.0506	0.4953	0.0263*
H1111	0.3233	−0.0524	0.4946	0.0475*
H1121	0.3788	−0.2470	0.5242	0.0598*
H1131	0.4235	−0.3674	0.4446	0.0570*
H1141	0.4138	−0.2959	0.3365	0.0521*
H1151	0.3546	−0.1055	0.3062	0.0426*
H1171	0.1932	0.2471	0.2614	0.0590*
H1181	0.0953	0.2078	0.1737	0.0872*
H1191	0.0486	0.0078	0.1491	0.0747*
H1201	0.0998	−0.1562	0.2170	0.0566*
H1211	0.2018	−0.1190	0.3079	0.0417*
H1231	0.4668	0.2728	0.4252	0.0672*
H1232	0.4509	0.1318	0.4315	0.0664*
H1233	0.4015	0.2263	0.4648	0.0678*
H1241	0.3711	0.4093	0.3573	0.0727*
H1242	0.2942	0.3572	0.3128	0.0727*
H1243	0.3004	0.3650	0.3918	0.0728*
H1281	0.0173	−0.2170	0.4720	0.0623*
H1291	0.1030	−0.3142	0.5558	0.1845*
H1292	0.1743	−0.2726	0.5226	0.1841*
H1293	0.1277	−0.1714	0.5573	0.1853*
H1301	0.0446	−0.3984	0.4247	0.2656*
H1302	0.0602	−0.2953	0.3730	0.2656*
H1303	0.1307	−0.3525	0.4223	0.2660*
H1331	0.4273	0.5142	0.5714	0.0744*
H1332	0.3594	0.4434	0.5249	0.0753*
H1333	0.4280	0.3667	0.5689	0.0745*
H1341	0.4376	0.4988	0.6959	0.0794*
H1342	0.4372	0.3521	0.6953	0.0795*
H1343	0.3727	0.4290	0.7274	0.0797*
H1371	0.2740	0.2420	0.7510	0.0450*
H1381	0.1945	0.2836	0.8290	0.0550*
H1391	0.0710	0.3800	0.7938	0.0669*
H1401	0.0352	0.4432	0.6844	0.0655*
H1411	0.1158	0.4078	0.6075	0.0532*
H1431	0.4336	0.1828	0.6146	0.0538*
H1441	0.4839	−0.0177	0.6323	0.0626*
H1451	0.4055	−0.1784	0.6598	0.0529*
H1461	0.2759	−0.1458	0.6626	0.0479*
H1471	0.2235	0.0561	0.6482	0.0414*
H1251	0.3341	0.6245	0.6241	0.0922*
H1252	0.2621	0.5606	0.5790	0.0916*
H1253	0.2694	0.5575	0.6573	0.0914*
H1481	0.4459	0.2468	0.2991	0.0723*
H1482	0.3638	0.1872	0.2623	0.0736*
H1483	0.4250	0.1035	0.3083	0.0731*
Si1	0.72364 (3)	0.30675 (6)	1.12684 (3)	0.0204

O2	0.75835 (7)	0.24766 (14)	1.06464 (8)	0.0260
C3	0.82073 (11)	0.26353 (19)	1.03004 (12)	0.0255
C4	0.90180 (11)	0.2759 (2)	1.07447 (12)	0.0309
O5	0.92895 (9)	0.15133 (16)	1.09127 (10)	0.0419
C6	0.87482 (11)	0.06489 (19)	1.05594 (11)	0.0262
C7	0.83186 (10)	0.13924 (18)	0.99583 (10)	0.0215
O8	0.76326 (7)	0.07700 (13)	0.96519 (7)	0.0229
Si9	0.71442 (3)	0.09575 (6)	0.88852 (3)	0.0208
C10	0.66986 (11)	0.25538 (19)	0.87472 (11)	0.0236
C11	0.59149 (12)	0.2803 (2)	0.87726 (12)	0.0348
C12	0.56001 (13)	0.3987 (2)	0.86442 (13)	0.0414
C13	0.60653 (14)	0.4952 (2)	0.84966 (12)	0.0371
C14	0.68474 (14)	0.4740 (2)	0.84830 (12)	0.0360
C15	0.71607 (12)	0.3554 (2)	0.86050 (12)	0.0302
C16	0.78341 (10)	0.07544 (18)	0.82865 (11)	0.0245
C17	0.85308 (12)	0.0067 (2)	0.84432 (13)	0.0321
C18	0.90013 (13)	−0.0147 (2)	0.79708 (15)	0.0405
C19	0.87767 (14)	0.0310 (2)	0.73354 (14)	0.0420
C20	0.80865 (14)	0.0981 (2)	0.71612 (13)	0.0404
C21	0.76297 (12)	0.1211 (2)	0.76376 (12)	0.0309
C22	0.64055 (12)	−0.0354 (2)	0.87710 (12)	0.0280
C23	0.59349 (14)	−0.0406 (2)	0.93337 (14)	0.0399
C24	0.68739 (15)	−0.1577 (2)	0.87864 (16)	0.0434
C25	0.58456 (13)	−0.0253 (3)	0.81001 (13)	0.0399
C26	0.91929 (10)	−0.04672 (19)	1.03593 (10)	0.0269
O27	0.88236 (9)	−0.15138 (14)	1.04527 (11)	0.0452
C28	0.91735 (14)	−0.2698 (2)	1.02870 (15)	0.0426
C29	0.9674 (3)	−0.3147 (4)	1.0886 (2)	0.1224
C30	0.8509 (2)	−0.3547 (4)	1.0019 (3)	0.1365
O31	0.97855 (9)	−0.04067 (15)	1.01401 (10)	0.0422
C32	0.64550 (11)	0.18924 (19)	1.13738 (12)	0.0259
C33	0.58200 (13)	0.1943 (2)	1.07413 (15)	0.0386
C34	0.60892 (14)	0.2200 (2)	1.19755 (14)	0.0396
C35	0.67821 (13)	0.0551 (2)	1.14394 (15)	0.0393
C36	0.80372 (10)	0.33135 (19)	1.20143 (11)	0.0252
C37	0.83211 (12)	0.4511 (2)	1.21847 (12)	0.0311
C38	0.89514 (12)	0.4715 (2)	1.27029 (13)	0.0395
C39	0.93142 (14)	0.3739 (3)	1.30614 (14)	0.0527
C40	0.90507 (16)	0.2544 (3)	1.29044 (16)	0.0646
C41	0.84217 (14)	0.2334 (2)	1.23836 (14)	0.0454
C42	0.67599 (10)	0.46124 (19)	1.10335 (11)	0.0232
C43	0.64981 (11)	0.5375 (2)	1.15032 (12)	0.0281
C44	0.61324 (11)	0.6509 (2)	1.13260 (13)	0.0327
C45	0.60239 (13)	0.6909 (2)	1.06750 (16)	0.0395
C46	0.62701 (13)	0.6172 (2)	1.02008 (14)	0.0409
C47	0.66296 (12)	0.5029 (2)	1.03770 (12)	0.0317
H31	0.8099	0.3330	0.9981	0.0353*
H41	0.9003	0.3225	1.1146	0.0440*

H42	0.9368	0.3186	1.0504	0.0445*
H61	0.8380	0.0319	1.0828	0.0346*
H71	0.8700	0.1499	0.9647	0.0290*
H111	0.5578	0.2129	0.8884	0.0487*
H121	0.5055	0.4116	0.8656	0.0588*
H131	0.5852	0.5746	0.8413	0.0519*
H141	0.7181	0.5375	0.8382	0.0517*
H151	0.7695	0.3425	0.8590	0.0445*
H171	0.8684	−0.0266	0.8870	0.0456*
H181	0.9472	−0.0615	0.8081	0.0594*
H191	0.9091	0.0150	0.7022	0.0637*
H201	0.7933	0.1303	0.6730	0.0597*
H211	0.7173	0.1693	0.7523	0.0443*
H231	0.5613	−0.1158	0.9258	0.0723*
H232	0.6271	−0.0484	0.9771	0.0717*
H233	0.5590	0.0293	0.9327	0.0716*
H241	0.6503	−0.2273	0.8742	0.0764*
H242	0.7251	−0.1668	0.9209	0.0763*
H243	0.7162	−0.1589	0.8413	0.0773*
H251	0.5511	−0.0992	0.8046	0.0684*
H252	0.5508	0.0490	0.8086	0.0689*
H253	0.6140	−0.0220	0.7725	0.0685*
H281	0.9427	−0.2555	0.9917	0.0645*
H291	1.0073	−0.3692	1.0765	0.2047*
H292	0.9275	−0.3628	1.1093	0.2041*
H293	0.9889	−0.2487	1.1179	0.2057*
H301	0.8700	−0.4403	1.0034	0.2369*
H302	0.8063	−0.3442	1.0243	0.2373*
H303	0.8342	−0.3322	0.9556	0.2374*
H331	0.5420	0.1350	1.0755	0.0679*
H332	0.5573	0.2752	1.0679	0.0661*
H333	0.6027	0.1747	1.0344	0.0669*
H341	0.5667	0.1604	1.1991	0.0727*
H342	0.6478	0.2112	1.2378	0.0729*
H343	0.5884	0.3041	1.1940	0.0739*
H351	0.6351	−0.0039	1.1449	0.0688*
H352	0.7169	0.0447	1.1836	0.0700*
H353	0.7019	0.0374	1.1068	0.0699*
H371	0.8103	0.5183	1.1929	0.0431*
H381	0.9109	0.5541	1.2814	0.0550*
H391	0.9746	0.3889	1.3415	0.0705*
H401	0.9275	0.1871	1.3145	0.0831*
H411	0.8261	0.1523	1.2278	0.0598*
H431	0.6578	0.5132	1.1955	0.0393*
H441	0.5950	0.7015	1.1651	0.0455*
H451	0.5773	0.7684	1.0554	0.0549*
H461	0.6197	0.6445	0.9761	0.0578*
H471	0.6791	0.4522	1.0050	0.0437*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si101	0.0227 (2)	0.0186 (2)	0.0240 (3)	−0.0011 (2)	0.0046 (2)	−0.0021 (2)
O102	0.0272 (6)	0.0222 (6)	0.0241 (8)	−0.0041 (6)	0.0043 (5)	−0.0013 (6)
C103	0.0180 (7)	0.0240 (9)	0.0234 (10)	−0.0005 (7)	0.0048 (7)	0.0006 (8)
C104	0.0231 (8)	0.0260 (9)	0.0356 (11)	0.0059 (8)	0.0058 (8)	0.0042 (9)
O105	0.0216 (6)	0.0347 (8)	0.0424 (10)	0.0025 (6)	−0.0060 (6)	0.0043 (7)
C106	0.0196 (7)	0.0302 (10)	0.0266 (10)	−0.0019 (8)	0.0033 (7)	−0.0003 (9)
C107	0.0174 (7)	0.0207 (9)	0.0215 (10)	0.0000 (6)	0.0025 (7)	0.0000 (7)
O108	0.0199 (6)	0.0256 (7)	0.0271 (8)	−0.0031 (5)	0.0075 (5)	−0.0054 (6)
Si109	0.0177 (2)	0.0211 (2)	0.0209 (3)	0.00225 (19)	0.00274 (18)	−0.0004 (2)
C110	0.0197 (8)	0.0244 (10)	0.0269 (11)	0.0029 (7)	−0.0007 (7)	−0.0015 (9)
C111	0.0326 (10)	0.0343 (12)	0.0329 (14)	0.0103 (9)	0.0039 (9)	0.0029 (11)
C112	0.0461 (13)	0.0406 (14)	0.0383 (16)	0.0147 (11)	0.0038 (11)	0.0136 (12)
C113	0.0386 (12)	0.0270 (11)	0.0535 (19)	0.0131 (9)	−0.0010 (11)	0.0052 (12)
C114	0.0324 (10)	0.0308 (11)	0.0453 (16)	0.0091 (9)	−0.0011 (10)	−0.0100 (11)
C115	0.0299 (9)	0.0302 (11)	0.0304 (13)	0.0042 (8)	0.0025 (9)	−0.0029 (10)
C116	0.0217 (8)	0.0289 (10)	0.0235 (10)	0.0038 (7)	0.0030 (7)	−0.0028 (8)
C117	0.0456 (13)	0.0344 (13)	0.0459 (16)	0.0044 (10)	−0.0142 (12)	0.0026 (12)
C118	0.0658 (18)	0.0546 (18)	0.061 (2)	0.0127 (15)	−0.0352 (16)	0.0082 (16)
C119	0.0435 (14)	0.0607 (18)	0.0529 (19)	0.0042 (13)	−0.0232 (12)	−0.0104 (15)
C120	0.0292 (10)	0.0434 (13)	0.0457 (16)	0.0021 (9)	−0.0034 (10)	−0.0142 (12)
C121	0.0265 (9)	0.0321 (11)	0.0313 (12)	0.0020 (8)	0.0001 (8)	−0.0038 (10)
C122	0.0220 (8)	0.0268 (10)	0.0310 (12)	−0.0033 (7)	0.0061 (8)	−0.0004 (9)
C123	0.0277 (10)	0.0477 (14)	0.0381 (15)	−0.0084 (10)	−0.0012 (10)	−0.0011 (12)
C124	0.0392 (12)	0.0282 (11)	0.0554 (18)	−0.0043 (9)	0.0125 (11)	0.0037 (12)
C125	0.0608 (16)	0.0212 (11)	0.072 (2)	−0.0071 (11)	0.0183 (15)	−0.0060 (13)
C148	0.0374 (11)	0.0452 (14)	0.0410 (15)	−0.0054 (10)	0.0200 (10)	−0.0018 (12)
C126	0.0194 (8)	0.0313 (10)	0.0335 (11)	−0.0057 (7)	0.0054 (7)	−0.0069 (8)
O127	0.0443 (8)	0.0288 (7)	0.0525 (11)	−0.0037 (6)	0.0299 (8)	−0.0047 (7)
C128	0.0444 (12)	0.0323 (11)	0.0546 (16)	−0.0044 (9)	0.0272 (11)	−0.0014 (11)
C129	0.079 (3)	0.126 (4)	0.107 (4)	−0.025 (3)	−0.016 (2)	0.060 (3)
C130	0.274 (7)	0.0324 (16)	0.135 (5)	−0.037 (3)	0.141 (5)	−0.023 (2)
O131	0.0464 (9)	0.0373 (9)	0.0866 (16)	−0.0035 (7)	0.0446 (10)	−0.0030 (9)
C132	0.0327 (10)	0.0257 (10)	0.0347 (13)	−0.0081 (8)	0.0069 (9)	−0.0047 (10)
C133	0.0458 (13)	0.0367 (13)	0.0440 (15)	−0.0163 (11)	0.0148 (11)	−0.0034 (12)
C134	0.0431 (13)	0.0474 (15)	0.0423 (16)	−0.0168 (11)	0.0040 (11)	−0.0145 (13)
C136	0.0283 (8)	0.0235 (9)	0.0251 (10)	−0.0022 (7)	0.0064 (7)	−0.0036 (9)
C137	0.0333 (10)	0.0305 (11)	0.0304 (12)	−0.0004 (8)	0.0058 (9)	0.0008 (9)
C138	0.0475 (12)	0.0409 (13)	0.0282 (12)	−0.0055 (11)	0.0117 (10)	0.0013 (11)
C139	0.0468 (13)	0.0491 (15)	0.0458 (16)	0.0011 (12)	0.0248 (12)	−0.0097 (13)
C140	0.0370 (12)	0.0566 (16)	0.0461 (16)	0.0141 (11)	0.0122 (11)	−0.0031 (13)
C141	0.0367 (11)	0.0416 (13)	0.0347 (14)	0.0114 (10)	0.0071 (9)	0.0004 (11)
C142	0.0245 (8)	0.0242 (9)	0.0276 (11)	0.0015 (7)	0.0041 (8)	−0.0020 (9)
C143	0.0261 (9)	0.0299 (12)	0.0578 (17)	0.0006 (8)	0.0099 (10)	0.0015 (12)
C144	0.0286 (10)	0.0372 (13)	0.063 (2)	0.0115 (10)	0.0090 (11)	0.0029 (13)
C145	0.0452 (12)	0.0266 (11)	0.0403 (16)	0.0090 (9)	0.0034 (11)	0.0025 (11)

C146	0.0416 (11)	0.0248 (10)	0.0356 (14)	−0.0010 (9)	0.0089 (10)	0.0029 (10)
C147	0.0273 (9)	0.0278 (11)	0.0347 (13)	0.0004 (8)	0.0061 (9)	0.0016 (10)
Si1	0.0194 (2)	0.0204 (2)	0.0210 (3)	0.00287 (19)	0.00248 (19)	0.0002 (2)
O2	0.0214 (6)	0.0279 (7)	0.0300 (9)	0.0009 (5)	0.0079 (6)	−0.0052 (6)
C3	0.0227 (8)	0.0230 (9)	0.0321 (12)	−0.0005 (7)	0.0087 (8)	−0.0007 (9)
C4	0.0224 (8)	0.0337 (11)	0.0373 (13)	−0.0061 (8)	0.0075 (8)	−0.0129 (9)
O5	0.0340 (8)	0.0385 (9)	0.0450 (11)	0.0072 (7)	−0.0137 (7)	−0.0127 (8)
C6	0.0234 (8)	0.0279 (10)	0.0259 (10)	0.0053 (7)	0.0008 (7)	−0.0031 (8)
C7	0.0214 (8)	0.0228 (9)	0.0211 (10)	−0.0007 (7)	0.0061 (7)	−0.0005 (8)
O8	0.0219 (6)	0.0235 (7)	0.0228 (7)	−0.0017 (5)	0.0027 (5)	−0.0005 (6)
Si9	0.0202 (2)	0.0204 (2)	0.0215 (3)	0.0002 (2)	0.00308 (19)	−0.0002 (2)
C10	0.0236 (8)	0.0208 (9)	0.0256 (11)	0.0006 (7)	0.0025 (8)	0.0027 (8)
C11	0.0267 (9)	0.0274 (11)	0.0508 (16)	0.0009 (8)	0.0088 (9)	0.0024 (11)
C12	0.0306 (10)	0.0328 (12)	0.0609 (19)	0.0066 (9)	0.0088 (11)	0.0019 (12)
C13	0.0464 (12)	0.0245 (11)	0.0393 (15)	0.0109 (9)	0.0050 (11)	0.0033 (10)
C14	0.0456 (12)	0.0233 (10)	0.0401 (15)	−0.0032 (9)	0.0107 (11)	0.0056 (10)
C15	0.0300 (9)	0.0261 (10)	0.0354 (13)	0.0024 (8)	0.0085 (9)	0.0026 (10)
C16	0.0241 (8)	0.0229 (9)	0.0269 (11)	−0.0011 (7)	0.0057 (7)	−0.0012 (8)
C17	0.0330 (10)	0.0345 (11)	0.0290 (12)	0.0060 (9)	0.0065 (9)	−0.0034 (10)
C18	0.0314 (11)	0.0421 (13)	0.0510 (16)	0.0080 (9)	0.0157 (10)	−0.0065 (12)
C19	0.0472 (13)	0.0433 (14)	0.0424 (15)	−0.0038 (11)	0.0261 (11)	−0.0056 (12)
C20	0.0535 (13)	0.0423 (13)	0.0295 (13)	−0.0007 (12)	0.0183 (10)	0.0041 (11)
C21	0.0319 (9)	0.0330 (11)	0.0290 (12)	0.0005 (8)	0.0085 (8)	0.0011 (10)
C22	0.0269 (9)	0.0235 (9)	0.0324 (12)	−0.0052 (8)	0.0028 (8)	−0.0024 (9)
C23	0.0401 (11)	0.0398 (13)	0.0420 (15)	−0.0148 (10)	0.0139 (10)	0.0014 (12)
C24	0.0445 (12)	0.0227 (11)	0.0623 (19)	−0.0024 (9)	0.0081 (12)	−0.0037 (12)
C25	0.0350 (11)	0.0483 (15)	0.0332 (14)	−0.0107 (10)	−0.0019 (10)	−0.0076 (12)
C26	0.0224 (8)	0.0296 (9)	0.0275 (10)	0.0059 (7)	0.0012 (7)	0.0008 (8)
O27	0.0384 (8)	0.0267 (7)	0.0776 (14)	0.0054 (6)	0.0291 (8)	0.0011 (8)
C28	0.0402 (12)	0.0272 (10)	0.0661 (18)	0.0077 (9)	0.0249 (12)	0.0032 (11)
C29	0.185 (5)	0.091 (3)	0.074 (3)	0.101 (3)	−0.020 (3)	−0.020 (2)
C30	0.079 (3)	0.063 (2)	0.246 (8)	0.021 (2)	−0.027 (3)	−0.054 (4)
O31	0.0328 (7)	0.0343 (8)	0.0643 (12)	0.0025 (6)	0.0219 (8)	−0.0004 (8)
C32	0.0229 (8)	0.0265 (10)	0.0290 (12)	0.0013 (7)	0.0068 (8)	0.0008 (9)
C33	0.0279 (10)	0.0429 (13)	0.0421 (16)	−0.0065 (9)	−0.0006 (10)	−0.0009 (12)
C34	0.0413 (12)	0.0411 (13)	0.0411 (15)	−0.0054 (10)	0.0198 (11)	0.0008 (12)
C35	0.0352 (11)	0.0235 (10)	0.0599 (19)	−0.0005 (9)	0.0105 (11)	0.0038 (12)
C36	0.0218 (8)	0.0286 (10)	0.0240 (10)	0.0035 (7)	0.0014 (7)	−0.0008 (8)
C37	0.0262 (9)	0.0303 (11)	0.0351 (13)	0.0026 (8)	0.0012 (9)	0.0003 (10)
C38	0.0304 (10)	0.0424 (13)	0.0409 (14)	−0.0078 (9)	−0.0054 (10)	−0.0061 (12)
C39	0.0389 (12)	0.0598 (17)	0.0489 (18)	−0.0090 (12)	−0.0194 (12)	0.0073 (14)
C40	0.0575 (17)	0.0462 (16)	0.072 (2)	0.0009 (13)	−0.0351 (16)	0.0166 (16)
C41	0.0458 (13)	0.0309 (12)	0.0504 (17)	0.0013 (10)	−0.0142 (12)	0.0076 (12)
C42	0.0202 (8)	0.0228 (9)	0.0254 (11)	0.0024 (7)	0.0008 (7)	−0.0002 (9)
C43	0.0276 (9)	0.0299 (11)	0.0247 (11)	0.0066 (8)	−0.0006 (8)	−0.0021 (9)
C44	0.0295 (10)	0.0291 (11)	0.0375 (14)	0.0068 (8)	0.0013 (9)	−0.0073 (10)
C45	0.0363 (11)	0.0297 (12)	0.0494 (18)	0.0111 (9)	0.0000 (11)	0.0063 (12)
C46	0.0480 (13)	0.0401 (14)	0.0337 (14)	0.0122 (11)	0.0055 (11)	0.0122 (12)

C47	0.0342 (10)	0.0355 (12)	0.0244 (12)	0.0065 (9)	0.0032 (9)	0.0016 (10)

Geometric parameters (Å, º)

Si101—O102	1.6478 (16)	Si1—O2	1.6354 (15)
Si101—C132	1.887 (2)	Si1—C32	1.891 (2)
Si101—C136	1.876 (2)	Si1—C36	1.879 (2)
Si101—C142	1.874 (2)	Si1—C42	1.876 (2)
O102—C103	1.411 (2)	O2—C3	1.408 (2)
C103—C104	1.515 (3)	C3—C4	1.528 (3)
C103—C107	1.540 (3)	C3—C7	1.537 (3)
C103—H1031	0.956	C3—H31	0.988
C104—O105	1.428 (3)	C4—O5	1.439 (3)
C104—H1041	0.986	C4—H41	0.968
C104—H1042	0.952	C4—H42	0.966
O105—C106	1.427 (2)	O5—C6	1.418 (2)
C106—C107	1.547 (3)	C6—C7	1.538 (3)
C106—C126	1.522 (3)	C6—C26	1.522 (3)
C106—H1061	0.981	C6—H61	0.983
C107—O108	1.408 (2)	C7—O8	1.404 (2)
C107—H1071	0.986	C7—H71	1.005
O108—Si109	1.6469 (15)	O8—Si9	1.6512 (16)
Si109—C110	1.879 (2)	Si9—C10	1.880 (2)
Si109—C116	1.880 (2)	Si9—C16	1.877 (2)
Si109—C122	1.893 (2)	Si9—C22	1.887 (2)
C110—C111	1.392 (3)	C10—C11	1.392 (3)
C110—C115	1.403 (3)	C10—C15	1.402 (3)
C111—C112	1.397 (3)	C11—C12	1.390 (3)
C111—H1111	0.937	C11—H111	0.983
C112—C113	1.381 (4)	C12—C13	1.380 (3)
C112—H1121	0.956	C12—H121	0.957
C113—C114	1.380 (4)	C13—C14	1.377 (3)
C113—H1131	0.935	C13—H131	0.932
C114—C115	1.386 (3)	C14—C15	1.390 (3)
C114—H1141	0.953	C14—H141	0.941
C115—H1151	0.946	C15—H151	0.940
C116—C117	1.390 (3)	C16—C17	1.398 (3)
C116—C121	1.402 (3)	C16—C21	1.399 (3)
C117—C118	1.379 (4)	C17—C18	1.395 (3)
C117—H1171	0.939	C17—H171	0.935
C118—C119	1.374 (5)	C18—C19	1.378 (4)
C118—H1181	0.921	C18—H181	0.947
C119—C120	1.373 (4)	C19—C20	1.383 (4)
C119—H1191	0.931	C19—H191	0.932
C120—C121	1.383 (3)	C20—C21	1.388 (3)
C120—H1201	0.963	C20—H201	0.939
C121—H1211	0.971	C21—H211	0.937
C122—C123	1.538 (3)	C22—C23	1.532 (3)

C122—C124	1.538 (3)	C22—C24	1.542 (3)
C122—C148	1.530 (3)	C22—C25	1.530 (3)
C123—H1231	0.971	C23—H231	0.977
C123—H1232	0.953	C23—H232	0.976
C123—H1233	0.965	C23—H233	0.957
C124—H1241	0.960	C24—H241	0.978
C124—H1242	0.975	C24—H242	0.987
C124—H1243	0.986	C24—H243	0.988
C125—C132	1.541 (3)	C25—H251	0.976
C125—H1251	0.964	C25—H252	0.986
C125—H1252	0.967	C25—H253	0.999
C125—H1253	0.969	C26—O27	1.325 (2)
C148—H1481	1.011	C26—O31	1.195 (2)
C148—H1482	0.967	O27—C28	1.475 (3)
C148—H1483	0.974	C28—C29	1.446 (5)
C126—O127	1.323 (2)	C28—C30	1.491 (5)
C126—O131	1.186 (2)	C28—H281	0.956
O127—C128	1.461 (3)	C29—H291	0.972
C128—C129	1.473 (5)	C29—H292	1.016
C128—C130	1.477 (4)	C29—H293	0.959
C128—H1281	1.006	C30—H301	0.977
C129—H1291	0.969	C30—H302	0.975
C129—H1292	0.987	C30—H303	0.968
C129—H1293	0.959	C32—C33	1.535 (3)
C130—H1301	0.962	C32—C34	1.524 (3)
C130—H1302	0.954	C32—C35	1.545 (3)
C130—H1303	0.958	C33—H331	0.945
C132—C133	1.528 (3)	C33—H332	0.966
C132—C134	1.541 (4)	C33—H333	0.971
C133—H1331	0.975	C34—H341	0.977
C133—H1332	0.970	C34—H342	0.967
C133—H1333	0.973	C34—H343	0.968
C134—H1341	0.969	C35—H351	0.982
C134—H1342	0.988	C35—H352	0.957
C134—H1343	0.991	C35—H353	0.949
C136—C137	1.395 (3)	C36—C37	1.399 (3)
C136—C141	1.400 (3)	C36—C41	1.391 (3)
C137—C138	1.389 (3)	C37—C38	1.389 (3)
C137—H1371	0.945	C37—H371	0.930
C138—C139	1.377 (4)	C38—C39	1.364 (4)
C138—H1381	0.957	C38—H381	0.944
C139—C140	1.380 (4)	C39—C40	1.381 (4)
C139—H1391	0.958	C39—H391	0.952
C140—C141	1.390 (3)	C40—C41	1.392 (4)
C140—H1401	0.938	C40—H401	0.919
C141—H1411	0.957	C41—H411	0.927
C142—C143	1.401 (3)	C42—C43	1.402 (3)
C142—C147	1.391 (3)	C42—C47	1.396 (3)

C143—C144	1.389 (3)	C43—C44	1.390 (3)
C143—H1431	0.967	C43—H431	0.946
C144—C145	1.374 (4)	C44—C45	1.381 (4)
C144—H1441	0.949	C44—H441	0.958
C145—C146	1.376 (3)	C45—C46	1.381 (4)
C145—H1451	0.938	C45—H451	0.951
C146—C147	1.397 (3)	C46—C47	1.394 (3)
C146—H1461	0.952	C46—H461	0.933
C147—H1471	0.945	C47—H471	0.945

O102—Si101—C132	104.35 (10)	O2—Si1—C32	101.78 (9)
O102—Si101—C136	109.85 (8)	O2—Si1—C36	111.48 (8)
C132—Si101—C136	109.81 (10)	C32—Si1—C36	115.76 (10)
O102—Si101—C142	110.31 (9)	O2—Si1—C42	110.57 (9)
C132—Si101—C142	115.03 (10)	C32—Si1—C42	109.35 (8)
C136—Si101—C142	107.44 (9)	C36—Si1—C42	107.80 (9)
Si101—O102—C103	125.33 (13)	Si1—O2—C3	140.64 (14)
O102—C103—C104	111.43 (16)	O2—C3—C4	114.49 (19)
O102—C103—C107	115.35 (14)	O2—C3—C7	107.31 (15)
C104—C103—C107	101.20 (17)	C4—C3—C7	99.66 (16)
O102—C103—H1031	109.4	O2—C3—H31	111.0
C104—C103—H1031	110.5	C4—C3—H31	111.7
C107—C103—H1031	108.7	C7—C3—H31	112.2
C103—C104—O105	103.81 (16)	C3—C4—O5	106.50 (16)
C103—C104—H1041	109.2	C3—C4—H41	112.6
O105—C104—H1041	110.8	O5—C4—H41	109.7
C103—C104—H1042	113.8	C3—C4—H42	109.2
O105—C104—H1042	111.0	O5—C4—H42	110.9
H1041—C104—H1042	108.2	H41—C4—H42	107.9
C104—O105—C106	108.85 (14)	C4—O5—C6	109.43 (15)
O105—C106—C107	107.59 (16)	O5—C6—C7	104.03 (16)
O105—C106—C126	110.81 (15)	O5—C6—C26	109.59 (15)
C107—C106—C126	109.67 (17)	C7—C6—C26	112.73 (17)
O105—C106—H1061	109.3	O5—C6—H61	112.7
C107—C106—H1061	111.3	C7—C6—H61	111.7
C126—C106—H1061	108.2	C26—C6—H61	106.2
C103—C107—C106	99.95 (14)	C6—C7—C3	99.74 (17)
C103—C107—O108	108.95 (15)	C6—C7—O8	110.60 (16)
C106—C107—O108	113.22 (17)	C3—C7—O8	116.78 (15)
C103—C107—H1071	112.3	C6—C7—H71	106.9
C106—C107—H1071	109.7	C3—C7—H71	110.0
O108—C107—H1071	112.2	O8—C7—H71	111.8
C107—O108—Si109	134.60 (13)	C7—O8—Si9	127.34 (13)
O108—Si109—C110	111.73 (9)	O8—Si9—C10	112.14 (9)
O108—Si109—C116	111.29 (8)	O8—Si9—C16	109.46 (8)
C110—Si109—C116	106.60 (9)	C10—Si9—C16	107.49 (9)
O108—Si109—C122	101.69 (9)	O8—Si9—C22	103.93 (9)
C110—Si109—C122	110.29 (9)	C10—Si9—C22	114.44 (9)

C116—Si109—C122	115.33 (10)	C16—Si9—C22	109.30 (10)
Si109—C110—C111	122.06 (16)	Si9—C10—C11	122.98 (15)
Si109—C110—C115	120.48 (17)	Si9—C10—C15	119.79 (14)
C111—C110—C115	117.5 (2)	C11—C10—C15	117.22 (19)
C110—C111—C112	121.1 (2)	C10—C11—C12	121.2 (2)
C110—C111—H1111	119.7	C10—C11—H111	119.4
C112—C111—H1111	119.2	C12—C11—H111	119.4
C111—C112—C113	120.2 (3)	C11—C12—C13	120.4 (2)
C111—C112—H1121	120.0	C11—C12—H121	118.7
C113—C112—H1121	119.8	C13—C12—H121	120.9
C112—C113—C114	119.8 (2)	C12—C13—C14	119.7 (2)
C112—C113—H1131	120.1	C12—C13—H131	120.1
C114—C113—H1131	120.2	C14—C13—H131	120.2
C113—C114—C115	120.1 (2)	C13—C14—C15	120.0 (2)
C113—C114—H1141	119.6	C13—C14—H141	122.0
C115—C114—H1141	120.3	C15—C14—H141	118.0
C110—C115—C114	121.4 (2)	C10—C15—C14	121.49 (19)
C110—C115—H1151	119.9	C10—C15—H151	119.7
C114—C115—H1151	118.7	C14—C15—H151	118.8
Si109—C116—C117	123.05 (17)	Si9—C16—C17	122.49 (17)
Si109—C116—C121	120.41 (16)	Si9—C16—C21	120.12 (14)
C117—C116—C121	116.3 (2)	C17—C16—C21	117.18 (19)
C116—C117—C118	121.5 (3)	C16—C17—C18	121.1 (2)
C116—C117—H1171	119.7	C16—C17—H171	119.9
C118—C117—H1171	118.8	C18—C17—H171	119.0
C117—C118—C119	121.0 (3)	C17—C18—C19	119.9 (2)
C117—C118—H1181	118.1	C17—C18—H181	120.5
C119—C118—H1181	120.9	C19—C18—H181	119.5
C118—C119—C120	119.2 (2)	C18—C19—C20	120.4 (2)
C118—C119—H1191	120.4	C18—C19—H191	119.2
C120—C119—H1191	120.3	C20—C19—H191	120.3
C119—C120—C121	119.9 (2)	C19—C20—C21	119.3 (2)
C119—C120—H1201	119.4	C19—C20—H201	120.9
C121—C120—H1201	120.7	C21—C20—H201	119.8
C116—C121—C120	122.1 (2)	C16—C21—C20	122.0 (2)
C116—C121—H1211	118.8	C16—C21—H211	118.9
C120—C121—H1211	119.1	C20—C21—H211	119.1
Si109—C122—C123	106.72 (16)	Si9—C22—C23	112.14 (16)
Si109—C122—C124	111.37 (13)	Si9—C22—C24	107.06 (14)
C123—C122—C124	108.2 (2)	C23—C22—C24	107.7 (2)
Si109—C122—C148	111.10 (16)	Si9—C22—C25	111.02 (16)
C123—C122—C148	109.55 (19)	C23—C22—C25	110.05 (18)
C124—C122—C148	109.8 (2)	C24—C22—C25	108.7 (2)
C122—C123—H1231	109.8	C22—C23—H231	106.2
C122—C123—H1232	110.4	C22—C23—H232	112.6
H1231—C123—H1232	107.3	H231—C23—H232	107.3
C122—C123—H1233	109.7	C22—C23—H233	112.2
H1231—C123—H1233	110.4	H231—C23—H233	108.1

H1232—C123—H1233	109.3	H232—C23—H233	110.1
C122—C124—H1241	110.2	C22—C24—H241	108.5
C122—C124—H1242	109.2	C22—C24—H242	111.1
H1241—C124—H1242	108.3	H241—C24—H242	108.7
C122—C124—H1243	109.1	C22—C24—H243	109.5
H1241—C124—H1243	110.2	H241—C24—H243	109.6
H1242—C124—H1243	109.8	H242—C24—H243	109.4
C132—C125—H1251	107.9	C22—C25—H251	107.8
C132—C125—H1252	109.8	C22—C25—H252	110.8
H1251—C125—H1252	108.2	H251—C25—H252	108.7
C132—C125—H1253	110.7	C22—C25—H253	111.5
H1251—C125—H1253	110.2	H251—C25—H253	108.5
H1252—C125—H1253	109.9	H252—C25—H253	109.4
C122—C148—H1481	111.8	C6—C26—O27	110.39 (16)
C122—C148—H1482	111.1	C6—C26—O31	124.78 (19)
H1481—C148—H1482	109.1	O27—C26—O31	124.82 (19)
C122—C148—H1483	109.8	C26—O27—C28	117.98 (16)
H1481—C148—H1483	107.4	O27—C28—C29	107.4 (3)
H1482—C148—H1483	107.5	O27—C28—C30	107.0 (2)
C106—C126—O127	108.69 (16)	C29—C28—C30	114.0 (4)
C106—C126—O131	125.83 (19)	O27—C28—H281	108.2
O127—C126—O131	125.5 (2)	C29—C28—H281	115.8
C126—O127—C128	118.79 (16)	C30—C28—H281	104.1
O127—C128—C129	109.0 (2)	C28—C29—H291	109.0
O127—C128—C130	105.8 (2)	C28—C29—H292	100.3
C129—C128—C130	116.6 (4)	H291—C29—H292	111.7
O127—C128—H1281	107.0	C28—C29—H293	112.7
C129—C128—H1281	108.1	H291—C29—H293	113.3
C130—C128—H1281	110.0	H292—C29—H293	109.2
C128—C129—H1291	110.9	C28—C30—H301	109.3
C128—C129—H1292	104.4	C28—C30—H302	112.3
H1291—C129—H1292	107.8	H301—C30—H302	112.8
C128—C129—H1293	111.6	C28—C30—H303	106.0
H1291—C129—H1293	111.4	H301—C30—H303	107.7
H1292—C129—H1293	110.4	H302—C30—H303	108.4
C128—C130—H1301	110.2	Si1—C32—C33	107.06 (16)
C128—C130—H1302	109.1	Si1—C32—C34	111.17 (16)
H1301—C130—H1302	112.1	C33—C32—C34	109.61 (19)
C128—C130—H1303	105.7	Si1—C32—C35	112.03 (13)
H1301—C130—H1303	110.5	C33—C32—C35	107.4 (2)
H1302—C130—H1303	109.0	C34—C32—C35	109.4 (2)
C125—C132—Si101	107.16 (15)	C32—C33—H331	111.3
C125—C132—C133	108.2 (2)	C32—C33—H332	111.8
Si101—C132—C133	112.32 (16)	H331—C33—H332	107.7
C125—C132—C134	108.9 (2)	C32—C33—H333	112.5
Si101—C132—C134	110.53 (17)	H331—C33—H333	105.3
C133—C132—C134	109.60 (19)	H332—C33—H333	107.9
C132—C133—H1331	111.0	C32—C34—H341	108.1

C132—C133—H1332	110.1	C32—C34—H342	109.9
H1331—C133—H1332	107.1	H341—C34—H342	108.3
C132—C133—H1333	110.7	C32—C34—H343	110.1
H1331—C133—H1333	109.0	H341—C34—H343	110.4
H1332—C133—H1333	108.9	H342—C34—H343	110.1
C132—C134—H1341	108.7	C32—C35—H351	109.7
C132—C134—H1342	112.8	C32—C35—H352	111.7
H1341—C134—H1342	107.4	H351—C35—H352	108.7
C132—C134—H1343	109.6	C32—C35—H353	108.9
H1341—C134—H1343	108.0	H351—C35—H353	109.3
H1342—C134—H1343	110.2	H352—C35—H353	108.6
Si101—C136—C137	120.42 (15)	Si1—C36—C37	120.23 (16)
Si101—C136—C141	122.15 (17)	Si1—C36—C41	122.72 (17)
C137—C136—C141	117.20 (19)	C37—C36—C41	116.8 (2)
C136—C137—C138	121.8 (2)	C36—C37—C38	121.6 (2)
C136—C137—H1371	117.9	C36—C37—H371	119.1
C138—C137—H1371	120.3	C38—C37—H371	119.1
C137—C138—C139	119.8 (2)	C37—C38—C39	120.4 (2)
C137—C138—H1381	119.6	C37—C38—H381	118.8
C139—C138—H1381	120.6	C39—C38—H381	120.7
C138—C139—C140	119.7 (2)	C38—C39—C40	119.4 (2)
C138—C139—H1391	121.2	C38—C39—H391	119.7
C140—C139—H1391	119.0	C40—C39—H391	120.8
C139—C140—C141	120.4 (2)	C39—C40—C41	120.4 (3)
C139—C140—H1401	119.9	C39—C40—H401	121.3
C141—C140—H1401	119.6	C41—C40—H401	118.3
C136—C141—C140	121.0 (2)	C40—C41—C36	121.3 (2)
C136—C141—H1411	119.8	C40—C41—H411	119.2
C140—C141—H1411	119.2	C36—C41—H411	119.4
Si101—C142—C143	123.59 (17)	Si1—C42—C43	121.59 (17)
Si101—C142—C147	119.75 (14)	Si1—C42—C47	121.01 (16)
C143—C142—C147	116.6 (2)	C43—C42—C47	117.36 (19)
C142—C143—C144	121.5 (2)	C42—C43—C44	121.5 (2)
C142—C143—H1431	120.1	C42—C43—H431	120.2
C144—C143—H1431	118.4	C44—C43—H431	118.2
C143—C144—C145	120.3 (2)	C43—C44—C45	119.9 (2)
C143—C144—H1441	120.2	C43—C44—H441	120.6
C145—C144—H1441	119.3	C45—C44—H441	119.5
C144—C145—C146	119.8 (2)	C44—C45—C46	119.8 (2)
C144—C145—H1451	121.3	C44—C45—H451	119.9
C146—C145—H1451	118.9	C46—C45—H451	120.3
C145—C146—C147	119.7 (2)	C45—C46—C47	120.3 (2)
C145—C146—H1461	118.3	C45—C46—H461	119.7
C147—C146—H1461	122.0	C47—C46—H461	120.0
C146—C147—C142	121.95 (19)	C42—C47—C46	121.1 (2)
C146—C147—H1471	118.1	C42—C47—H471	118.8
C142—C147—H1471	119.8	C46—C47—H471	120.1