

Table 3. Bond lengths [Å] and angles [deg] for (34).

O1-C5	1.340(4)	C18-C19	1.389(5)
O1-C2	1.458(4)	C18-H18	0.83(4)
C2-C10	1.515(4)	C19-C20	1.370(6)
C2-C3	1.561(4)	C19-H19	1.07(5)
C2-H2	0.97(3)	C20-C21	1.367(5)
C3-O29	1.383(4)	C20-H20	0.90(4)
C3-C34	1.547(4)	C21-C22	1.391(5)
C3-C4	1.556(4)	C21-H21	0.99(4)
C4-O6	1.422(4)	C22-H22	0.88(3)
C4-C9	1.504(5)	C23-C28	1.389(5)
C4-C5	1.529(5)	C23-C24	1.411(5)
C5-O39	1.188(4)	C24-C25	1.366(6)
O6-C7	1.388(4)	C24-H24	0.84(4)
C7-O38	1.197(4)	C25-C26	1.361(6)
C7-C8	1.465(6)	C25-H25	0.87(5)
C8-C9	1.307(5)	C26-C27	1.376(6)
C8-H8	0.89(4)	C26-H26	0.85(4)
C9-H9	0.85(4)	C27-C28	1.387(5)
C10-O11	1.418(4)	C27-H27	0.93(4)
C10-H10A	0.89(3)	C28-H28	1.02(5)
C10-H10B	0.95(3)	O29-Si30	1.667(2)
O11-S12	1.659(2)	Si30-C32	1.839(4)
S12-C17	1.873(3)	Si30-C31	1.853(4)
S12-C23	1.876(3)	Si30-C33	1.854(4)
S12-C13	1.880(3)	C31-H31A	0.96
C13-C16	1.524(5)	C31-H31B	0.96
C13-C15	1.537(5)	C31-H31C	0.96
C13-C14	1.544(5)	C32-H32A	0.96
C14-H14A	0.96	C32-H32B	0.96
C14-H14B	0.96	C32-H32C	0.96
C14-H14C	0.96	C33-H33A	0.96
C15-H15A	0.96	C33-H33B	0.96
C15-H15B	0.96	C33-H33C	0.96
C15-H15C	0.96	C34-O35	1.193(4)
C16-H16A	0.96	C34-O36	1.332(4)
C16-H16B	0.96	O36-C37	1.452(4)
C16-H16C	0.96	C37-H37A	0.96
C17-C18	1.395(5)	C37-H37B	0.96
C17-C22	1.400(5)	C37-H37C	0.96
C5-O1-C2	112.5(2)	O6-C4-C5	111.6(3)
O1-C2-C10	110.0(3)	C9-C4-C5	111.6(3)
O1-C2-C3	105.1(2)	O6-C4-C3	111.4(2)
C10-C2-C3	114.4(3)	C9-C4-C3	115.0(3)
O1-C2-H2	107(2)	C5-C4-C3	102.8(3)
C10-C2-H2	112(2)	O39-C5-O1	122.4(3)
C3-C2-H2	108(2)	O39-C5-C4	127.9(3)
O29-C3-C34	112.8(3)	O1-C5-C4	109.6(3)
O29-C3-C4	111.4(3)	C7-O6-C4	109.0(3)
C34-C3-C4	106.1(2)	O38-C7-O6	120.4(3)
O29-C3-C2	112.7(3)	O38-C7-C8	131.9(4)
C34-C3-C2	111.3(3)	O6-C7-C8	107.7(3)
C4-C3-C2	101.8(2)	C9-C8-C7	109.1(3)
O6-C4-C9	104.7(3)	C9-C8-H8	132(3)

C7-C8-H8	119(2)	C21-C22-C17	121.9(3)
C8-C9-C4	109.4(3)	C21-C22-H22	120(2)
C8-C9-H9	129(3)	C17-C22-H22	118(2)
C4-C9-H9	121(3)	C28-C23-C24	115.9(3)
O11-C10-C2	107.6(3)	C28-C23-S12	119.6(3)
O11-C10-H10A	112(2)	C24-C23-S12	124.5(3)
C2-C10-H10A	109(2)	C25-C24-C23	121.3(4)
O11-C10-H10B	106(2)	C25-C24-H24	118(3)
C2-C10-H10B	112(2)	C23-C24-H24	120(3)
H10A-C10-H10B	110(3)	C26-C25-C24	121.7(4)
C10-O11-S12	127.6(2)	C26-C25-H25	121(3)
O11-S12-C17	108.14(13)	C24-C25-H25	117(3)
O11-S12-C23	108.07(13)	C25-C26-C27	118.7(4)
C17-S12-C23	113.0(2)	C25-C26-H26	123(3)
O11-S12-C13	103.52(13)	C27-C26-H26	118(3)
C17-S12-C13	111.7(2)	C26-C27-C28	120.3(4)
C23-S12-C13	111.8(2)	C26-C27-H27	121(2)
C16-C13-C15	109.1(3)	C28-C27-H27	119(2)
C16-C13-C14	109.6(3)	C27-C28-C23	122.0(4)
C15-C13-C14	109.9(3)	C27-C28-H28	118(3)
C16-C13-S12	110.7(2)	C23-C28-H28	120(3)
C15-C13-S12	109.3(3)	C3-O29-Si30	138.8(2)
C14-C13-S12	108.3(2)	O29-Si30-C32	112.0(2)
C13-C14-H14A	109.4(2)	O29-Si30-C31	108.7(2)
C13-C14-H14B	110.0(2)	C32-Si30-C31	113.6(2)
H14A-C14-H14B	109.5	O29-Si30-C33	101.9(2)
C13-C14-H14C	109.0(2)	C32-Si30-C33	110.8(2)
H14A-C14-H14C	109.5	C31-Si30-C33	109.3(2)
H14B-C14-H14C	109.5	Si30-C31-H31A	109.2(2)
C13-C15-H15A	109.5(2)	Si30-C31-H31B	109.94(14)
C13-C15-H15B	109.5(2)	H31A-C31-H31B	109.5
H15A-C15-H15B	109.5	Si30-C31-H31C	109.2(2)
C13-C15-H15C	109.5(2)	H31A-C31-H31C	109.5
H15A-C15-H15C	109.5	H31B-C31-H31C	109.5
H15B-C15-H15C	109.5	Si30-C32-H32A	109.58(13)
C13-C16-H16A	109.5(2)	Si30-C32-H32B	109.3(2)
C13-C16-H16B	109.8(2)	H32A-C32-H32B	109.5
H16A-C16-H16B	109.5	Si30-C32-H32C	109.55(14)
C13-C16-H16C	109.1(2)	H32A-C32-H32C	109.5
H16A-C16-H16C	109.5	H32B-C32-H32C	109.5
H16B-C16-H16C	109.5	Si30-C33-H33A	109.2(2)
C18-C17-C22	116.2(3)	Si30-C33-H33B	109.61(14)
C18-C17-S12	126.3(3)	H33A-C33-H33B	109.5
C22-C17-S12	117.4(3)	Si30-C33-H33C	109.6(2)
C19-C18-C17	121.9(3)	H33A-C33-H33C	109.5
C19-C18-H18	123(3)	H33B-C33-H33C	109.5
C17-C18-H18	115(3)	O35-C34-O36	126.6(3)
C20-C19-C18	119.8(4)	O35-C34-C3	123.6(3)
C20-C19-H19	113(2)	O36-C34-C3	109.7(3)
C18-C19-H19	127(2)	C34-O36-C37	115.4(3)
C21-C20-C19	120.4(4)	O36-C37-H37A	109.5(2)
C21-C20-H20	120(3)	O36-C37-H37B	109.4(2)
C19-C20-H20	119(3)	H37A-C37-H37B	109.5
C20-C21-C22	119.7(4)	O36-C37-H37C	109.5(2)
C20-C21-H21	122(3)	H37A-C37-H37C	109.5
C22-C21-H21	118(3)	H37B-C37-H37C	109.5

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (34).
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O1	23(1)	27(1)	27(1)	-8(1)	7(1)	-5(1)
C2	26(2)	20(2)	20(2)	-3(1)	2(1)	0(1)
C3	27(2)	20(2)	18(2)	-2(1)	0(1)	-5(1)
C4	25(2)	21(2)	20(2)	-4(1)	2(1)	-1(1)
C5	27(2)	25(2)	21(2)	-3(1)	2(1)	-6(1)
O6	26(1)	26(1)	24(1)	-6(1)	1(1)	2(1)
C7	28(2)	30(2)	37(2)	8(2)	6(2)	7(2)
C8	25(2)	44(2)	38(2)	8(2)	-3(2)	0(2)
C9	32(2)	30(2)	26(2)	1(2)	-8(2)	-5(2)
C10	25(2)	24(2)	22(2)	-2(1)	3(1)	2(1)
O11	25(1)	27(1)	19(1)	-6(1)	0(1)	2(1)
Si12	27(1)	26(1)	26(1)	-2(1)	1(1)	0(1)
C13	21(2)	36(2)	25(2)	-4(2)	3(1)	-2(2)
C14	28(2)	53(3)	66(3)	-24(2)	10(2)	-17(2)
C15	34(2)	59(3)	50(3)	7(2)	2(2)	19(2)
C16	33(2)	64(3)	31(2)	-9(2)	10(2)	-4(2)
C17	20(2)	21(2)	24(2)	-4(1)	5(1)	1(1)
C18	43(2)	28(2)	23(2)	2(2)	2(2)	-7(2)
C19	48(3)	31(2)	41(2)	-8(2)	-1(2)	-13(2)
C20	39(2)	23(2)	45(2)	-5(2)	6(2)	-6(2)
C21	42(2)	28(2)	38(2)	6(2)	6(2)	-2(2)
C22	33(2)	27(2)	28(2)	1(2)	-3(2)	-1(2)
C23	22(2)	22(2)	23(2)	3(1)	1(1)	-3(1)
C24	51(2)	29(2)	32(2)	-1(2)	-9(2)	1(2)
C25	54(3)	46(3)	33(2)	7(2)	-14(2)	-1(2)
C26	52(3)	32(2)	42(2)	18(2)	-3(2)	10(2)
C27	61(3)	22(2)	39(2)	4(2)	3(2)	9(2)
C28	43(2)	25(2)	28(2)	2(1)	-3(2)	-2(2)
O29	34(1)	27(1)	23(1)	-2(1)	1(1)	-9(1)
Si30	33(1)	28(1)	28(1)	5(1)	2(1)	-5(1)
C31	40(2)	82(3)	36(2)	12(2)	8(2)	0(2)
C32	64(3)	25(2)	47(2)	4(2)	-11(2)	9(2)
C33	62(3)	44(2)	49(2)	10(2)	-11(2)	-24(2)
C34	32(2)	22(2)	22(2)	-4(1)	-1(2)	3(2)
O35	55(2)	37(1)	19(1)	-3(1)	3(1)	-6(1)
O36	29(1)	41(1)	24(1)	-8(1)	-5(1)	-7(1)
C37	42(2)	58(3)	33(2)	-19(2)	-8(2)	-10(2)
O38	47(2)	52(2)	44(2)	1(1)	12(1)	23(1)
O39	42(2)	30(1)	45(2)	2(1)	13(1)	-8(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (34).

	x	y	z	U(eq)
H14A	13197(6)	651(2)	470(2)	73
H14B	11339(6)	1098(2)	369(2)	73
H14C	11746(6)	731(2)	955(2)	73
H15A	13134(6)	-802(3)	596(2)	72
H15B	11699(6)	-697(3)	1083(2)	72
H15C	11232(6)	-1239(3)	577(2)	72
H16A	12530(5)	-230(3)	-336(2)	64
H16B	10634(5)	-668(3)	-370(2)	64
H16C	10693(5)	227(3)	-448(2)	64
H31A	2439(6)	895(3)	3561(2)	79
H31B	938(6)	842(3)	3088(2)	79
H31C	1187(6)	160(3)	3511(2)	79
H32A	6012(7)	-56(2)	3469(2)	68
H32B	4890(7)	-826(2)	3420(2)	68
H32C	6308(7)	-596(2)	2951(2)	68
H33A	3268(7)	-782(3)	2099(2)	78
H33B	1734(7)	-948(3)	2548(2)	78
H33C	1486(7)	-267(3)	2124(2)	78
H37A	9795(6)	2643(3)	3342(2)	67
H37B	7768(6)	2638(3)	3580(2)	67
H37C	9081(6)	1934(3)	3686(2)	67
H2	8447(47)	788(18)	2239(13)	16(8)
H8	1302(52)	2543(21)	1671(15)	29(10)
H9	3839(57)	1706(22)	1382(17)	38(12)
H10A	5941(46)	605(18)	1365(13)	10(8)
H10B	6510(45)	-73(20)	1724(13)	20(8)
H18	6617(59)	-1069(22)	-259(17)	36(11)
H19	4931(64)	-2324(26)	-287(19)	55(13)
H20	4878(63)	-2879(26)	553(18)	56(14)
H21	6287(63)	-2426(25)	1376(18)	57(13)
H22	7663(45)	-1234(18)	1307(14)	12(8)
H24	6542(63)	176(25)	-561(18)	53(13)
H25	5147(76)	1081(28)	-1016(22)	73(17)
H26	4941(62)	2283(26)	-646(18)	56(14)
H27	5914(50)	2512(23)	236(15)	29(10)
H28	7446(64)	1581(25)	750(19)	55(13)

Figure 1. View of C₂₉H₃₆O₈SSi (34) showing the atom labeling scheme. Thermal ellipsoids are scaled to the 50% probability level. Hydrogen atoms shown are drawn to an arbitrary scale. The methyl hydrogen atoms have been omitted for clarity.

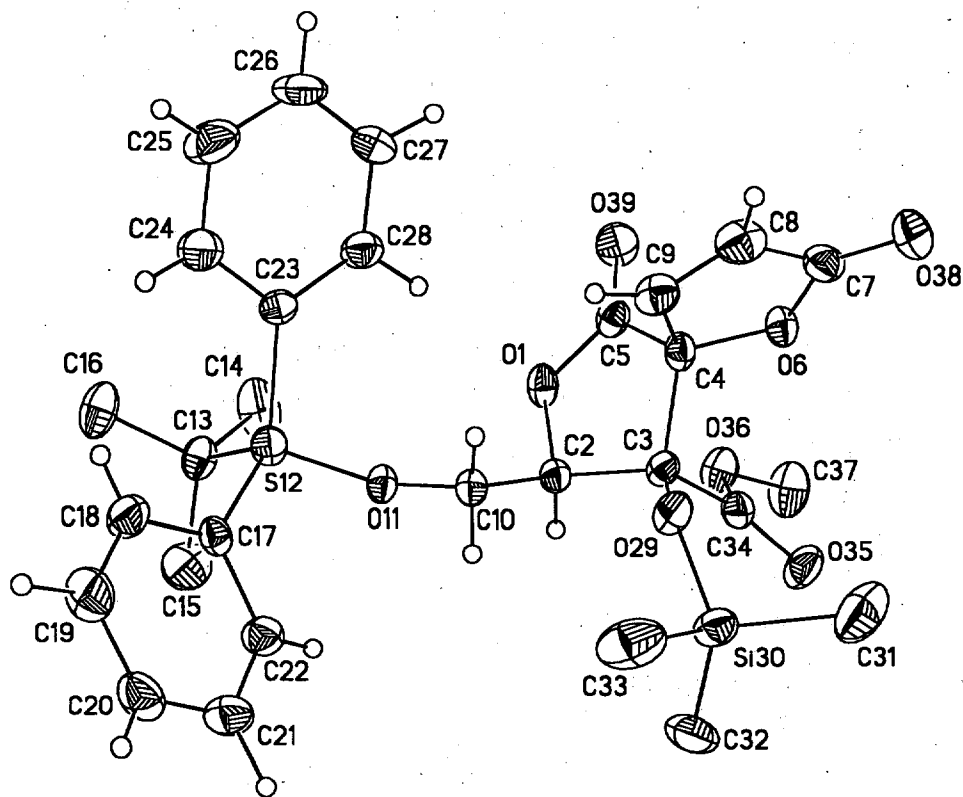
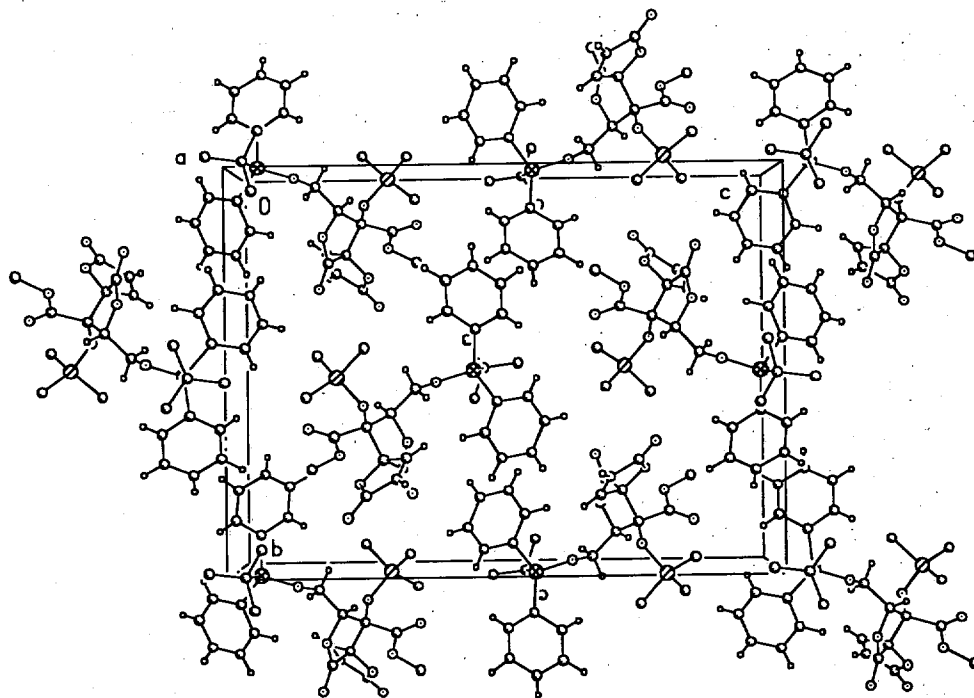


Figure 2. Unit cell packing diagram for $C_{29}H_{36}O_8SSi$ (**34**). The view is approximately down the **a** axis.



Crystallographic Material for $C_{29}H_{36}O_8Si_2$ (36).

X-ray Experimental.

Table 1. Crystallographic Data for $C_{29}H_{36}O_8Si_2$ (36).

Table 2. Fractional coordinates and equivalent isotropic thermal parameters ($\text{\AA}^2$) for the non-hydrogen atoms of $C_{29}H_{36}O_8Si_2$ (36).

Table 3. Bond Lengths ($\text{\AA}$) and Angles ($^\circ$) for the non-hydrogen atoms of $C_{29}H_{36}O_8Si_2$ (36).

Table 4. Anisotropic thermal parameters for the non-hydrogen atoms of $C_{29}H_{36}O_8Si_2$ (36).

Table 5. Fractional coordinates and isotropic thermal parameters ($\text{\AA}^2$) for the hydrogen atoms of $C_{29}H_{36}O_8Si_2$ (36).

Figure 1. View of $C_{29}H_{36}O_8Si_2$ (36) showing the atom labeling scheme. Thermal ellipsoids are scaled to the 30% probability level. Hydrogen atoms shown are drawn to an arbitrary scale.

Figure 2. Unit cell packing diagram for $C_{29}H_{36}O_8Si_2$ (36). The view is approximately down the *a* axis.

X-ray Experimental for $C_{29}H_{36}O_8Si_2$ (**36**): Crystals grew as clusters of thin colorless needles and lathes by slow cooling of a hexane solution. The data were collected using the ω -scan technique at $6^\circ/\text{min.}$, with a scan range of 1.2° in ω to a $2\theta_{\text{max}} = 45^\circ$ at room temperature on a Enraf-Nonius CAD4 diffractometer using a graphite monochromator with $MoK\alpha$ radiation ($\lambda = 0.71073\text{\AA}$). Details of crystal data, data collection and structure refinement are listed in Table 1. Three reflections were remeasured every 96 reflections to monitor instrument and crystal stability. A smoothed curve of the intensities of these check reflections was used to scale the data. No significant correction was applied to the data. The data were corrected for Lp effects but not for absorption. Data reduction, decay correction, structure solution and refinement were performed using the SHELXTL/PC software package.¹ The structure was solved by direct methods and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms. The hydrogen atoms were calculated in ideal positions with isotropic displacement parameters set to $1.2 \times U_{eq}$ of the attached atom ($1.5 \times U_{eq}$ for methyl hydrogen atoms). The function, $\sum w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.0553 \times P)^2]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. The data were checked for secondary extinction effects but no correction was found to be warranted. The absolute configuration was determined by internal comparison. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).² All figures were generated using SHELXTL/PC.¹ Tables of positional and thermal parameters, bond lengths and angles, figures and lists of observed and calculated structure factors are located in tables 1 through 5.

References

- 1) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.
- 2) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.

Table 1. Crystal data and structure refinement for (36).

Empirical formula	C ₂₉ H ₃₆ O ₈ Si ₂
Formula weight	568.76
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P212121
Unit cell dimensions	a = 7.547(1) Å alpha = 90° b = 12.788(1) Å beta = 90° c = 32.3644(4) Å gamma = 90°
Volume, Z	3123.3(5) Å ³ , 4
Density (calculated)	1.210 Mg/m ³
Absorption coefficient	0.158 mm ⁻¹
F(000)	1208
Theta range for data collection	1.26 to 22.48 deg.
Limiting indices	-4 ≤ h ≤ 8, 0 ≤ k ≤ 13, -34 ≤ l ≤ 34
Reflections collected	2375
Independent reflections	2356 [R(int) = 0.3380]
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2349 / 0 / 352
Goodness-of-fit on F ²	1.01
Final R indices [I > 2sigma(I)]	R1 = 0.0757, wR2 = 0.118
R indices (all data)	R1 = 0.2032, wR2 = 0.162
Absolute structure parameter	-1.0(5)
Largest diff. peak and hole	0.22 and -0.22 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (36). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O1	2940(12)	1504(6)	2430(2)	53(3)
C2	2099(24)	2048(12)	2741(4)	67(5)
C3	580(21)	2591(11)	2563(5)	63(5)
C4	531(20)	2391(10)	2171(4)	52(4)
C5	1991(20)	1672(9)	2053(4)	41(4)
C6	1204(20)	643(12)	1903(5)	55(5)
O7	1135(11)	704(6)	1482(3)	48(3)
C8	2033(20)	1643(10)	1331(3)	42(4)
C9	3128(18)	2081(10)	1691(4)	38(3)
O10	2629(17)	2022(8)	3093(3)	95(4)
O11	674(14)	-80(7)	2089(3)	71(3)
O12	3198(13)	3135(6)	1668(2)	57(3)
Si13	4423(7)	4104(3)	1860(1)	73(2)
C14	5869(25)	4572(12)	1444(4)	143(9)
C15	2762(23)	5112(9)	2002(4)	95(6)
C16	5624(19)	3712(11)	2323(4)	89(6)
C17	4974(21)	1556(11)	1691(4)	50(4)
O18	6308(14)	2024(7)	1651(3)	76(4)
O19	4830(12)	534(7)	1753(3)	54(3)
C20	6460(18)	-65(12)	1733(4)	79(5)
C21	3006(21)	1393(10)	941(4)	62(5)
O22	1803(14)	1155(6)	624(2)	58(3)
Si23	1594(6)	51(3)	366(1)	53(1)
C24	2318(27)	-1049(11)	699(4)	59(5)
C25	1255(30)	-1434(12)	1013(5)	107(8)
C26	1840(45)	-2188(20)	1292(8)	132(13)
C27	3544(46)	-2507(21)	1250(7)	132(13)
C28	4665(31)	-2202(16)	950(7)	117(8)
C29	3982(29)	-1452(14)	680(5)	92(6)
C30	3046(18)	114(13)	-100(4)	55(4)
C31	3616(25)	1081(14)	-239(5)	89(6)
C32	4562(32)	1160(20)	-601(6)	133(11)
C33	4980(40)	335(27)	-829(8)	163(19)
C34	4377(31)	-607(21)	-703(7)	124(10)
C35	3445(23)	-755(14)	-337(5)	80(5)
C36	-795(21)	42(17)	189(4)	79(5)
C37	-959(21)	909(15)	-131(5)	120(7)
C38	-1309(23)	-1013(14)	5(5)	129(7)
C39	-2019(20)	363(15)	549(5)	148(10)

Table 3. Bond lengths [Å] and angles [deg] for (36).

O1-C2	1.38(2)	C21-H21C	0.96
O1-C5	1.431(12)	O22-Si23	1.649(9)
C2-O10	1.208(14)	Si23-C24	1.85(2)
C2-C3	1.46(2)	Si23-C30	1.866(13)
C3-C4	1.294(14)	Si23-C36	1.89(2)
C3-H3	0.96	C24-C29	1.36(2)
C4-C5	1.49(2)	C24-C25	1.39(2)
C4-H4	0.96	C25-C26	1.39(3)
C5-C6	1.52(2)	C25-H25	0.96
C5-C9	1.54(2)	C26-C27	1.36(3)
C6-O11	1.17(2)	C26-H26	0.96
C6-O7	1.37(2)	C27-C28	1.35(3)
O7-C8	1.462(13)	C27-H27	0.96
C8-C21	1.50(2)	C28-C29	1.40(2)
C8-C9	1.53(2)	C28-H28	0.96
C8-H8	0.96	C29-H29	0.96
C9-O12	1.352(13)	C30-C31	1.38(2)
C9-C17	1.55(2)	C30-C35	1.38(2)
O12-Si13	1.667(9)	C31-C32	1.38(2)
Si13-C16	1.822(14)	C31-H31	0.96
Si13-C14	1.833(14)	C32-C33	1.33(3)
Si13-C15	1.855(14)	C32-H32	0.96
C14-H14A	0.96	C33-C34	1.35(3)
C14-H14B	0.96	C33-H33	0.96
C14-H14C	0.96	C34-C35	1.39(2)
C15-H15A	0.96	C34-H34	0.96
C15-H15B	0.96	C35-H35	0.96
C15-H15C	0.96	C36-C38	1.52(2)
C16-H16A	0.96	C36-C37	1.52(2)
C16-H16B	0.96	C36-C39	1.54(2)
C16-H16C	0.96	C37-H37A	0.96
C17-O18	1.178(14)	C37-H37B	0.96
C17-O19	1.328(14)	C37-H37C	0.96
O19-C20	1.451(13)	C38-H38A	0.96
C20-H20A	0.96	C38-H38B	0.96
C20-H20B	0.96	C38-H38C	0.96
C20-H20C	0.96	C39-H39A	0.96
C21-O22	1.403(14)	C39-H39B	0.96
C21-H21B	0.96	C39-H39C	0.96
C2-O1-C5	108.5(10)	C4-C5-C9	113.4(11)
O10-C2-O1	122(2)	C6-C5-C9	105.4(11)
O10-C2-C3	130(2)	O11-C6-O7	123(2)
O1-C2-C3	108.3(11)	O11-C6-C5	131(2)
C4-C3-C2	108(2)	O7-C6-C5	106.5(13)
C4-C3-H3	125.8(10)	C6-O7-C8	111.2(11)
C2-C3-H3	125.8(9)	O7-C8-C21	109.5(10)
C3-C4-C5	110.7(14)	O7-C8-C9	107.2(9)
C3-C4-H4	124.7(10)	C21-C8-C9	117.0(12)
C5-C4-H4	124.7(7)	O7-C8-H8	107.6(7)
O1-C5-C4	104.2(10)	C21-C8-H8	107.5(8)
O1-C5-C6	109.8(11)	C9-C8-H8	107.6(7)
C4-C5-C6	109.1(12)	O12-C9-C8	110.1(11)
O1-C5-C9	114.9(11)	O12-C9-C5	113.6(11)

C8-C9-C5	98.9(10)	C24-C25-H25	118.8(12)
O12-C9-C17	113.4(12)	C26-C25-H25	119(2)
C8-C9-C17	109.1(10)	C27-C26-C25	116(3)
C5-C9-C17	110.7(11)	C27-C26-H26	122(2)
C9-O12-Si13	138.0(10)	C25-C26-H26	122(2)
O12-Si13-C16	112.3(6)	C28-C27-C26	126(3)
O12-Si13-C14	107.4(6)	C28-C27-H27	117(2)
C16-Si13-C14	113.4(8)	C26-C27-H27	117(2)
O12-Si13-C15	103.5(6)	C27-C28-C29	115(2)
C16-Si13-C15	108.9(6)	C27-C28-H28	123(2)
C14-Si13-C15	110.9(7)	C29-C28-H28	123(2)
Si13-C14-H14A	109.5(6)	C24-C29-C28	125(2)
Si13-C14-H14B	109.4(5)	C24-C29-H29	117.4(11)
H14A-C14-H14B	109.5	C28-C29-H29	118(2)
Si13-C14-H14C	109.5(6)	C31-C30-C35	118.1(14)
H14A-C14-H14C	109.5	C31-C30-Si23	118.9(14)
H14B-C14-H14C	109.5	C35-C30-Si23	122.7(14)
Si13-C15-H15A	109.6(4)	C32-C31-C30	120(2)
Si13-C15-H15B	109.4(4)	C32-C31-H31	119.9(14)
H15A-C15-H15B	109.5	C30-C31-H31	120.0(10)
Si13-C15-H15C	109.5(5)	C33-C32-C31	123(3)
H15A-C15-H15C	109.5	C33-C32-H32	119(2)
H15B-C15-H15C	109.5	C31-C32-H32	118.7(14)
Si13-C16-H16A	109.4(4)	C32-C33-C34	118(3)
Si13-C16-H16B	109.4(5)	C32-C33-H33	121(2)
H16A-C16-H16B	109.5	C34-C33-H33	121(2)
Si13-C16-H16C	109.5(4)	C33-C34-C35	123(3)
H16A-C16-H16C	109.5	C33-C34-H34	118(2)
H16B-C16-H16C	109.5	C35-C34-H34	118.4(14)
O18-C17-O19	126(2)	C30-C35-C34	118(2)
O18-C17-C9	123.4(12)	C30-C35-H35	120.8(10)
O19-C17-C9	110.7(13)	C34-C35-H35	121.0(14)
C17-O19-C20	116.3(12)	C38-C36-C37	111.1(13)
O19-C20-H20A	109.4(7)	C38-C36-C39	112(2)
O19-C20-H20B	109.5(7)	C37-C36-C39	106(2)
H20A-C20-H20B	109.5	C38-C36-Si23	111.5(13)
O19-C20-H20C	109.5(7)	C37-C36-Si23	106.2(13)
H20A-C20-H20C	109.5	C39-C36-Si23	109.8(10)
H20B-C20-H20C	109.5	C36-C37-H37A	109.7(9)
O22-C21-C8	110.2(13)	C36-C37-H37B	109.5(9)
O22-C21-H21B	109.7(7)	H37A-C37-H37B	109.5
C8-C21-H21B	109.6(8)	C36-C37-H37C	109.3(9)
O22-C21-H21C	109.6(7)	H37A-C37-H37C	109.5
C8-C21-H21C	109.6(7)	H37B-C37-H37C	109.5
H21B-C21-H21C	108.2	C36-C38-H38A	109.5(9)
C21-O22-Si23	128.2(9)	C36-C38-H38B	109.6(10)
O22-Si23-C24	109.1(5)	H38A-C38-H38B	109.5
O22-Si23-C30	108.4(7)	C36-C38-H38C	109.3(10)
C24-Si23-C30	109.2(8)	H38A-C38-H38C	109.5
O22-Si23-C36	104.5(7)	H38B-C38-H38C	109.5
C24-Si23-C36	116.9(9)	C36-C39-H39A	109.6(8)
C30-Si23-C36	108.4(6)	C36-C39-H39B	109.3(11)
C29-C24-C25	116(2)	H39A-C39-H39B	109.5
C29-C24-Si23	122.3(14)	C36-C39-H39C	109.6(10)
C25-C24-Si23	122(2)	H39A-C39-H39C	109.5
C24-C25-C26	123(2)	H39B-C39-H39C	109.5

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (36).
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O1	65(7)	62(6)	32(5)	-2(5)	-5(6)	3(6)
C2	88(15)	80(12)	33(9)	4(9)	4(11)	1(12)
C3	64(13)	66(11)	59(10)	4(9)	3(11)	18(11)
C4	49(10)	58(10)	48(9)	4(8)	3(10)	4(10)
C5	50(11)	29(8)	45(9)	-14(7)	-21(9)	12(9)
C6	45(12)	51(11)	71(11)	-7(10)	-11(11)	17(10)
O7	44(7)	49(6)	49(6)	-6(5)	-5(6)	-7(5)
C8	42(10)	41(9)	42(8)	-15(7)	-5(8)	-1(9)
C9	31(9)	41(9)	43(8)	-4(8)	1(9)	3(8)
O10	136(12)	104(8)	45(6)	4(6)	-3(7)	6(9)
O11	75(8)	50(6)	86(7)	18(6)	11(7)	-8(7)
O12	78(7)	32(5)	61(5)	1(5)	-7(7)	-21(6)
Si13	94(4)	56(3)	68(3)	-19(3)	13(3)	-27(3)
C14	192(22)	104(14)	134(15)	-38(12)	97(17)	-69(16)
C15	153(17)	40(8)	90(11)	-13(9)	11(12)	12(13)
C16	80(13)	97(12)	90(11)	-55(11)	-20(11)	-21(12)
C17	55(13)	44(10)	50(9)	-9(9)	-24(10)	-19(10)
O18	61(8)	71(7)	97(8)	-27(7)	11(8)	-31(7)
O19	48(7)	47(6)	67(7)	2(5)	-1(6)	11(6)
C20	60(11)	108(12)	70(10)	6(11)	1(11)	35(12)
C21	77(13)	54(9)	53(9)	-11(8)	-7(11)	11(10)
O22	71(7)	48(6)	55(6)	1(5)	-17(6)	1(6)
Si23	60(3)	54(2)	45(2)	-8(2)	0(2)	-6(3)
C24	99(16)	52(10)	25(8)	-3(8)	3(11)	-2(12)
C25	200(25)	65(12)	55(11)	5(10)	28(15)	-24(16)
C26	239(37)	82(19)	75(16)	-9(14)	53(26)	-64(26)
C27	244(43)	86(17)	65(17)	29(14)	-14(23)	-36(26)
C28	125(21)	98(17)	128(18)	-2(15)	-30(19)	27(17)
C29	109(19)	67(13)	101(14)	26(12)	-34(15)	-10(13)
C30	41(10)	77(10)	47(8)	11(10)	10(8)	-2(12)
C31	101(17)	103(14)	64(12)	44(11)	3(11)	-2(14)
C32	109(21)	207(29)	84(16)	87(18)	6(16)	-59(22)
C33	74(21)	349(60)	67(18)	9(25)	22(15)	21(29)
C34	72(18)	227(33)	74(18)	-30(18)	19(14)	20(22)
C35	68(13)	104(14)	67(10)	-19(11)	-12(11)	20(13)
C36	47(11)	117(14)	73(11)	-31(13)	1(10)	9(14)
C37	67(14)	145(18)	147(17)	-11(16)	-37(13)	57(15)
C38	105(17)	147(18)	136(15)	-44(15)	-16(15)	-51(16)
C39	61(12)	246(28)	138(16)	-70(17)	20(14)	23(18)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (36).

	x	y	z	U(eq)
H3	-241(21)	3025(11)	2711(5)	76
H4	-332(20)	2669(10)	1983(4)	62
H8	1139(20)	2149(10)	1264(3)	50
H14A	6717(25)	4040(12)	1376(4)	215
H14B	6480(25)	5190(12)	1534(4)	215
H14C	5167(25)	4732(12)	1205(4)	215
H15A	2019(23)	4851(9)	2220(4)	142
H15B	2047(23)	5274(9)	1765(4)	142
H15C	3360(23)	5732(9)	2094(4)	142
H16A	6487(19)	3190(11)	2253(4)	134
H16B	4807(19)	3431(11)	2522(4)	134
H16C	6212(19)	4310(11)	2440(4)	134
H20A	6206(18)	-790(12)	1783(4)	119
H20B	7272(18)	185(12)	1939(4)	119
H20C	6981(18)	12(12)	1464(4)	119
H21B	3721(21)	1980(10)	861(4)	74
H21C	3777(21)	807(10)	986(4)	74
H25	68(30)	-1172(12)	1040(5)	128
H26	1081(45)	-2462(20)	1504(8)	158
H27	3981(46)	-3000(21)	1449(7)	158
H28	5845(31)	-2475(16)	925(7)	140
H29	4743(29)	-1202(14)	464(5)	111
H31	3354(25)	1699(14)	-81(5)	107
H32	4939(32)	1839(20)	-692(6)	160
H33	5679(40)	406(27)	-1076(8)	196
H34	4608(31)	-1204(21)	-875(7)	149
H35	3087(23)	-1442(14)	-251(5)	95
H37A	-2154(21)	939(15)	-232(5)	180
H37B	-167(21)	772(15)	-357(5)	180
H37C	-655(21)	1565(15)	-6(5)	180
H38A	-2526(23)	-994(14)	-81(5)	194
H38B	-1155(23)	-1551(14)	209(5)	194
H38C	-567(23)	-1158(14)	-229(5)	194
H39A	-3230(20)	356(15)	458(5)	222
H39B	-1711(20)	1055(15)	639(5)	222
H39C	-1875(20)	-119(15)	774(5)	222

Figure 1. View of C₂₉H₃₆O₈Si₂ (**36**) showing the atom labeling scheme. Thermal ellipsoids are scaled to the 30% probability level. Hydrogen atoms shown are drawn to an arbitrary scale.

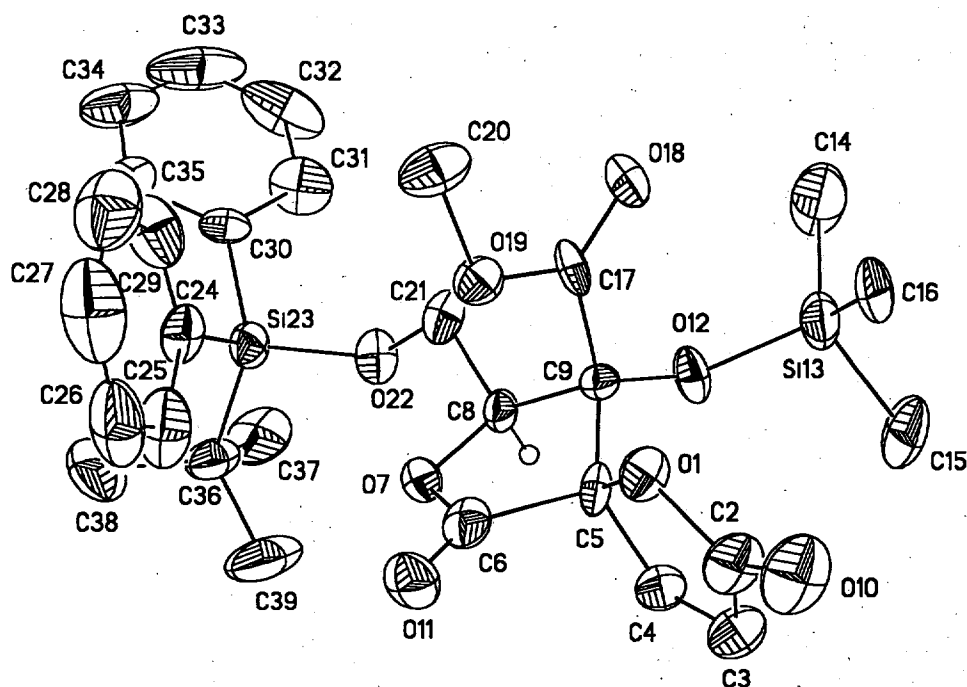
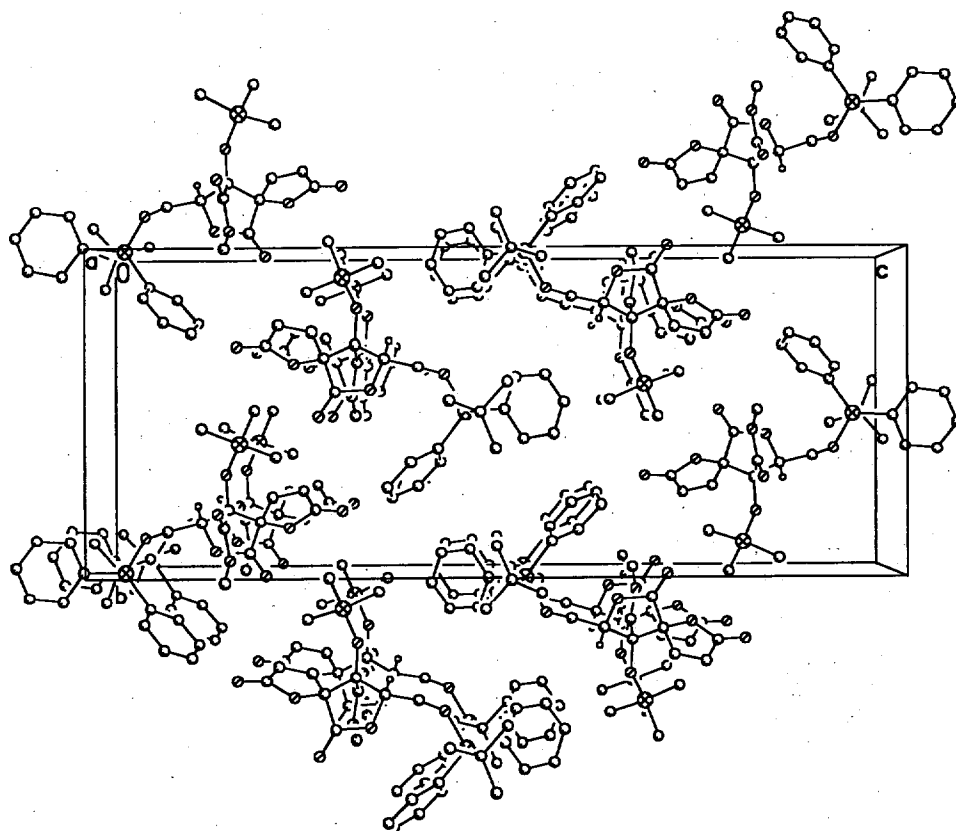


Figure 2. Unit cell packing diagram for $C_{29}H_{36}O_8Si_2$ (**36**). The view is approximately down the *a* axis.



Crystallographic Material for C₂₉H₃₆O₈Si₂ (37).

X-ray Experimental.

Table 1. Crystallographic Data for C₂₉H₃₆O₈Si₂ (37).

Table 2. Fractional coordinates and equivalent isotropic thermal parameters ($\text{\AA}^2$) for the non-hydrogen atoms of C₂₉H₃₆O₈Si₂ (37).

Table 3. Bond Lengths ($\text{\AA}$) and Angles ($^\circ$) for the non-hydrogen atoms of C₂₉H₃₆O₈Si₂ (37).

Table 4. Anisotropic thermal parameters for the non-hydrogen atoms of C₂₉H₃₆O₈Si₂ (37).

Table 5. Fractional coordinates and isotropic thermal parameters ($\text{\AA}^2$) for the hydrogen atoms of C₂₉H₃₆O₈Si₂ (37).

Figure 1. View of C₂₉H₃₆O₈Si₂ (37) showing the atom labeling scheme. Thermal ellipsoids are scaled to the 30% probability level. Most hydrogen atoms have been omitted for clarity.

Figure 2. Unit cell packing diagram for C₂₉H₃₆O₈Si₂ (37). The view is approximately down the **b** axis.

X-ray Experimental for C₂₉H₃₆O₈Si₂ (37): Crystals grew as clusters of thin colorless plates and lathes by slow cooling of a hexane solution. The data crystal was cut from a larger crystal and had approximate dimensions; 0.29 x 0.41 x 0.58 mm. The data were collected using the ω -scan technique at 6 - 12°/min., with a scan range of 1.0° in ω to a $2\theta_{\max} = 50^\circ$ at room temperature on a Siemens P4 diffractometer, equipped with a Nicolet LT-2 low-temperature device and using a graphite monochromator with MoK α radiation ($\lambda = 0.71073\text{\AA}$). Details of crystal data, data collection and structure refinement are listed in Table 1. Three reflections (1,2,-2; 2,-2,-2; 3,-7,0) were remeasured every 96 reflections to monitor instrument and crystal stability. A smoothed curve of the intensities of these check reflections was used to scale the data. The scaling factor ranged from 0.964 - 1.00. The data were corrected for Lp effects but not for absorption. Data reduction, decay correction, structure solution and refinement were performed using the SHELXTL/PC software package.¹ The structure was solved by direct methods and refined by full-matrix least-squares on F² with anisotropic displacement parameters for the non-H atoms. The hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms). The function, $\sum w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.0444*P)^2 + (0.2032*P)]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. The data were corrected for secondary extinction effects. The correction takes the form: $F_{\text{corr}} = kF_c/[1 + (1.0(2)\times 10^{-5}) * F_c^2 \lambda^3/(\sin 2\theta)]^{0.25}$ where k is the overall scale factor. The absolute configuration was assigned on the basis of internal comparison. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).² All figures were generated using SHELXTL/PC.¹ Tables of positional and thermal parameters, bond lengths and angles, figures and lists of observed and calculated structure factors are located in tables 1 through 5.

References

- 1) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.
- 2) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.

Table 1. Crystal data and structure refinement for (37).

Empirical formula	C ₂₉ H ₃₆ O ₈ Si ₂
Formula weight	568.76
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 2 ₁
Unit cell dimensions	a = 12.131(1) Å alpha = 90° b = 7.849(1) Å beta = 102.03(1)° c = 17.062(1) Å gamma = 90°
Volume, Z	1588.9(3) Å ³ , 2
Density (calculated)	1.189 Mg/m ³
Absorption coefficient	0.156 mm ⁻¹
F(000)	604
Crystal size	0.58 x 0.41 x 0.29 mm
Theta range for data collection	2.30 to 25.00 deg.
Limiting indices	-14 ≤ h ≤ 11, 0 ≤ k ≤ 9, -20 ≤ l ≤ 20
Reflections collected	5772
Independent reflections	3032 [R(int) = 0.0291]
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3031 / 1 / 353
Goodness-of-fit on F ²	1.040
Final R indices [I > 2σ(I)]	R ₁ = 0.0414, wR ₂ = 0.0900
R indices (all data)	R ₁ = 0.0609, wR ₂ = 0.0986
Absolute structure parameter	0.1(2)
Extinction coefficient	1.0(2) × 10 ⁻⁵
Largest diff. peak and hole	0.177 and -0.131 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (37). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O1	3235(2)	2632(4)	5653(1)	68(1)
C2	3246(5)	2393(7)	4855(2)	79(1)
C3	4148(5)	1220(7)	4809(3)	86(2)
C4	4667(4)	767(7)	5535(2)	74(1)
C5	4087(3)	1596(5)	6126(2)	58(1)
C6	4823(4)	2804(6)	6722(2)	69(1)
O7	4454(2)	2831(4)	7406(1)	65(1)
C8	3492(3)	1731(5)	7361(2)	53(1)
C9	3543(3)	451(5)	6685(2)	50(1)
O10	2599(3)	3147(5)	4347(2)	115(1)
O11	5604(3)	3639(5)	6614(2)	99(1)
O12	2465(2)	-57(4)	6349(2)	63(1)
Si13	1767(1)	-1669(2)	5844(1)	64(1)
C14	1343(5)	-3170(9)	6547(3)	128(2)
C15	525(4)	-574(9)	5242(3)	110(2)
C16	2553(5)	-2730(8)	5179(3)	113(2)
C17	4321(4)	-1047(6)	6991(2)	60(1)
O18	3989(3)	-2455(5)	7027(3)	116(1)
O19	5370(2)	-562(4)	7219(2)	77(1)
C20	6187(4)	-1893(9)	7543(3)	110(2)
C21	3507(3)	989(6)	8175(2)	57(1)
O22	3378(2)	2294(4)	8717(1)	64(1)
Si23	2300(1)	2613(2)	9144(1)	51(1)
C24	2444(3)	1197(6)	10031(2)	58(1)
C25	3472(4)	409(6)	10344(2)	70(1)
C26	3637(5)	-544(7)	11037(3)	94(2)
C27	2785(6)	-724(8)	11430(3)	108(2)
C28	1767(5)	22(10)	11151(3)	112(2)
C29	1598(4)	990(8)	10454(2)	86(2)
C30	970(3)	2070(6)	8409(2)	63(1)
C31	430(4)	545(9)	8457(3)	95(2)
C32	-519(5)	63(11)	7881(3)	126(2)
C33	-919(5)	1122(13)	7251(3)	124(3)
C34	-404(5)	2647(12)	7197(3)	115(2)
C35	535(3)	3123(8)	7762(2)	86(2)
C36	2484(4)	4896(7)	9494(2)	72(1)
C37	3542(4)	4973(7)	10154(3)	92(2)
C38	2696(8)	6078(9)	8821(4)	169(4)
C39	1495(5)	5496(11)	9831(4)	152(3)

Table 3. Bond lengths [Å] and angles [deg] for (37).

O1-C2	1.377(4)	C21-H21B	0.96
O1-C5	1.425(5)	O22-Si23	1.644(2)
C2-O10	1.197(5)	Si23-C24	1.855(4)
C2-C3	1.445(7)	Si23-C30	1.875(4)
C3-C4	1.316(6)	Si23-C36	1.887(5)
C3-H3	0.96	C24-C29	1.383(5)
C4-C5	1.493(5)	C24-C25	1.395(6)
C4-H4	0.96	C25-C26	1.377(6)
C5-C6	1.534(6)	C25-H25	0.96
C5-C9	1.554(5)	C26-C27	1.352(7)
C6-O11	1.198(5)	C26-H26	0.96
C6-O7	1.333(4)	C27-C28	1.360(8)
O7-C8	1.441(4)	C27-H27	0.96
C8-C21	1.503(5)	C28-C29	1.389(7)
C8-C9	1.540(5)	C28-H28	0.96
C8-H8	0.96	C29-H29	0.96
C9-O12	1.373(4)	C30-C31	1.375(7)
C9-C17	1.530(6)	C30-C35	1.392(6)
O12-Si13	1.661(3)	C31-C32	1.400(7)
Si13-C16	1.827(5)	C31-H31	0.96
Si13-C14	1.831(5)	C32-C33	1.365(9)
Si13-C15	1.848(5)	C32-H32	0.96
C14-H14A	0.96	C33-C34	1.362(10)
C14-H14B	0.96	C33-H33	0.96
C14-H14C	0.96	C34-C35	1.382(7)
C15-H15A	0.96	C34-H34	0.96
C15-H15B	0.96	C35-H35	0.96
C15-H15C	0.96	C36-C39	1.509(7)
C16-H16A	0.96	C36-C37	1.521(6)
C16-H16B	0.96	C36-C38	1.539(7)
C16-H16C	0.96	C37-H37A	0.96
C17-O18	1.182(5)	C37-H37B	0.96
C17-O19	1.307(5)	C37-H37C	0.96
O19-C20	1.467(6)	C38-H38A	0.96
C20-H20A	0.96	C38-H38B	0.96
C20-H20B	0.96	C38-H38C	0.96
C20-H20C	0.96	C39-H39A	0.96
C21-O22	1.410(5)	C39-H39B	0.96
C21-H21A	0.96	C39-H39C	0.96
C2-O1-C5	109.1(3)	C4-C5-C9	118.8(4)
O10-C2-O1	120.6(5)	C6-C5-C9	102.3(3)
O10-C2-C3	131.8(4)	O11-C6-O7	123.2(4)
O1-C2-C3	107.7(4)	O11-C6-C5	127.3(4)
C4-C3-C2	109.9(4)	O7-C6-C5	109.6(4)
C4-C3-H3	125.7(3)	C6-O7-C8	111.1(3)
C2-C3-H3	124.4(2)	O7-C8-C21	109.2(3)
C3-C4-C5	108.5(4)	O7-C8-C9	105.8(3)
C3-C4-H4	126.3(3)	C21-C8-C9	116.4(3)
C5-C4-H4	125.2(2)	O7-C8-H8	108.4(2)
O1-C5-C4	104.7(3)	C21-C8-H8	108.0(2)
O1-C5-C6	106.0(3)	C9-C8-H8	108.8(2)
C4-C5-C6	115.2(3)	O12-C9-C17	112.6(3)
O1-C5-C9	109.1(3)	O12-C9-C8	108.6(3)

C17-C9-C8	111.3(3)	C26-C25-H25	120.8(3)
O12-C9-C5	113.6(3)	C24-C25-H25	117.3(2)
C17-C9-C5	110.1(3)	C27-C26-C25	119.6(5)
C8-C9-C5	99.9(3)	C27-C26-H26	120.9(3)
C9-O12-Si13	140.9(3)	C25-C26-H26	119.4(3)
O12-Si13-C16	113.2(2)	C26-C27-C28	120.8(5)
O12-Si13-C14	109.4(2)	C26-C27-H27	118.5(3)
C16-Si13-C14	111.6(3)	C28-C27-H27	120.6(3)
O12-Si13-C15	101.7(2)	C27-C28-C29	119.8(5)
C16-Si13-C15	109.7(3)	C27-C28-H28	118.7(3)
C14-Si13-C15	110.9(3)	C29-C28-H28	121.5(3)
Si13-C14-H14A	110.2(2)	C24-C29-C28	121.2(5)
Si13-C14-H14B	108.0(2)	C24-C29-H29	118.6(3)
H14A-C14-H14B	109.5	C28-C29-H29	120.2(3)
Si13-C14-H14C	110.3(2)	C31-C30-C35	117.2(4)
H14A-C14-H14C	109.5	C31-C30-Si23	120.8(4)
H14B-C14-H14C	109.5	C35-C30-Si23	121.8(4)
Si13-C15-H15A	110.1(2)	C30-C31-C32	121.7(6)
Si13-C15-H15B	109.5(2)	C30-C31-H31	117.8(3)
H15A-C15-H15B	109.5	C32-C31-H31	120.4(4)
Si13-C15-H15C	108.8(2)	C33-C32-C31	119.5(7)
H15A-C15-H15C	109.5	C33-C32-H32	119.4(4)
H15B-C15-H15C	109.5	C31-C32-H32	121.1(4)
Si13-C16-H16A	110.1(2)	C34-C33-C32	119.7(6)
Si13-C16-H16B	109.5(2)	C34-C33-H33	119.1(4)
H16A-C16-H16B	109.5	C32-C33-H33	121.1(4)
Si13-C16-H16C	108.8(2)	C33-C34-C35	120.9(6)
H16A-C16-H16C	109.5	C33-C34-H34	119.3(4)
H16B-C16-H16C	109.5	C35-C34-H34	119.8(4)
O18-C17-O19	125.3(4)	C34-C35-C30	120.9(6)
O18-C17-C9	122.9(4)	C34-C35-H35	121.1(4)
O19-C17-C9	111.7(4)	C30-C35-H35	118.0(3)
C17-O19-C20	116.3(4)	C39-C36-C37	108.7(4)
O19-C20-H20A	109.4(3)	C39-C36-C38	111.5(6)
O19-C20-H20B	109.2(2)	C37-C36-C38	106.3(5)
H20A-C20-H20B	109.5	C39-C36-Si23	111.5(4)
O19-C20-H20C	109.7(2)	C37-C36-Si23	107.3(3)
H20A-C20-H20C	109.5	C38-C36-Si23	111.3(3)
H20B-C20-H20C	109.5	C36-C37-H37A	110.3(3)
O22-C21-C8	110.1(3)	C36-C37-H37B	109.7(3)
O22-C21-H21A	109.5(2)	H37A-C37-H37B	109.5
C8-C21-H21A	108.9(2)	C36-C37-H37C	108.3(3)
O22-C21-H21B	109.4(2)	H37A-C37-H37C	109.5
C8-C21-H21B	110.3(2)	H37B-C37-H37C	109.5
H21A-C21-H21B	108.7	C36-C38-H38A	109.4(4)
C21-O22-Si23	127.5(2)	C36-C38-H38B	109.4(3)
O22-Si23-C24	108.8(2)	H38A-C38-H38B	109.5
O22-Si23-C30	108.76(14)	C36-C38-H38C	109.6(4)
C24-Si23-C30	109.3(2)	H38A-C38-H38C	109.5
O22-Si23-C36	103.5(2)	H38B-C38-H38C	109.5
C24-Si23-C36	109.0(2)	C36-C39-H39A	109.5(3)
C30-Si23-C36	117.1(2)	C36-C39-H39B	109.5(3)
C29-C24-C25	116.7(4)	H39A-C39-H39B	109.5
C29-C24-Si23	122.9(3)	C36-C39-H39C	109.4(4)
C25-C24-Si23	120.2(3)	H39A-C39-H39C	109.5
C26-C25-C24	121.9(5)	H39B-C39-H39C	109.5

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (37).
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O1	101(2)	61(2)	43(1)	1(1)	16(1)	13(2)
C2	128(4)	61(3)	47(2)	0(2)	17(2)	-1(3)
C3	143(4)	75(3)	49(2)	-10(2)	40(3)	-3(3)
C4	90(3)	78(3)	67(3)	-5(2)	44(2)	5(3)
C5	75(3)	61(3)	41(2)	4(2)	19(2)	4(2)
C6	89(3)	67(3)	52(2)	1(2)	22(2)	-18(3)
O7	85(2)	66(2)	47(1)	-13(1)	24(1)	-23(2)
C8	60(2)	55(2)	44(2)	-10(2)	12(2)	-5(2)
C9	61(2)	47(2)	43(2)	-3(2)	11(2)	-4(2)
O10	176(3)	100(3)	55(2)	15(2)	-3(2)	18(3)
O11	123(3)	107(3)	74(2)	-1(2)	39(2)	-53(3)
O12	59(2)	58(2)	65(2)	-14(1)	2(1)	-2(1)
Si13	78(1)	60(1)	48(1)	1(1)	-3(1)	-12(1)
C14	160(5)	131(5)	77(3)	30(4)	-12(3)	-76(5)
C15	96(4)	103(4)	109(4)	1(4)	-30(3)	-5(4)
C16	132(4)	94(5)	113(4)	-51(4)	23(3)	-8(4)
C17	75(3)	52(3)	51(2)	-5(2)	11(2)	1(2)
O18	106(3)	62(2)	161(4)	21(3)	-16(2)	4(2)
O19	62(2)	87(2)	80(2)	5(2)	10(2)	11(2)
C20	94(3)	145(6)	84(3)	12(4)	1(3)	53(4)
C21	64(2)	64(3)	45(2)	-4(2)	20(2)	-3(2)
O22	61(1)	85(2)	51(1)	-21(2)	24(1)	-16(2)
Si23	49(1)	66(1)	39(1)	-1(1)	13(1)	-1(1)
C24	53(2)	75(3)	46(2)	2(2)	14(2)	-7(2)
C25	71(3)	76(3)	57(2)	0(2)	-2(2)	3(2)
C26	117(4)	74(3)	75(3)	7(3)	-19(3)	6(3)
C27	152(6)	96(4)	61(3)	24(3)	-8(4)	-38(4)
C28	102(4)	161(7)	76(3)	25(4)	23(3)	-43(4)
C29	67(3)	131(5)	61(2)	24(3)	17(2)	-17(3)
C30	54(2)	90(4)	48(2)	-2(2)	14(2)	1(2)
C31	79(3)	122(5)	74(3)	0(3)	-7(2)	-23(4)
C32	101(4)	168(7)	98(4)	-6(5)	-3(3)	-50(5)
C33	84(4)	211(9)	67(3)	-12(5)	-7(3)	-33(5)
C34	93(4)	175(7)	66(3)	26(4)	-6(3)	-2(5)
C35	72(3)	127(5)	54(2)	13(3)	0(2)	-5(3)
C36	76(3)	80(3)	56(2)	-3(2)	7(2)	8(3)
C37	91(4)	80(4)	98(4)	-20(3)	5(3)	-13(3)
C38	328(11)	70(4)	100(4)	19(4)	21(6)	-28(6)
C39	84(4)	161(7)	204(7)	-93(6)	18(4)	24(5)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (37).

	x	y	z	U(eq)
H3	4331(5)	833(7)	4318(3)	103
H4	5325(4)	60(7)	5670(2)	89
H8	2821(3)	2405(5)	7210(2)	63
H14A	1995(5)	-3721(9)	6861(3)	191
H14B	963(5)	-2540(9)	6894(3)	191
H14C	842(5)	-4014(9)	6262(3)	191
H15A	106(4)	-21(9)	5588(3)	165
H15B	769(4)	259(9)	4902(3)	165
H15C	56(4)	-1402(9)	4918(3)	165
H16A	3202(5)	-3294(8)	5488(3)	170
H16B	2077(5)	-3552(8)	4855(3)	170
H16C	2790(5)	-1891(8)	4839(3)	170
H20A	6925(4)	-1400(9)	7694(3)	165
H20B	5980(4)	-2395(9)	8005(3)	165
H20C	6191(4)	-2755(9)	7144(3)	165
H21A	4214(3)	422(6)	8362(2)	68
H21B	2910(3)	174(6)	8146(2)	68
H25	4072(4)	574(6)	10063(2)	84
H26	4352(5)	-1083(7)	11229(3)	113
H27	2914(6)	-1393(8)	11912(3)	129
H28	1180(5)	-134(10)	11445(3)	135
H29	885(4)	1534(8)	10259(2)	103
H31	746(4)	-215(9)	8885(3)	114
H32	-911(5)	-979(11)	7933(3)	151
H33	-1545(5)	796(13)	6835(3)	149
H34	-708(5)	3405(12)	6764(3)	138
H35	901(3)	4195(8)	7724(2)	104
H37A	3666(4)	6114(7)	10356(3)	138
H37B	3465(4)	4220(7)	10582(3)	138
H37C	4170(4)	4619(7)	9932(3)	138
H38A	3327(8)	5660(9)	8620(4)	254
H38B	2855(8)	7208(9)	9029(4)	254
H38C	2039(8)	6101(9)	8395(4)	254
H39A	821(5)	5448(11)	9421(4)	228
H39B	1623(5)	6647(11)	10018(4)	228
H39C	1412(5)	4773(11)	10269(4)	228

Figure 1. View of C₂₉H₃₆O₈Si₂ (**37**) showing the atom labeling scheme. Thermal ellipsoids are scaled to the 30% probability level. Most hydrogen atoms have been omitted for clarity.

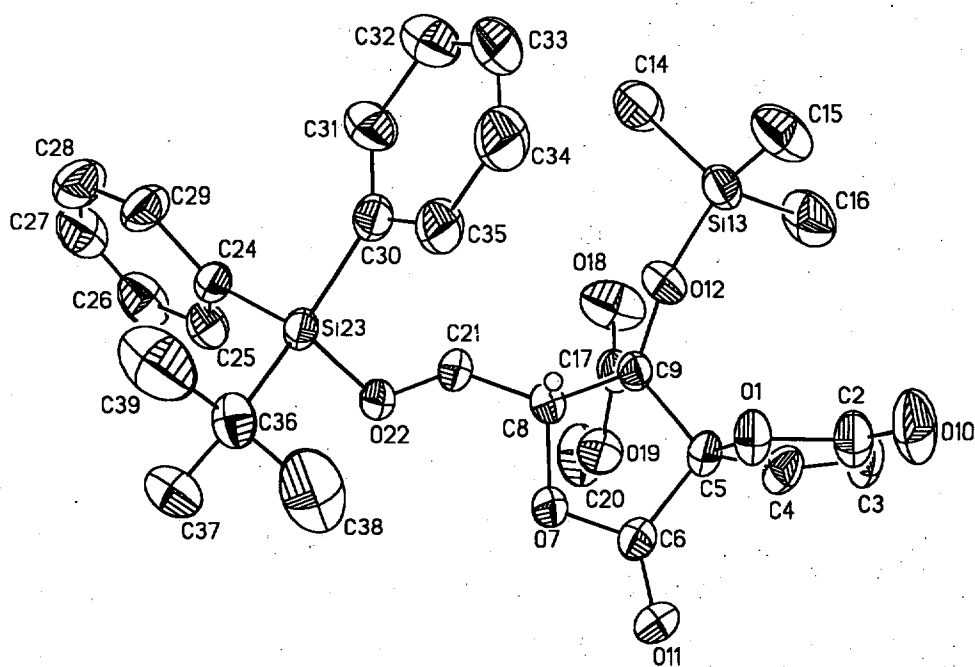
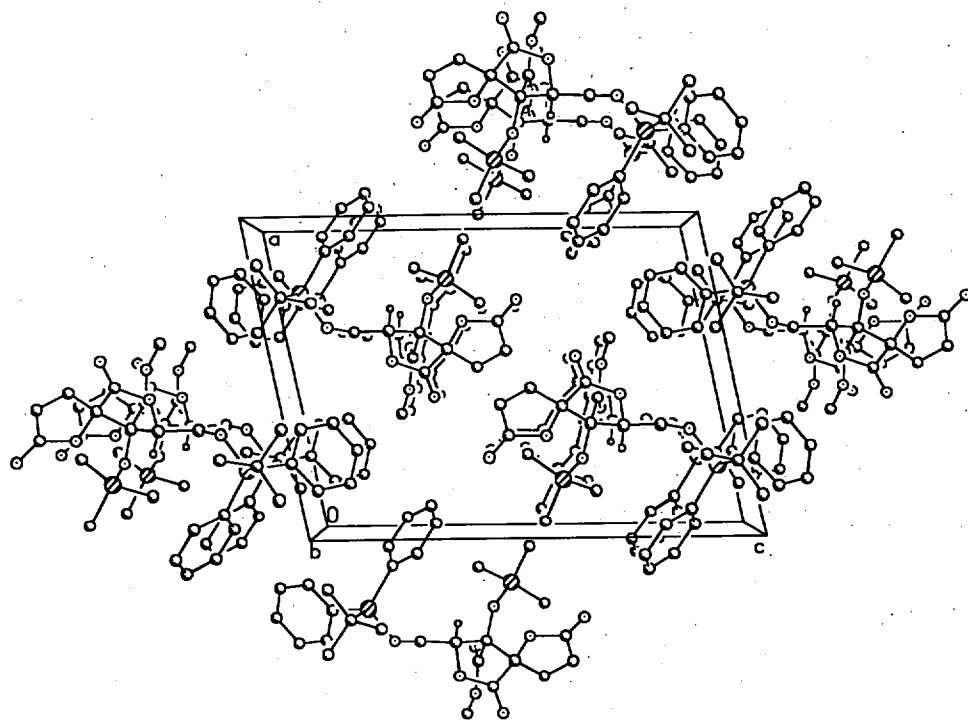


Figure 2. Unit cell packing diagram for $C_{29}H_{36}O_8Si_2$ (**37**). The view is approximately down the **b** axis.



Crystallographic Material for (39).

X-ray Experimental.

Table 1. Crystallographic Data for (39).

Table 2. Fractional coordinates and equivalent isotropic thermal parameters ($\text{\AA}^2$) for the non-hydrogen atoms of (39).

Table 3. Bond Lengths ($\text{\AA}$) and Angles ($^\circ$) for the non-hydrogen atoms of (39).

Table 4. Anisotropic thermal parameters for the non-hydrogen atoms of (39).

Table 5. Fractional coordinates and isotropic thermal parameters ($\text{\AA}^2$) for the hydrogen atoms of (39).

Table 6. Torsion Angles ($^\circ$) for the non-hydrogen atoms of (39).

Figure 1. View of (39) showing the atom labeling scheme. Displacement ellipsoids are scaled to the 30% probability level. Hydrogen atoms are drawn to an arbitrary size.

Figure 2. Unit cell packing diagram for (39). The view is approximately down the **a** axis.

X-ray Experimental for C₂₉H₃₈O₈Si₂ (39): Crystals grew as clusters of colorless lathes and needles by slow cooling of a hexanes/ethyl acetate solution. The data were collected using the ω -scan technique at 3 - 6°/min., with a scan range of 1.0° in ω to a $2\theta_{\max} = 45^\circ$ at -90 °C on a Siemens P4 diffractometer, equipped with a Nicolet LT-2 low-temperature device and using a graphite monochromator with MoK α radiation ($\lambda = 0.71073\text{\AA}$). Details of crystal data, data collection and structure refinement are listed in Table 1. Three reflections (0,0,4; 0,0,-4, 0,1,4) were remeasured every 97 reflections to monitor instrument and crystal stability. A smoothed curve of the intensities of these check reflections was used to scale the data. The scaling factor ranged from 0.943 - 1.03. The data were corrected for Lp effects but not for absorption. Data reduction, decay correction, structure solution and refinement were performed using the SHELXTL/PC software package.¹ The structure was solved by direct methods and refined by full-matrix least-squares on F² with anisotropic displacement parameters for the non-H atoms. The hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms). The function, $\sum w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.0444*P)^2 + (0.2032*P)]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. The data were corrected for secondary extinction effects. The correction takes the form: $F_{\text{corr}} = kF_c/[1 + (4.7(6)\times 10^{-6}) * F_c^2 \lambda^3/(\sin 2\theta)]^{0.25}$ where k is the overall scale factor. The absolute configuration was assigned on the basis of internal comparison. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).² All figures were generated using SHELXTL/PC.¹ Tables of positional and thermal parameters, bond lengths and angles, figures and lists of observed and calculated structure factors are located in tables 1 through 5.

References

- 1) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.
- 2) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.

Table 1. Crystal data and structure refinement for (39).

Empirical formula	C ₂₉ H ₃₈ O ₈ Si ₂	
Formula weight	570.77	
Temperature	183(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	a = 7.1540(10) Å	α = 90°.
	b = 17.573(3) Å	β = 90°.
	c = 23.968(3) Å	γ = 90°.
Volume	3013.2(8) Å ³	
Z	4	
Density (calculated)	1.258 Mg/m ³	
Absorption coefficient	0.164 mm ⁻¹	
F(000)	1216	
Theta range for data collection	2.06 to 22.51°	
Index ranges	-7 ≤ h ≤ 7, -1 ≤ k ≤ 18, -1 ≤ l ≤ 25	
Reflections collected	4724	
Independent reflections	3928 [R(int) = 0.0676]	
Completeness to theta = 22.51°	99.9 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3928 / 0 / 354	
Goodness-of-fit on F ²	1.010	
Final R indices [I > 2σ(I)]	R1 = 0.0726, wR2 = 0.1123	
R indices (all data)	R1 = 0.1511, wR2 = 0.1378	
Absolute structure parameter	0.2(3)	
Extinction coefficient	4.7(6) × 10 ⁻⁶	
Largest diff. peak and hole	0.26 and -0.30 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (39). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O1	5380(8)	2437(3)	2474(2)	37(2)
C2	6994(12)	2101(5)	2322(4)	38(2)
C3	7587(14)	2418(6)	1766(4)	67(3)
C4	6392(12)	3090(5)	1658(3)	42(2)
C5	4795(11)	3001(5)	2081(3)	28(2)
C6	3019(12)	2741(5)	1779(3)	31(2)
O7	1843(7)	3333(3)	1717(2)	31(1)
C8	2534(12)	4004(4)	1992(3)	29(2)
C9	4132(10)	3735(4)	2381(3)	24(2)
O10	7729(9)	1627(4)	2605(3)	58(2)
O11	2664(9)	2123(3)	1605(2)	51(2)
O12	5564(7)	4258(3)	2421(2)	39(2)
Si13	6433(3)	4877(1)	2875(1)	37(1)
C14	4600(12)	5379(5)	3270(4)	61(3)
C15	7645(14)	5549(5)	2407(4)	61(3)
C16	8164(11)	4393(5)	3319(3)	54(3)
C17	3383(12)	3480(4)	2951(3)	27(2)
O18	4065(8)	3661(3)	3386(2)	46(2)
O19	1923(7)	3018(3)	2884(2)	34(2)
C20	1241(12)	2648(5)	3391(3)	53(3)
C21	3153(11)	4592(4)	1555(3)	31(2)
O22	1577(7)	4751(2)	1220(2)	27(1)
Si23	1563(3)	5039(1)	560(1)	23(1)
C24	2809(11)	4292(4)	137(3)	27(2)
C25	3599(12)	4424(5)	-386(3)	40(2)
C26	4488(12)	3840(5)	-673(4)	42(3)
C27	4552(13)	3117(5)	-462(4)	44(3)
C28	3778(13)	2977(5)	42(4)	47(3)
C29	2871(11)	3552(4)	339(3)	33(2)
C30	2682(11)	6004(4)	524(3)	26(2)
C31	2842(11)	6414(5)	1015(3)	33(2)

C32	3681(12)	7126(4)	1036(4)	38(2)
C33	4357(11)	7448(5)	556(4)	41(2)
C34	4248(12)	7038(5)	62(4)	44(3)
C35	3370(12)	6345(4)	37(3)	35(2)
C36	-993(10)	5082(5)	383(3)	34(2)
C37	-1895(12)	4314(5)	524(4)	71(3)
C38	-1273(11)	5266(5)	-228(3)	51(3)
C39	-1915(13)	5709(6)	732(4)	74(4)

Table 3. Bond lengths [Å] and angles [°] for (39).

O1-C2	1.347(9)	C17-O19	1.333(9)
O1-C5	1.429(8)	O19-C20	1.462(8)
C2-O10	1.197(9)	C20-H20A	0.96
C2-C3	1.504(12)	C20-H20B	0.96
C3-C4	1.480(11)	C20-H20C	0.96
C3-H3A	0.96	C21-O22	1.414(8)
C3-H3B	0.96	C21-H21A	0.96
C4-C5	1.535(10)	C21-H21B	0.96
C4-H4A	0.96	O22-Si23	1.659(5)
C4-H4B	0.96	Si23-C30	1.878(8)
C5-C6	1.532(11)	Si23-C36	1.879(7)
C5-C9	1.552(10)	Si23-C24	1.882(8)
C6-O11	1.191(9)	C24-C29	1.390(10)
C6-O7	1.347(9)	C24-C25	1.395(10)
O7-C8	1.439(8)	C25-C26	1.390(10)
C8-C21	1.536(9)	C25-H25	0.96
C8-C9	1.549(10)	C26-C27	1.369(10)
C8-H8A	0.96	C26-H26	0.96
C9-O12	1.380(8)	C27-C28	1.350(11)
C9-C17	1.535(10)	C27-H27	0.96
O12-Si13	1.660(6)	C28-C29	1.396(10)
Si13-C14	1.842(8)	C28-H28	0.96
Si13-C16	1.842(8)	C29-H29	0.96
Si13-C15	1.846(9)	C30-C31	1.384(10)
C14-H14A	0.96	C30-C35	1.402(10)
C14-H14B	0.96	C31-C32	1.388(10)
C14-H14C	0.96	C31-H31	0.96
C15-H15A	0.96	C32-C33	1.372(10)
C15-H15B	0.96	C32-H32	0.96
C15-H15C	0.96	C33-C34	1.388(11)
C16-H16A	0.96	C33-H33	0.96
C16-H16B	0.96	C34-C35	1.371(10)
C16-H16C	0.96	C34-H34	0.96
C17-O18	1.193(8)	C35-H35	0.96

C36-C38	1.514(9)	C38-H38A	0.96
C36-C37	1.532(10)	C38-H38B	0.96
C36-C39	1.533(10)	C38-H38C	0.96
C37-H37A	0.96	C39-H39A	0.96
C37-H37B	0.96	C39-H39B	0.96
C37-H37C	0.96	C39-H39C	0.96
C2-O1-C5	112.1(6)	O7-C8-H8A	109.6
O10-C2-O1	121.8(8)	C21-C8-H8A	107.9
O10-C2-C3	129.5(9)	C9-C8-H8A	109.6
O1-C2-C3	108.7(8)	O12-C9-C17	113.1(7)
C4-C3-C2	106.6(8)	O12-C9-C8	112.8(6)
C4-C3-H3A	111.3	C17-C9-C8	111.6(6)
C2-C3-H3A	111.3	O12-C9-C5	111.0(6)
C4-C3-H3B	109.7	C17-C9-C5	106.1(6)
C2-C3-H3B	109.1	C8-C9-C5	101.5(6)
H3A-C3-H3B	108.8	C9-O12-Si13	139.5(5)
C3-C4-C5	103.5(7)	O12-Si13-C14	112.6(4)
C3-C4-H4A	110.6	O12-Si13-C16	109.1(4)
C5-C4-H4A	110.7	C14-Si13-C16	113.8(4)
C3-C4-H4B	112.1	O12-Si13-C15	101.3(3)
C5-C4-H4B	110.8	C14-Si13-C15	109.9(4)
H4A-C4-H4B	109.0	C16-Si13-C15	109.3(4)
O1-C5-C6	110.3(7)	Si13-C14-H14A	109.4
O1-C5-C4	106.7(6)	Si13-C14-H14B	109.4
C6-C5-C4	109.6(7)	H14A-C14-H14B	109.5
O1-C5-C9	111.2(6)	Si13-C14-H14C	109.7
C6-C5-C9	102.3(6)	H14A-C14-H14C	109.5
C4-C5-C9	116.7(7)	H14B-C14-H14C	109.5
O11-C6-O7	122.2(8)	Si13-C15-H15A	110.3
O11-C6-C5	127.9(8)	Si13-C15-H15B	108.6
O7-C6-C5	109.9(7)	H15A-C15-H15B	109.5
C6-O7-C8	111.6(6)	Si13-C15-H15C	109.5
O7-C8-C21	109.7(6)	H15A-C15-H15C	109.5
O7-C8-C9	106.3(6)	H15B-C15-H15C	109.5
C21-C8-C9	113.7(7)	Si13-C16-H16A	109.9

Si13-C16-H16B	109.3	C25-C26-H26	119.8
H16A-C16-H16B	109.5	C28-C27-C26	119.0(9)
Si13-C16-H16C	109.2	C28-C27-H27	119.8
H16A-C16-H16C	109.5	C26-C27-H27	121.1
H16B-C16-H16C	109.5	C27-C28-C29	121.1(8)
O18-C17-O19	126.1(7)	C27-C28-H28	120.4
O18-C17-C9	123.8(8)	C29-C28-H28	118.5
O19-C17-C9	110.1(6)	C24-C29-C28	121.0(8)
C17-O19-C20	115.6(6)	C24-C29-H29	118.8
O19-C20-H20A	108.4	C28-C29-H29	120.2
O19-C20-H20B	109.2	C31-C30-C35	117.1(7)
H20A-C20-H20B	109.5	C31-C30-Si23	117.8(6)
O19-C20-H20C	110.8	C35-C30-Si23	125.1(6)
H20A-C20-H20C	109.5	C30-C31-C32	122.4(8)
H20B-C20-H20C	109.5	C30-C31-H31	117.8
O22-C21-C8	106.9(6)	C32-C31-H31	119.8
O22-C21-H21A	110.8	C33-C32-C31	119.6(8)
C8-C21-H21A	108.4	C33-C32-H32	119.7
O22-C21-H21B	110.2	C31-C32-H32	120.7
C8-C21-H21B	111.2	C32-C33-C34	118.8(8)
H21A-C21-H21B	109.2	C32-C33-H33	121.3
C21-O22-Si23	127.4(4)	C34-C33-H33	119.9
O22-Si23-C30	108.5(3)	C35-C34-C33	121.6(8)
O22-Si23-C36	103.5(3)	C35-C34-H34	118.9
C30-Si23-C36	111.6(4)	C33-C34-H34	119.5
O22-Si23-C24	107.3(3)	C34-C35-C30	120.3(8)
C30-Si23-C24	113.7(3)	C34-C35-H35	121.1
C36-Si23-C24	111.5(4)	C30-C35-H35	118.5
C29-C24-C25	117.1(7)	C38-C36-C37	110.2(7)
C29-C24-Si23	118.7(6)	C38-C36-C39	108.5(7)
C25-C24-Si23	124.1(6)	C37-C36-C39	109.4(7)
C26-C25-C24	120.5(8)	C38-C36-Si23	110.8(5)
C26-C25-H25	120.6	C37-C36-Si23	108.9(5)
C24-C25-H25	118.9	C39-C36-Si23	108.9(6)
C27-C26-C25	121.2(8)	C36-C37-H37A	111.8
C27-C26-H26	119.0	C36-C37-H37B	107.7

H37A-C37-H37B	109.5	H38A-C38-H38C	109.5
C36-C37-H37C	108.9	H38B-C38-H38C	109.5
H37A-C37-H37C	109.5	C36-C39-H39A	111.0
H37B-C37-H37C	109.5	C36-C39-H39B	108.0
C36-C38-H38A	111.4	H39A-C39-H39B	109.5
C36-C38-H38B	109.0	C36-C39-H39C	109.5
H38A-C38-H38B	109.5	H39A-C39-H39C	109.5
C36-C38-H38C	108.1	H39B-C39-H39C	109.5

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (39). 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}
O1	41(4)	44(4)	26(3)	15(3)	1(3)	14(3)
C2	28(6)	44(6)	42(6)	-16(5)	-3(5)	3(5)
C3	45(6)	79(8)	78(8)	13(7)	33(6)	3(6)
C4	43(6)	48(6)	34(5)	9(5)	13(5)	0(5)
C5	26(5)	37(5)	22(5)	5(5)	-2(4)	5(4)
C6	38(6)	25(5)	31(5)	11(5)	7(5)	-8(5)
O7	27(3)	29(3)	38(4)	4(3)	-4(3)	-4(3)
C8	33(5)	29(5)	25(5)	-4(4)	-5(4)	-2(4)
C9	18(5)	27(5)	28(5)	7(4)	5(4)	-6(4)
O10	55(4)	60(5)	58(4)	11(4)	-18(4)	24(4)
O11	68(5)	35(4)	48(4)	1(3)	-3(4)	-6(4)
O12	37(4)	48(4)	31(3)	5(3)	-4(3)	-13(3)
Si13	38(2)	38(2)	36(1)	-1(1)	-1(1)	3(1)
C14	65(7)	47(6)	72(7)	-8(6)	12(7)	19(6)
C15	79(8)	57(6)	46(6)	-10(6)	-7(6)	-28(6)
C16	44(7)	82(7)	36(5)	-4(6)	0(5)	13(6)
C17	31(5)	27(5)	24(5)	1(4)	1(5)	4(5)
O18	60(4)	53(4)	24(3)	8(3)	-5(3)	-14(3)
O19	36(4)	38(3)	29(3)	9(3)	7(3)	-6(3)
C20	58(7)	49(6)	51(6)	25(5)	9(6)	-9(6)
C21	41(6)	24(5)	28(5)	3(4)	0(5)	-1(5)
O22	25(3)	32(3)	25(3)	2(3)	-2(3)	4(3)
Si23	25(1)	23(1)	20(1)	3(1)	-2(1)	1(1)
C24	28(5)	33(5)	18(5)	0(4)	0(4)	-1(4)
C25	54(6)	29(5)	37(6)	-1(4)	8(5)	1(5)
C26	48(6)	40(6)	38(6)	-6(5)	12(5)	-5(5)
C27	51(7)	37(6)	44(7)	-19(6)	-2(6)	12(5)
C28	58(7)	34(6)	48(6)	1(6)	-14(6)	5(6)
C29	39(6)	28(5)	30(5)	-1(4)	9(4)	2(5)
C30	24(5)	27(5)	27(5)	-4(5)	0(4)	7(4)
C31	29(5)	34(5)	36(6)	6(5)	5(4)	3(5)

C32	40(6)	29(5)	44(6)	-1(5)	-6(5)	2(5)
C33	41(6)	18(5)	64(7)	-5(6)	2(6)	-9(4)
C34	51(7)	32(6)	48(7)	15(5)	16(5)	-7(5)
C35	50(6)	28(5)	28(5)	2(5)	-3(5)	0(5)
C36	25(5)	44(6)	32(5)	18(5)	0(4)	2(5)
C37	30(7)	80(7)	102(9)	45(8)	-9(6)	-23(6)
C38	38(6)	81(7)	35(5)	17(5)	-7(5)	-12(6)
C39	40(7)	107(9)	74(8)	-15(7)	-7(6)	44(7)
