APPENDIX SIX

X-Ray Crystallographic Data Relevant to Chapter Three

CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Crystal Structure Analysis of:

Allylic Alcohol 211 (DCB30)

(CCDC 277462)

Contents:

Figure A6.1 Representation of Allylic Alcohol **211**

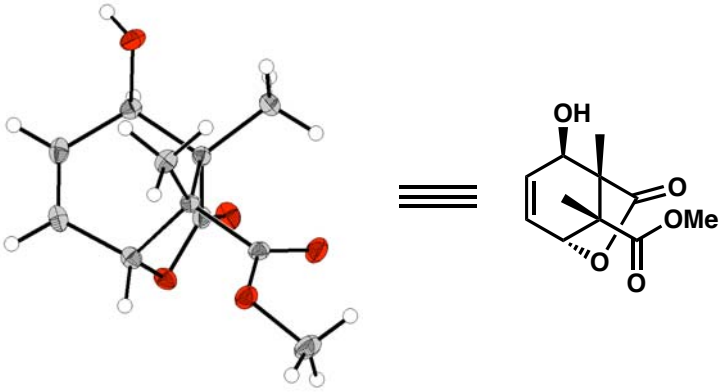

Table 1. Crystal data and structure refinement for DCB30 (CCDC 277462).

Empirical formula	$C_{11}H_{14}O_5$
Formula weight	226.22
Crystallization Solvent	Heptane/diethylether
Crystal Habit	Fragment
Crystal size	0.41 x 0.24 x 0.16 mm^3
Crystal color	Colorless

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 8068 reflections used in lattice determination	2.74 to 39.14°
Unit cell dimensions	a = 8.5469(4) Å b = 8.7203(4) Å c = 14.1988(6) Å
Volume	1058.26(8) $Å^3$
Z	4
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Density (calculated)	1.420 Mg/m^3
F(000)	480
Data collection program	Bruker SMART v5.630
θ range for data collection	2.74 to 40.70°
Completeness to θ = 40.70°	92.3 %
Index ranges	$-15 \le h \le 13$, $-15 \le k \le 15$, $-25 \le l \le 23$
Data collection scan type	ω scans at 5 ϕ settings
Data reduction program	Bruker SAINT v6.45A
Reflections collected	19516
Independent reflections	6114 [R_{int}= 0.0607]
Absorption coefficient	0.113 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9822 and 0.9553

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	Bruker XS v6.12
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	Bruker XL v6.12
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	6114 / 0 / 201
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.304
Final R indices [I>2σ(I), 4485 reflections]	R1 = 0.0415, *w*R2 = 0.0690
R indices (all data)	R1 = 0.0621, *w*R2 = 0.0715
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Absolute structure determination	Not possible to reliably determine absolute configuration
Absolute structure parameter	-0.2(6)
Largest diff. peak and hole	0.427 and -0.273 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for DCB30 (CCDC 277462). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
O(1)	1165(1)	11191(1)	7918(1)	16(1)
O(2)	1872(1)	13004(1)	8946(1)	21(1)
O(3)	4173(1)	9617(1)	8803(1)	21(1)
O(4)	3237(1)	7678(1)	7931(1)	18(1)
O(5)	-878(1)	9680(1)	10618(1)	19(1)
C(1)	-1241(1)	9774(1)	8195(1)	17(1)
C(2)	492(1)	9626(1)	8002(1)	15(1)
C(3)	1380(1)	8989(1)	8868(1)	12(1)
C(4)	1180(1)	10414(1)	9520(1)	12(1)
C(5)	-565(1)	10628(1)	9813(1)	14(1)
C(6)	-1706(1)	10259(1)	9031(1)	17(1)
C(7)	1471(1)	11701(1)	8802(1)	14(1)
C(8)	2214(1)	10544(1)	10395(1)	16(1)
C(9)	763(1)	7465(1)	9253(1)	16(1)
C(10)	3095(1)	8815(1)	8558(1)	14(1)
C(11)	4809(1)	7460(1)	7566(1)	23(1)

Table 3. Bond lengths [Å] and angles [°] for DCB30 (CCDC 277462).

O(1)-C(7)	1.3559(11)	C(8)-C(4)-C(7)	113.05(7)
O(1)-C(2)	1.4855(11)	C(8)-C(4)-C(3)	118.58(7)
O(2)-C(7)	1.2050(11)	C(7)-C(4)-C(3)	99.84(6)
O(3)-C(10)	1.2082(11)	C(8)-C(4)-C(5)	109.06(7)
O(4)-C(10)	1.3387(11)	C(7)-C(4)-C(5)	104.16(7)
O(4)-C(11)	1.4519(12)	C(3)-C(4)-C(5)	111.03(7)
O(5)-C(5)	1.4350(11)	O(5)-C(5)-C(6)	110.00(7)
O(5)-H(5A)	0.783(13)	O(5)-C(5)-C(4)	108.75(7)
C(1)-C(6)	1.3223(13)	C(6)-C(5)-C(4)	113.26(7)
C(1)-C(2)	1.5115(13)	O(5)-C(5)-H(5)	109.9(6)
C(1)-H(1)	0.973(11)	C(6)-C(5)-H(5)	108.8(6)
C(2)-C(3)	1.5486(12)	C(4)-C(5)-H(5)	106.0(6)
C(2)-H(2)	0.989(9)	C(1)-C(6)-C(5)	122.26(8)
C(3)-C(9)	1.5301(12)	C(1)-C(6)-H(6)	120.8(6)
C(3)-C(10)	1.5380(13)	C(5)-C(6)-H(6)	116.9(6)
C(3)-C(4)	1.5586(12)	O(2)-C(7)-O(1)	121.44(8)
C(4)-C(8)	1.5294(12)	O(2)-C(7)-C(4)	128.47(8)
C(4)-C(7)	1.5365(12)	O(1)-C(7)-C(4)	110.07(7)
C(4)-C(5)	1.5600(12)	C(4)-C(8)-H(8A)	108.8(6)
C(5)-C(6)	1.5120(13)	C(4)-C(8)-H(8B)	108.5(7)
C(5)-H(5)	0.994(11)	H(8A)-C(8)-H(8B)	109.1(9)
C(6)-H(6)	0.951(10)	C(4)-C(8)-H(8C)	112.1(7)
C(8)-H(8A)	1.025(12)	H(8A)-C(8)-H(8C)	105.7(10)
C(8)-H(8B)	0.977(11)	H(8B)-C(8)-H(8C)	112.6(10)
C(8)-H(8C)	0.976(12)	C(3)-C(9)-H(9A)	110.7(6)
C(9)-H(9A)	0.987(11)	C(3)-C(9)-H(9B)	111.9(7)
C(9)-H(9B)	0.952(11)	H(9A)-C(9)-H(9B)	104.0(9)
C(9)-H(9C)	0.952(12)	C(3)-C(9)-H(9C)	110.2(7)
C(11)-H(11A)	0.967(12)	H(9A)-C(9)-H(9C)	108.6(9)
C(11)-H(11B)	0.940(13)	H(9B)-C(9)-H(9C)	111.2(10)
C(11)-H(11C)	0.962(12)	O(3)-C(10)-O(4)	123.45(8)
		O(3)-C(10)-C(3)	125.99(8)
C(7)-O(1)-C(2)	107.57(7)	O(4)-C(10)-C(3)	110.48(7)
C(10)-O(4)-C(11)	114.73(8)	O(4)-C(11)-H(11A)	107.9(7)
C(5)-O(5)-H(5A)	104.1(10)	O(4)-C(11)-H(11B)	106.0(8)
C(6)-C(1)-C(2)	119.00(8)	H(11A)-C(11)-H(11B)	111.7(10)
C(6)-C(1)-H(1)	122.2(6)	O(4)-C(11)-H(11C)	108.7(7)
C(2)-C(1)-H(1)	118.8(6)	H(11A)-C(11)-H(11C)	111.6(9)
O(1)-C(2)-C(1)	108.39(7)	H(11B)-C(11)-H(11C)	110.6(10)
O(1)-C(2)-C(3)	101.75(7)		
C(1)-C(2)-C(3)	111.51(7)		
O(1)-C(2)-H(2)	105.7(6)		
C(1)-C(2)-H(2)	112.9(6)		
C(3)-C(2)-H(2)	115.6(5)		
C(9)-C(3)-C(10)	110.19(7)		
C(9)-C(3)-C(2)	115.23(8)		
C(10)-C(3)-C(2)	105.96(7)		
C(9)-C(3)-C(4)	116.29(7)		
C(10)-C(3)-C(4)	110.65(7)		
C(2)-C(3)-C(4)	97.55(7)		

Table 4. Anisotropic displacement parameters ($Å^2 x 10^4$) for DCB30 (CCDC 277462). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	203(3)	149(3)	142(3)	30(2)	-26(3)	-27(3)
O(2)	239(4)	146(3)	239(3)	28(3)	-42(3)	-47(3)
O(3)	154(3)	239(4)	236(3)	-25(3)	30(3)	-54(3)
O(4)	154(3)	204(3)	196(3)	-37(3)	29(3)	16(3)
O(5)	178(3)	213(3)	185(3)	47(3)	60(3)	34(3)
C(1)	159(4)	156(4)	203(4)	11(3)	-58(3)	-11(4)
C(2)	167(4)	130(4)	149(4)	-4(3)	-18(3)	-17(4)
C(3)	129(4)	116(4)	122(3)	8(3)	3(3)	-2(3)
C(4)	120(4)	119(4)	124(3)	11(3)	-4(3)	0(3)
C(5)	147(4)	127(4)	144(4)	9(3)	21(3)	14(3)
C(6)	129(4)	162(4)	230(4)	24(3)	-19(3)	10(4)
C(7)	118(4)	149(4)	157(4)	18(3)	-10(3)	3(3)
C(8)	163(4)	190(5)	138(4)	6(3)	-24(3)	-5(4)
C(9)	154(4)	117(4)	201(4)	11(3)	21(4)	-5(4)
C(10)	148(4)	151(4)	120(4)	32(3)	18(3)	10(4)
C(11)	191(5)	259(6)	230(5)	-5(4)	75(4)	52(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for DCB30 (CCDC 277462).

	x	y	z	U_{iso}
H(5A)	-1603(15)	10067(15)	10856(9)	35(4)
H(1)	-1977(13)	9484(13)	7703(7)	18(3)
H(2)	719(11)	9112(11)	7397(7)	6(2)
H(5)	-680(12)	11727(13)	9986(7)	15(3)
H(6)	-2786(12)	10404(12)	9164(7)	14(3)
H(8A)	1942(13)	11540(14)	10742(8)	23(3)
H(8B)	1993(13)	9673(14)	10807(7)	23(3)
H(8C)	3321(14)	10627(15)	10235(8)	29(3)
H(9A)	1386(12)	7128(12)	9800(8)	17(3)
H(9B)	-271(13)	7561(12)	9496(8)	17(3)
H(9C)	815(14)	6693(14)	8779(8)	27(3)
H(11A)	5491(14)	7243(13)	8093(8)	20(3)
H(11B)	4748(14)	6625(15)	7148(9)	29(3)
H(11C)	5121(13)	8376(14)	7239(8)	20(3)

Table 6. Hydrogen bonds for DCB30 (CCDC 277462) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5A)...O(2)#1	0.783(13)	2.147(13)	2.8567(10)	151.0(13)

Symmetry transformations used to generate equivalent atoms:
#1 x-1/2,-y+5/2,-z+2

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Crystal Structure Analysis of:

Allylic Alcohol 217 (DCB31)

(CCDC 283708)

Contents:

Figure A6.2 Representation of Allylic Alcohol **217**

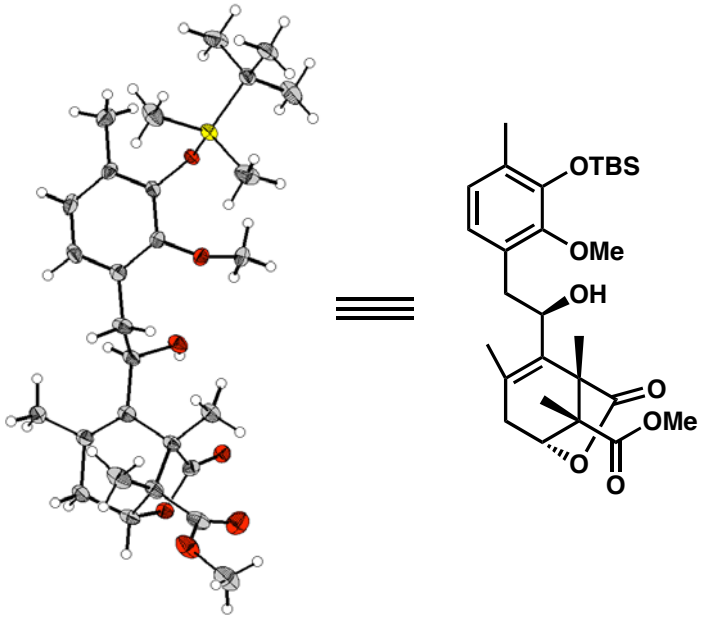

Table 1. Crystal data and structure refinement for DCB31 (CCDC 283708).

Empirical formula	$C_{28}H_{42}O_7$ Si	
Formula weight	518.71	
Crystallization Solvent	EtOAc/heptane	
Crystal Habit	Block	
Crystal size	0.32 x 0.31 x 0.22 mm^3	
Crystal color	Colorless	

Data Collection

Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	100(2) K	
θ range for 15772 reflections used in lattice determination	2.32 to 28.21°	
Unit cell dimensions	a = 12.6604(8) Å b = 15.4100(10) Å c = 15.7147(10) Å	α= 81.0750(10)° β= 66.6280(10)° γ = 87.6100(10)°
Volume	2779.6(3) $Å^3$	
Z	4	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.240 Mg/m^3	
F(000)	1120	
Data collection program	Bruker SMART v5.630	
θ range for data collection	1.75 to 28.27°	
Completeness to θ = 28.27°	92.1 %	
Index ranges	$-16 \le h \le 16, -20 \le k \le 19, -20 \le l \le 20$	
Data collection scan type	ω scans at 7 ϕ settings	
Data reduction program	Bruker SAINT v6.45A	
Reflections collected	56601	
Independent reflections	12691 [R_{int}= 0.0626]	
Absorption coefficient	0.127 mm^{-1}	
Absorption correction	None	
Max. and min. transmission	0.9725 and 0.9604	

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	12691 / 0 / 985
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.502
Final R indices [$I>2\sigma(I)$, 7901 reflections]	R1 = 0.0455, *w*R2 = 0.0721
R indices (all data)	R1 = 0.0839, *w*R2 = 0.0763
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.003
Average shift/error	0.000
Largest diff. peak and hole	0.492 and -0.382 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for DCB31 (CCDC 283708). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Si(1)	-42(1)	510(1)	2060(1)	21(1)
O(1A)	816(1)	1084(1)	2346(1)	19(1)
O(2A)	1297(1)	2515(1)	937(1)	23(1)
O(3A)	3033(1)	4131(1)	770(1)	26(1)
O(4A)	3980(1)	6315(1)	-2542(1)	37(1)
O(5A)	2422(1)	7069(1)	-2515(1)	38(1)
O(6A)	4208(1)	6810(1)	-903(1)	21(1)
O(7A)	4924(1)	5456(1)	-917(1)	22(1)
C(1A)	646(1)	1925(1)	2572(1)	18(1)
C(2A)	899(1)	2648(1)	1864(1)	18(1)
C(3A)	719(1)	3501(1)	2073(1)	21(1)
C(4A)	306(2)	3607(1)	3011(1)	27(1)
C(5A)	107(2)	2895(1)	3709(1)	26(1)
C(6A)	276(1)	2039(1)	3508(1)	20(1)
C(7A)	81(2)	1260(1)	4263(1)	29(1)
C(8A)	2448(2)	2186(2)	597(2)	28(1)
C(9A)	166(2)	811(2)	810(2)	38(1)
C(10A)	-1553(2)	709(2)	2806(2)	35(1)
C(11A)	375(1)	-659(1)	2268(1)	22(1)
C(12A)	-338(2)	-1258(1)	1990(2)	30(1)
C(13A)	1656(2)	-771(2)	1691(2)	37(1)
C(14A)	138(2)	-938(1)	3311(1)	34(1)
C(15A)	999(2)	4291(1)	1317(1)	25(1)
C(16A)	2140(1)	4736(1)	1130(1)	21(1)
C(17A)	2349(1)	5629(1)	503(1)	20(1)
C(18A)	2866(1)	5673(1)	-583(1)	20(1)
C(19A)	2473(1)	6519(1)	-1042(1)	24(1)
C(20A)	3079(2)	7190(1)	-749(1)	24(1)
C(21A)	2454(2)	7262(1)	276(1)	24(1)
C(22A)	2158(1)	6374(1)	879(1)	22(1)
C(23A)	1640(2)	6435(1)	1910(1)	29(1)
C(24A)	2706(2)	4851(1)	-947(1)	25(1)
C(25A)	4114(2)	5923(1)	-833(1)	20(1)
C(26A)	1171(2)	6613(2)	-701(2)	35(1)
C(27A)	3055(2)	6601(1)	-2107(1)	28(1)
C(28A)	2900(3)	7207(2)	-3527(2)	44(1)
Si(2)	5149(1)	9590(1)	2638(1)	21(1)
O(1B)	4218(1)	9004(1)	2444(1)	20(1)
O(2B)	3743(1)	7599(1)	3860(1)	24(1)
O(3B)	1918(1)	5944(1)	4116(1)	26(1)
O(4B)	1344(1)	3774(1)	7408(1)	34(1)
O(5B)	2918(1)	2985(1)	7232(1)	32(1)
O(6B)	863(1)	3261(1)	5877(1)	21(1)
O(7B)	126(1)	4607(1)	5934(1)	23(1)
C(1B)	4350(1)	8159(1)	2224(1)	17(1)
C(2B)	4097(1)	7444(1)	2943(1)	18(1)

C(3B)	4225(1)	6587(1)	2749(1)	21(1)
C(4B)	4584(1)	6466(1)	1817(1)	24(1)
C(5B)	4779(1)	7171(1)	1112(1)	24(1)
C(6B)	4666(1)	8032(1)	1295(1)	19(1)
C(7B)	4854(2)	8801(1)	525(1)	26(1)
C(8B)	2574(2)	7893(1)	4228(1)	29(1)
C(9B)	5680(2)	8968(1)	3484(2)	29(1)
C(10B)	6404(2)	9919(2)	1510(2)	33(1)
C(11B)	4327(2)	10573(1)	3092(1)	25(1)
C(12B)	5122(2)	11175(1)	3282(2)	32(1)
C(13B)	3289(2)	10289(2)	4020(2)	46(1)
C(14B)	3894(2)	11088(2)	2385(2)	46(1)
C(15B)	3966(2)	5805(1)	3514(1)	25(1)
C(16B)	2821(1)	5350(1)	3733(1)	19(1)
C(17B)	2636(1)	4457(1)	4354(1)	19(1)
C(18B)	2219(1)	4416(1)	5438(1)	19(1)
C(19B)	2690(1)	3582(1)	5839(1)	22(1)
C(20B)	2018(2)	2897(1)	5624(1)	22(1)
C(21B)	2507(2)	2827(1)	4603(1)	22(1)
C(22B)	2764(1)	3713(1)	3988(1)	20(1)
C(23B)	3189(2)	3634(1)	2963(1)	26(1)
C(24B)	2419(2)	5244(1)	5771(1)	23(1)
C(25B)	955(2)	4150(1)	5785(1)	19(1)
C(26B)	3999(2)	3506(2)	5394(2)	29(1)
C(27B)	2231(2)	3484(1)	6908(1)	25(1)
C(28B)	2541(2)	2794(2)	8236(1)	35(1)

Table 3. Bond lengths [Å] and angles [°] for DCB31 (CCDC 283708).

Si(1)-O(1A)	1.6602(11)	C(15A)-H(15B)	1.012(16)
Si(1)-C(10A)	1.847(2)	C(16A)-C(17A)	1.529(2)
Si(1)-C(9A)	1.860(2)	C(16A)-H(16A)	1.032(13)
Si(1)-C(11A)	1.8719(17)	C(17A)-C(22A)	1.342(2)
O(1A)-C(1A)	1.3834(18)	C(17A)-C(18A)	1.559(2)
O(2A)-C(2A)	1.3854(18)	C(18A)-C(25A)	1.520(2)
O(2A)-C(8A)	1.440(2)	C(18A)-C(24A)	1.519(2)
O(3A)-C(16A)	1.4266(19)	C(18A)-C(19A)	1.552(2)
O(3A)-H(3A)	0.92(2)	C(19A)-C(26A)	1.525(2)
O(4A)-C(27A)	1.203(2)	C(19A)-C(27A)	1.525(2)
O(5A)-C(27A)	1.337(2)	C(19A)-C(20A)	1.538(2)
O(5A)-C(28A)	1.442(2)	C(20A)-C(21A)	1.506(2)
O(6A)-C(25A)	1.3611(19)	C(20A)-H(20A)	1.015(16)
O(6A)-C(20A)	1.4637(19)	C(21A)-C(22A)	1.505(2)
O(7A)-C(25A)	1.2020(18)	C(21A)-H(21A)	0.976(15)
C(1A)-C(2A)	1.394(2)	C(21A)-H(21B)	1.002(16)
C(1A)-C(6A)	1.393(2)	C(22A)-C(23A)	1.505(2)
C(2A)-C(3A)	1.392(2)	C(23A)-H(23A)	0.95(2)
C(3A)-C(4A)	1.389(2)	C(23A)-H(23B)	0.963(19)
C(3A)-C(15A)	1.508(2)	C(23A)-H(23C)	0.98(2)
C(4A)-C(5A)	1.378(2)	C(24A)-H(24A)	0.973(16)
C(4A)-H(4A)	0.933(16)	C(24A)-H(24B)	1.022(16)
C(5A)-C(6A)	1.392(2)	C(24A)-H(24C)	0.984(16)
C(5A)-H(5A)	0.918(15)	C(26A)-H(26A)	1.042(16)
C(6A)-C(7A)	1.504(2)	C(26A)-H(26B)	0.994(18)
C(7A)-H(7A1)	0.978(19)	C(26A)-H(26C)	0.944(18)
C(7A)-H(7A2)	0.991(17)	C(28A)-H(28A)	0.96(2)
C(7A)-H(7A3)	0.977(17)	C(28A)-H(28B)	1.00(2)
C(8A)-H(8A1)	0.96(2)	C(28A)-H(28C)	0.95(2)
C(8A)-H(8A2)	0.96(2)	Si(2)-O(1B)	1.6614(12)
C(8A)-H(8A3)	0.980(18)	Si(2)-C(9B)	1.844(2)
C(9A)-H(9A1)	0.96(2)	Si(2)-C(10B)	1.864(2)
C(9A)-H(9A2)	0.99(2)	Si(2)-C(11B)	1.8712(17)
C(9A)-H(9A3)	1.04(2)	O(1B)-C(1B)	1.3842(18)
C(10A)-H(10A)	1.032(18)	O(2B)-C(2B)	1.3868(18)
C(10A)-H(10B)	0.95(2)	O(2B)-C(8B)	1.441(2)
C(10A)-H(10C)	0.91(2)	O(3B)-C(16B)	1.4298(19)
C(11A)-C(13A)	1.530(2)	O(3B)-H(3B)	0.98(3)
C(11A)-C(14A)	1.537(2)	O(4B)-C(27B)	1.2025(19)
C(11A)-C(12A)	1.539(2)	O(5B)-C(27B)	1.3347(19)
C(12A)-H(12A)	0.995(16)	O(5B)-C(28B)	1.441(2)
C(12A)-H(12B)	1.002(16)	O(6B)-C(25B)	1.3590(19)
C(12A)-H(12C)	0.939(17)	O(6B)-C(20B)	1.4668(19)
C(13A)-H(13A)	0.986(18)	O(7B)-C(25B)	1.2030(18)
C(13A)-H(13B)	0.990(17)	C(1B)-C(6B)	1.396(2)
C(13A)-H(13C)	1.072(16)	C(1B)-C(2B)	1.396(2)
C(14A)-H(14A)	1.043(18)	C(2B)-C(3B)	1.389(2)
C(14A)-H(14B)	1.016(17)	C(3B)-C(4B)	1.391(2)
C(14A)-H(14C)	0.982(18)	C(3B)-C(15B)	1.509(2)
C(15A)-C(16A)	1.525(2)	C(4B)-C(5B)	1.378(2)
C(15A)-H(15A)	0.967(16)	C(4B)-H(4B)	0.941(15)

C(5B)-C(6B)	1.391(2)	C(26B)-H(26F)	0.902(18)
C(5B)-H(5B)	0.956(15)	C(28B)-H(28D)	0.973(19)
C(6B)-C(7B)	1.508(2)	C(28B)-H(28E)	1.01(2)
C(7B)-H(7B1)	0.984(18)	C(28B)-H(28F)	1.005(18)
C(7B)-H(7B2)	0.973(18)		
C(7B)-H(7B3)	0.959(18)	O(1A)-Si(1)-C(10A)	108.83(9)
C(8B)-H(8B1)	0.994(16)	O(1A)-Si(1)-C(9A)	112.73(9)
C(8B)-H(8B2)	0.949(17)	C(10A)-Si(1)-C(9A)	108.59(12)
C(8B)-H(8B3)	0.976(19)	O(1A)-Si(1)-C(11A)	104.53(7)
C(9B)-H(9B1)	1.021(19)	C(10A)-Si(1)-C(11A)	112.83(9)
C(9B)-H(9B2)	0.968(18)	C(9A)-Si(1)-C(11A)	109.35(9)
C(9B)-H(9B3)	0.910(18)	C(1A)-O(1A)-Si(1)	126.87(10)
C(10B)-H(10D)	0.929(19)	C(2A)-O(2A)-C(8A)	112.94(13)
C(10B)-H(10E)	0.972(19)	C(16A)-O(3A)-H(3A)	109.0(14)
C(10B)-H(10F)	1.041(19)	C(27A)-O(5A)-C(28A)	116.14(17)
C(11B)-C(14B)	1.529(3)	C(25A)-O(6A)-C(20A)	108.79(12)
C(11B)-C(12B)	1.537(3)	O(1A)-C(1A)-C(2A)	119.97(14)
C(11B)-C(13B)	1.541(3)	O(1A)-C(1A)-C(6A)	119.17(14)
C(12B)-H(12D)	0.961(18)	C(2A)-C(1A)-C(6A)	120.77(16)
C(12B)-H(12E)	0.976(16)	O(2A)-C(2A)-C(3A)	119.27(15)
C(12B)-H(12F)	1.036(18)	O(2A)-C(2A)-C(1A)	119.52(15)
C(13B)-H(13D)	0.99(2)	C(3A)-C(2A)-C(1A)	121.17(15)
C(13B)-H(13E)	0.97(2)	C(4A)-C(3A)-C(2A)	117.57(16)
C(13B)-H(13F)	0.988(19)	C(4A)-C(3A)-C(15A)	120.43(17)
C(14B)-H(14D)	1.009(19)	C(2A)-C(3A)-C(15A)	121.96(16)
C(14B)-H(14E)	0.99(2)	C(5A)-C(4A)-C(3A)	121.26(18)
C(14B)-H(14F)	1.010(19)	C(5A)-C(4A)-H(4A)	120.0(10)
C(15B)-C(16B)	1.526(2)	C(3A)-C(4A)-H(4A)	118.7(10)
C(15B)-H(15C)	0.983(16)	C(4A)-C(5A)-C(6A)	121.60(17)
C(15B)-H(15D)	0.969(15)	C(4A)-C(5A)-H(5A)	120.6(10)
C(16B)-C(17B)	1.527(2)	C(6A)-C(5A)-H(5A)	117.8(10)
C(16B)-H(16B)	1.061(14)	C(5A)-C(6A)-C(1A)	117.47(16)
C(17B)-C(22B)	1.336(2)	C(5A)-C(6A)-C(7A)	121.95(16)
C(17B)-C(18B)	1.562(2)	C(1A)-C(6A)-C(7A)	120.58(16)
C(18B)-C(24B)	1.519(2)	C(6A)-C(7A)-H(7A1)	113.2(11)
C(18B)-C(25B)	1.524(2)	C(6A)-C(7A)-H(7A2)	110.5(10)
C(18B)-C(19B)	1.545(2)	H(7A1)-C(7A)-H(7A2)	109.8(14)
C(19B)-C(27B)	1.528(2)	C(6A)-C(7A)-H(7A3)	111.4(10)
C(19B)-C(26B)	1.530(2)	H(7A1)-C(7A)-H(7A3)	105.1(15)
C(19B)-C(20B)	1.538(2)	H(7A2)-C(7A)-H(7A3)	106.4(13)
C(20B)-C(21B)	1.494(2)	O(2A)-C(8A)-H(8A1)	109.8(11)
C(20B)-H(20B)	0.966(15)	O(2A)-C(8A)-H(8A2)	107.6(11)
C(21B)-C(22B)	1.511(2)	H(8A1)-C(8A)-H(8A2)	113.2(16)
C(21B)-H(21C)	1.005(15)	O(2A)-C(8A)-H(8A3)	111.8(10)
C(21B)-H(21D)	0.945(15)	H(8A1)-C(8A)-H(8A3)	106.8(15)
C(22B)-C(23B)	1.505(2)	H(8A2)-C(8A)-H(8A3)	107.7(15)
C(23B)-H(23D)	1.002(18)	Si(1)-C(9A)-H(9A1)	110.4(11)
C(23B)-H(23E)	0.977(19)	Si(1)-C(9A)-H(9A2)	110.6(11)
C(23B)-H(23F)	0.991(17)	H(9A1)-C(9A)-H(9A2)	107.4(16)
C(24B)-H(24D)	0.991(16)	Si(1)-C(9A)-H(9A3)	112.4(11)
C(24B)-H(24E)	0.985(17)	H(9A1)-C(9A)-H(9A3)	108.1(16)
C(24B)-H(24F)	0.994(16)	H(9A2)-C(9A)-H(9A3)	107.9(16)
C(26B)-H(26D)	1.02(2)	Si(1)-C(10A)-H(10A)	108.2(10)
C(26B)-H(26E)	1.022(17)	Si(1)-C(10A)-H(10B)	108.1(11)

H(10A)-C(10A)-H(10B)	104.5(15)	C(20A)-C(19A)-C(18A)	97.74(13)
Si(1)-C(10A)-H(10C)	108.5(13)	O(6A)-C(20A)-C(21A)	109.08(14)
H(10A)-C(10A)-H(10C)	115.9(16)	O(6A)-C(20A)-C(19A)	103.63(13)
H(10B)-C(10A)-H(10C)	111.3(17)	C(21A)-C(20A)-C(19A)	110.94(15)
C(13A)-C(11A)-C(14A)	108.50(17)	O(6A)-C(20A)-H(20A)	107.1(9)
C(13A)-C(11A)-C(12A)	109.27(16)	C(21A)-C(20A)-H(20A)	112.5(9)
C(14A)-C(11A)-C(12A)	108.78(16)	C(19A)-C(20A)-H(20A)	113.0(9)
C(13A)-C(11A)-Si(1)	110.65(13)	C(22A)-C(21A)-C(20A)	112.11(15)
C(14A)-C(11A)-Si(1)	110.17(12)	C(22A)-C(21A)-H(21A)	108.0(9)
C(12A)-C(11A)-Si(1)	109.44(13)	C(20A)-C(21A)-H(21A)	111.1(9)
C(11A)-C(12A)-H(12A)	110.6(9)	C(22A)-C(21A)-H(21B)	111.3(9)
C(11A)-C(12A)-H(12B)	110.9(9)	C(20A)-C(21A)-H(21B)	107.9(9)
H(12A)-C(12A)-H(12B)	109.3(13)	H(21A)-C(21A)-H(21B)	106.3(13)
C(11A)-C(12A)-H(12C)	109.0(11)	C(17A)-C(22A)-C(21A)	121.63(16)
H(12A)-C(12A)-H(12C)	110.9(14)	C(17A)-C(22A)-C(23A)	125.70(16)
H(12B)-C(12A)-H(12C)	106.0(14)	C(21A)-C(22A)-C(23A)	112.67(16)
C(11A)-C(13A)-H(13A)	109.7(10)	C(22A)-C(23A)-H(23A)	115.5(12)
C(11A)-C(13A)-H(13B)	111.0(9)	C(22A)-C(23A)-H(23B)	108.7(11)
H(13A)-C(13A)-H(13B)	106.6(14)	H(23A)-C(23A)-H(23B)	102.7(15)
C(11A)-C(13A)-H(13C)	107.1(9)	C(22A)-C(23A)-H(23C)	113.8(11)
H(13A)-C(13A)-H(13C)	113.9(14)	H(23A)-C(23A)-H(23C)	108.7(17)
H(13B)-C(13A)-H(13C)	108.6(13)	H(23B)-C(23A)-H(23C)	106.5(16)
C(11A)-C(14A)-H(14A)	111.0(10)	C(18A)-C(24A)-H(24A)	112.1(10)
C(11A)-C(14A)-H(14B)	108.8(9)	C(18A)-C(24A)-H(24B)	110.3(9)
H(14A)-C(14A)-H(14B)	107.3(14)	H(24A)-C(24A)-H(24B)	107.2(13)
C(11A)-C(14A)-H(14C)	110.1(10)	C(18A)-C(24A)-H(24C)	111.6(9)
H(14A)-C(14A)-H(14C)	111.2(14)	H(24A)-C(24A)-H(24C)	107.9(13)
H(14B)-C(14A)-H(14C)	108.3(14)	H(24B)-C(24A)-H(24C)	107.4(13)
C(3A)-C(15A)-C(16A)	112.34(15)	O(7A)-C(25A)-O(6A)	121.67(15)
C(3A)-C(15A)-H(15A)	110.7(9)	O(7A)-C(25A)-C(18A)	129.29(16)
C(16A)-C(15A)-H(15A)	105.5(9)	O(6A)-C(25A)-C(18A)	108.93(14)
C(3A)-C(15A)-H(15B)	110.2(9)	C(19A)-C(26A)-H(26A)	110.5(9)
C(16A)-C(15A)-H(15B)	110.8(9)	C(19A)-C(26A)-H(26B)	107.7(10)
H(15A)-C(15A)-H(15B)	107.2(13)	H(26A)-C(26A)-H(26B)	107.1(13)
O(3A)-C(16A)-C(15A)	107.75(15)	C(19A)-C(26A)-H(26C)	109.7(11)
O(3A)-C(16A)-C(17A)	112.97(13)	H(26A)-C(26A)-H(26C)	109.4(14)
C(15A)-C(16A)-C(17A)	113.83(14)	H(26B)-C(26A)-H(26C)	112.4(15)
O(3A)-C(16A)-H(16A)	99.6(7)	O(4A)-C(27A)-O(5A)	123.21(17)
C(15A)-C(16A)-H(16A)	112.7(7)	O(4A)-C(27A)-C(19A)	125.58(16)
C(17A)-C(16A)-H(16A)	109.1(7)	O(5A)-C(27A)-C(19A)	111.16(16)
C(22A)-C(17A)-C(16A)	120.51(15)	O(5A)-C(28A)-H(28A)	110.6(12)
C(22A)-C(17A)-C(18A)	119.78(15)	O(5A)-C(28A)-H(28B)	103.5(13)
C(16A)-C(17A)-C(18A)	119.58(15)	H(28A)-C(28A)-H(28B)	109.6(18)
C(25A)-C(18A)-C(24A)	114.37(15)	O(5A)-C(28A)-H(28C)	110.8(11)
C(25A)-C(18A)-C(19A)	100.28(13)	H(28A)-C(28A)-H(28C)	112.4(17)
C(24A)-C(18A)-C(19A)	113.17(14)	H(28B)-C(28A)-H(28C)	109.6(17)
C(25A)-C(18A)-C(17A)	101.39(12)	O(1B)-Si(2)-C(9B)	112.15(8)
C(24A)-C(18A)-C(17A)	116.05(14)	O(1B)-Si(2)-C(10B)	109.07(9)
C(19A)-C(18A)-C(17A)	109.92(14)	C(9B)-Si(2)-C(10B)	108.51(10)
C(26A)-C(19A)-C(27A)	112.09(16)	O(1B)-Si(2)-C(11B)	104.44(7)
C(26A)-C(19A)-C(20A)	114.62(16)	C(9B)-Si(2)-C(11B)	111.62(9)
C(27A)-C(19A)-C(20A)	106.69(14)	C(10B)-Si(2)-C(11B)	111.00(9)
C(26A)-C(19A)-C(18A)	114.66(15)	C(1B)-O(1B)-Si(2)	127.35(10)
C(27A)-C(19A)-C(18A)	109.97(14)	C(2B)-O(2B)-C(8B)	112.18(13)

C(16B)-O(3B)-H(3B)	107.7(14)	C(11B)-C(12B)-H(12F)	112.8(10)
C(27B)-O(5B)-C(28B)	116.43(15)	H(12D)-C(12B)-H(12F)	105.8(14)
C(25B)-O(6B)-C(20B)	108.58(13)	H(12E)-C(12B)-H(12F)	110.6(14)
O(1B)-C(1B)-C(6B)	119.68(14)	C(11B)-C(13B)-H(13D)	109.3(12)
O(1B)-C(1B)-C(2B)	119.45(14)	C(11B)-C(13B)-H(13E)	110.6(12)
C(6B)-C(1B)-C(2B)	120.76(16)	H(13D)-C(13B)-H(13E)	108.2(17)
O(2B)-C(2B)-C(3B)	119.92(14)	C(11B)-C(13B)-H(13F)	108.0(10)
O(2B)-C(2B)-C(1B)	118.93(15)	H(13D)-C(13B)-H(13F)	110.4(16)
C(3B)-C(2B)-C(1B)	121.12(15)	H(13E)-C(13B)-H(13F)	110.3(16)
C(2B)-C(3B)-C(4B)	117.72(16)	C(11B)-C(14B)-H(14D)	109.6(10)
C(2B)-C(3B)-C(15B)	121.99(16)	C(11B)-C(14B)-H(14E)	110.8(12)
C(4B)-C(3B)-C(15B)	120.27(17)	H(14D)-C(14B)-H(14E)	105.5(15)
C(5B)-C(4B)-C(3B)	121.15(17)	C(11B)-C(14B)-H(14F)	108.6(12)
C(5B)-C(4B)-H(4B)	119.8(9)	H(14D)-C(14B)-H(14F)	115.0(16)
C(3B)-C(4B)-H(4B)	119.0(9)	H(14E)-C(14B)-H(14F)	107.3(17)
C(4B)-C(5B)-C(6B)	121.71(17)	C(3B)-C(15B)-C(16B)	112.59(15)
C(4B)-C(5B)-H(5B)	120.8(10)	C(3B)-C(15B)-H(15C)	108.3(10)
C(6B)-C(5B)-H(5B)	117.5(10)	C(16B)-C(15B)-H(15C)	110.0(9)
C(5B)-C(6B)-C(1B)	117.39(16)	C(3B)-C(15B)-H(15D)	110.1(9)
C(5B)-C(6B)-C(7B)	121.52(16)	C(16B)-C(15B)-H(15D)	107.5(9)
C(1B)-C(6B)-C(7B)	121.08(16)	H(15C)-C(15B)-H(15D)	108.3(13)
C(6B)-C(7B)-H(7B1)	113.2(10)	O(3B)-C(16B)-C(17B)	112.54(13)
C(6B)-C(7B)-H(7B2)	112.6(10)	O(3B)-C(16B)-C(15B)	108.21(14)
H(7B1)-C(7B)-H(7B2)	104.5(15)	C(17B)-C(16B)-C(15B)	114.24(14)
C(6B)-C(7B)-H(7B3)	111.5(11)	O(3B)-C(16B)-H(16B)	98.2(7)
H(7B1)-C(7B)-H(7B3)	109.7(14)	C(17B)-C(16B)-H(16B)	110.5(8)
H(7B2)-C(7B)-H(7B3)	104.8(14)	C(15B)-C(16B)-H(16B)	112.1(7)
O(2B)-C(8B)-H(8B1)	110.8(9)	C(22B)-C(17B)-C(16B)	120.84(15)
O(2B)-C(8B)-H(8B2)	107.1(10)	C(22B)-C(17B)-C(18B)	119.74(14)
H(8B1)-C(8B)-H(8B2)	110.8(14)	C(16B)-C(17B)-C(18B)	119.31(14)
O(2B)-C(8B)-H(8B3)	109.1(11)	C(24B)-C(18B)-C(25B)	113.84(15)
H(8B1)-C(8B)-H(8B3)	107.0(14)	C(24B)-C(18B)-C(19B)	113.46(14)
H(8B2)-C(8B)-H(8B3)	112.0(14)	C(25B)-C(18B)-C(19B)	100.43(13)
Si(2)-C(9B)-H(9B1)	110.4(11)	C(24B)-C(18B)-C(17B)	116.12(14)
Si(2)-C(9B)-H(9B2)	109.6(10)	C(25B)-C(18B)-C(17B)	102.22(12)
H(9B1)-C(9B)-H(9B2)	106.8(15)	C(19B)-C(18B)-C(17B)	109.14(13)
Si(2)-C(9B)-H(9B3)	109.9(11)	C(27B)-C(19B)-C(26B)	112.00(15)
H(9B1)-C(9B)-H(9B3)	110.6(15)	C(27B)-C(19B)-C(20B)	105.71(14)
H(9B2)-C(9B)-H(9B3)	109.6(15)	C(26B)-C(19B)-C(20B)	114.79(16)
Si(2)-C(10B)-H(10D)	109.2(11)	C(27B)-C(19B)-C(18B)	110.73(14)
Si(2)-C(10B)-H(10E)	110.5(10)	C(26B)-C(19B)-C(18B)	114.56(14)
H(10D)-C(10B)-H(10E)	107.8(15)	C(20B)-C(19B)-C(18B)	97.96(13)
Si(2)-C(10B)-H(10F)	113.3(10)	O(6B)-C(20B)-C(21B)	108.63(14)
H(10D)-C(10B)-H(10F)	108.2(15)	O(6B)-C(20B)-C(19B)	103.56(13)
H(10E)-C(10B)-H(10F)	107.7(14)	C(21B)-C(20B)-C(19B)	111.22(14)
C(14B)-C(11B)-C(12B)	109.06(17)	O(6B)-C(20B)-H(20B)	107.2(9)
C(14B)-C(11B)-C(13B)	108.9(2)	C(21B)-C(20B)-H(20B)	112.0(9)
C(12B)-C(11B)-C(13B)	108.43(17)	C(19B)-C(20B)-H(20B)	113.7(9)
C(14B)-C(11B)-Si(2)	111.31(14)	C(20B)-C(21B)-C(22B)	112.67(15)
C(12B)-C(11B)-Si(2)	108.80(13)	C(20B)-C(21B)-H(21C)	110.0(8)
C(13B)-C(11B)-Si(2)	110.29(13)	C(22B)-C(21B)-H(21C)	110.7(8)
C(11B)-C(12B)-H(12D)	110.8(11)	C(20B)-C(21B)-H(21D)	108.8(9)
C(11B)-C(12B)-H(12E)	111.3(10)	C(22B)-C(21B)-H(21D)	110.2(9)
H(12D)-C(12B)-H(12E)	105.1(14)	H(21C)-C(21B)-H(21D)	104.2(12)

C(17B)-C(22B)-C(23B)	126.52(16)
C(17B)-C(22B)-C(21B)	121.36(15)
C(23B)-C(22B)-C(21B)	112.11(15)
C(22B)-C(23B)-H(23D)	115.8(10)
C(22B)-C(23B)-H(23E)	113.2(10)
H(23D)-C(23B)-H(23E)	108.1(14)
C(22B)-C(23B)-H(23F)	108.3(9)
H(23D)-C(23B)-H(23F)	104.7(13)
H(23E)-C(23B)-H(23F)	105.9(14)
C(18B)-C(24B)-H(24D)	113.2(9)
C(18B)-C(24B)-H(24E)	110.4(10)
H(24D)-C(24B)-H(24E)	108.6(13)
C(18B)-C(24B)-H(24F)	110.5(9)
H(24D)-C(24B)-H(24F)	108.5(13)
H(24E)-C(24B)-H(24F)	105.3(13)
O(7B)-C(25B)-O(6B)	121.65(16)
O(7B)-C(25B)-C(18B)	129.16(16)
O(6B)-C(25B)-C(18B)	109.13(14)
C(19B)-C(26B)-H(26D)	109.0(11)
C(19B)-C(26B)-H(26E)	109.2(9)
H(26D)-C(26B)-H(26E)	111.8(14)
C(19B)-C(26B)-H(26F)	110.8(11)
H(26D)-C(26B)-H(26F)	105.9(15)
H(26E)-C(26B)-H(26F)	110.2(15)
O(4B)-C(27B)-O(5B)	123.36(17)
O(4B)-C(27B)-C(19B)	125.61(16)
O(5B)-C(27B)-C(19B)	110.94(15)
O(5B)-C(28B)-H(28D)	112.0(11)
O(5B)-C(28B)-H(28E)	107.3(11)
H(28D)-C(28B)-H(28E)	117.1(16)
O(5B)-C(28B)-H(28F)	112.6(10)
H(28D)-C(28B)-H(28F)	96.4(14)
H(28E)-C(28B)-H(28F)	111.3(15)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for DCB31 (CCDC 283708). The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2 a^{*2} U^{11}$ + ... + 2 h k a* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si(1)	246(3)	166(3)	247(3)	-46(2)	-122(2)	20(2)
O(1A)	218(7)	140(6)	209(6)	-42(5)	-89(5)	25(5)
O(2A)	235(7)	253(7)	173(6)	-30(5)	-67(5)	39(6)
O(3A)	198(7)	203(7)	373(8)	-42(6)	-118(6)	22(6)
O(4A)	350(8)	465(9)	301(8)	4(7)	-165(6)	64(7)
O(5A)	562(9)	293(8)	437(9)	-82(7)	-372(7)	140(7)
O(6A)	189(7)	196(7)	260(7)	-20(5)	-99(5)	-15(5)
O(7A)	170(7)	244(7)	230(7)	-32(5)	-82(5)	31(6)
C(1A)	140(9)	163(10)	236(10)	-59(8)	-64(8)	2(8)
C(2A)	125(9)	219(10)	200(10)	-34(8)	-58(7)	3(8)
C(3A)	99(9)	196(10)	304(11)	-37(8)	-44(8)	0(8)
C(4A)	175(10)	184(11)	378(12)	-115(10)	-14(9)	-18(8)
C(5A)	205(10)	327(12)	211(11)	-121(9)	0(8)	-51(9)
C(6A)	156(9)	238(11)	176(10)	-32(8)	-27(8)	-46(8)
C(7A)	308(13)	319(13)	205(11)	-27(9)	-78(9)	-47(11)
C(8A)	227(12)	296(13)	235(12)	-65(10)	4(9)	37(10)
C(9A)	642(18)	241(13)	365(13)	-23(10)	-322(13)	-22(12)
C(10A)	281(12)	289(13)	538(16)	-137(12)	-195(11)	40(10)
C(11A)	254(10)	188(10)	231(10)	-56(8)	-103(8)	11(8)
C(12A)	390(14)	169(12)	358(13)	-41(10)	-182(11)	1(10)
C(13A)	351(13)	250(13)	550(16)	-136(11)	-187(12)	57(10)
C(14A)	506(15)	206(12)	379(13)	22(10)	-264(12)	-19(11)
C(15A)	157(10)	174(11)	395(13)	2(9)	-100(9)	-11(8)
C(16A)	163(10)	150(10)	287(11)	-20(8)	-78(8)	13(8)
C(17A)	116(9)	190(10)	297(10)	-27(8)	-78(8)	-11(8)
C(18A)	178(10)	160(10)	270(10)	-26(8)	-103(8)	10(8)
C(19A)	222(10)	189(10)	341(11)	-43(8)	-145(9)	34(8)
C(20A)	242(11)	139(10)	339(11)	8(9)	-143(9)	4(8)
C(21A)	213(11)	162(10)	324(11)	-52(9)	-93(9)	17(9)
C(22A)	140(9)	178(10)	300(11)	-25(8)	-48(8)	10(8)
C(23A)	272(12)	208(12)	307(12)	-50(10)	-27(10)	10(10)
C(24A)	238(12)	217(11)	321(12)	-52(9)	-141(10)	12(9)
C(25A)	220(10)	213(11)	163(9)	-8(8)	-94(8)	-19(8)
C(26A)	263(12)	263(13)	599(16)	-47(12)	-252(12)	52(10)
C(27A)	365(12)	184(11)	394(12)	-14(9)	-269(10)	-28(9)
C(28A)	750(20)	329(15)	444(15)	-103(12)	-428(14)	111(14)
Si(2)	224(3)	166(3)	247(3)	-30(2)	-96(2)	14(2)
O(1B)	223(7)	140(7)	237(7)	-21(5)	-98(5)	13(5)
O(2B)	255(7)	269(7)	176(7)	0(6)	-64(5)	-3(6)
O(3B)	237(8)	179(7)	385(8)	-45(6)	-133(6)	34(6)
O(4B)	300(8)	425(9)	267(7)	-10(6)	-100(6)	72(7)
O(5B)	431(8)	303(8)	273(7)	-35(6)	-207(6)	95(6)
O(6B)	175(7)	173(7)	257(7)	-21(5)	-58(5)	-15(5)
O(7B)	179(7)	243(7)	246(7)	-58(6)	-74(5)	33(6)
C(1B)	149(9)	135(9)	218(10)	-21(8)	-63(8)	1(7)
C(2B)	141(9)	212(10)	167(9)	1(8)	-48(7)	7(8)

C(3B)	121(9)	188(10)	273(10)	15(8)	-54(8)	-24(8)
C(4B)	182(10)	150(11)	346(12)	-63(9)	-58(9)	-11(8)
C(5B)	171(10)	289(12)	213(11)	-96(9)	-15(8)	-23(8)
C(6B)	149(9)	212(10)	178(9)	-1(8)	-37(7)	-24(8)
C(7B)	294(12)	270(12)	189(11)	31(9)	-89(9)	-29(10)
C(8B)	303(13)	269(13)	222(12)	-62(10)	-26(9)	15(10)
C(9B)	321(13)	249(12)	356(13)	-55(10)	-177(11)	25(10)
C(10B)	290(12)	329(13)	334(13)	-78(11)	-82(10)	-43(11)
C(11B)	242(10)	183(10)	341(11)	-73(8)	-111(9)	19(8)
C(12B)	332(13)	219(12)	412(14)	-126(10)	-134(11)	19(10)
C(13B)	329(14)	304(14)	624(18)	-215(13)	7(12)	17(12)
C(14B)	586(17)	253(13)	755(19)	-156(13)	-461(16)	154(13)
C(15B)	181(11)	171(11)	348(12)	48(9)	-92(9)	-14(9)
C(16B)	171(10)	135(10)	264(10)	2(8)	-92(8)	-13(8)
C(17B)	128(9)	179(10)	227(10)	0(8)	-58(8)	-16(8)
C(18B)	186(10)	141(10)	236(10)	-8(8)	-88(8)	-2(8)
C(19B)	231(10)	186(10)	232(10)	-4(8)	-93(8)	9(8)
C(20B)	213(10)	139(10)	267(11)	27(8)	-74(8)	0(8)
C(21B)	215(11)	154(10)	265(11)	-55(8)	-66(9)	22(9)
C(22B)	169(10)	174(10)	218(10)	-17(8)	-50(8)	-14(8)
C(23B)	279(12)	219(12)	218(11)	-32(9)	-31(9)	14(10)
C(24B)	243(12)	193(11)	284(12)	-45(9)	-124(9)	-5(9)
C(25B)	231(10)	207(10)	142(9)	-28(8)	-79(8)	-4(9)
C(26B)	214(11)	284(13)	350(13)	20(10)	-119(10)	53(10)
C(27B)	272(11)	193(10)	312(11)	-10(9)	-156(9)	-17(9)
C(28B)	468(15)	337(13)	264(12)	-40(10)	-188(11)	62(12)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for DCB31 (CCDC 283708).

	x	y	z	U_{iso}
H(3A)	3688(19)	4314(14)	814(14)	78(8)
H(4A)	201(13)	4175(11)	3162(11)	30(5)
H(5A)	-132(13)	2974(10)	4325(11)	25(5)
H(7A1)	-544(16)	867(12)	4330(12)	46(6)
H(7A2)	-69(13)	1455(11)	4872(12)	32(5)
H(7A3)	760(15)	894(11)	4127(11)	40(6)
H(8A1)	2967(16)	2594(13)	644(12)	53(7)
H(8A2)	2642(16)	2081(13)	-37(14)	60(7)
H(8A3)	2505(14)	1627(12)	968(12)	41(6)
H(9A1)	45(16)	1427(14)	673(13)	59(7)
H(9A2)	-397(16)	488(13)	676(13)	58(7)
H(9A3)	985(18)	670(14)	351(14)	71(8)
H(10A)	-1676(14)	505(12)	3497(13)	46(6)
H(10B)	-2032(17)	324(13)	2692(13)	55(7)
H(10C)	-1708(17)	1284(14)	2659(14)	66(8)
H(12A)	-171(13)	-1113(10)	1309(12)	28(5)
H(12B)	-1181(15)	-1199(10)	2360(11)	29(5)
H(12C)	-170(14)	-1847(12)	2143(11)	33(5)
H(13A)	1874(15)	-1379(12)	1840(12)	45(6)
H(13B)	2135(14)	-385(11)	1849(11)	29(5)
H(13C)	1796(13)	-581(11)	968(12)	34(5)
H(14A)	-721(16)	-845(12)	3734(12)	49(6)
H(14B)	627(14)	-554(11)	3490(11)	31(5)
H(14C)	355(14)	-1552(12)	3421(12)	43(6)
H(15A)	425(13)	4736(10)	1503(10)	25(5)
H(15B)	998(13)	4120(11)	721(11)	30(5)
H(16A)	2236(11)	4803(8)	1738(9)	3(4)
H(20A)	3219(13)	7783(11)	-1165(11)	34(5)
H(21A)	2915(13)	7589(10)	494(10)	21(5)
H(21B)	1745(13)	7611(10)	350(10)	26(5)
H(23A)	1387(17)	5894(14)	2315(14)	64(7)
H(23B)	941(17)	6760(13)	2048(12)	54(7)
H(23C)	2132(17)	6743(13)	2117(13)	60(7)
H(24A)	3128(14)	4891(11)	-1621(12)	33(5)
H(24B)	1857(15)	4754(10)	-810(11)	32(5)
H(24C)	2960(13)	4324(11)	-645(11)	28(5)
H(26A)	782(14)	6455(11)	27(12)	33(5)
H(26B)	880(14)	6179(12)	-967(11)	39(6)
H(26C)	997(14)	7196(12)	-883(12)	40(6)
H(28A)	3459(16)	7683(14)	-3771(13)	55(7)
H(28B)	2220(20)	7377(15)	-3685(15)	87(9)
H(28C)	3208(16)	6680(13)	-3761(13)	53(7)
H(3B)	1220(20)	5723(16)	4087(17)	114(10)
H(4B)	4665(12)	5890(10)	1672(10)	19(5)
H(5B)	5010(13)	7083(10)	475(11)	26(5)
H(7B1)	5590(16)	9117(12)	338(12)	44(6)
H(7B2)	4273(15)	9247(12)	709(12)	45(6)

H(7B3)	4798(14)	8624(11)	-15(12)	39(6)
H(8B1)	2458(13)	8392(11)	3792(11)	29(5)
H(8B2)	2434(13)	8067(11)	4816(12)	32(5)
H(8B3)	2056(16)	7416(13)	4285(12)	51(6)
H(9B1)	5015(17)	8795(12)	4117(14)	58(7)
H(9B2)	6204(15)	9337(12)	3590(11)	43(6)
H(9B3)	6052(15)	8483(12)	3257(12)	41(6)
H(10D)	6756(15)	9418(13)	1273(12)	47(6)
H(10E)	6969(15)	10252(12)	1610(12)	45(6)
H(10F)	6179(15)	10302(12)	1002(13)	52(6)
H(12D)	4742(15)	11708(12)	3470(12)	43(6)
H(12E)	5801(14)	11364(11)	2713(12)	30(5)
H(12F)	5359(15)	10891(12)	3820(13)	47(6)
H(13D)	3564(17)	9949(14)	4480(14)	66(8)
H(13E)	2761(17)	9917(13)	3923(13)	60(7)
H(13F)	2901(15)	10825(12)	4254(12)	44(6)
H(14D)	3408(15)	11588(12)	2666(12)	48(6)
H(14E)	3379(17)	10716(13)	2251(13)	62(7)
H(14F)	4577(18)	11267(13)	1777(14)	62(8)
H(15C)	3961(13)	6006(11)	4080(11)	29(5)
H(15D)	4563(13)	5374(10)	3328(10)	20(5)
H(16B)	2690(11)	5298(9)	3116(10)	13(4)
H(20B)	1938(12)	2330(10)	6009(10)	21(5)
H(21C)	1972(13)	2468(10)	4457(10)	21(5)
H(21D)	3183(13)	2494(10)	4462(10)	19(5)
H(23D)	3419(14)	4199(12)	2518(12)	43(6)
H(23E)	2648(16)	3318(12)	2812(12)	47(6)
H(23F)	3899(15)	3285(11)	2794(11)	34(5)
H(24D)	2117(13)	5778(11)	5512(10)	26(5)
H(24E)	3246(15)	5340(11)	5603(11)	34(5)
H(24F)	2058(13)	5180(10)	6467(12)	29(5)
H(26D)	4364(16)	3949(13)	5623(12)	55(7)
H(26E)	4271(14)	3613(11)	4680(12)	42(6)
H(26F)	4218(15)	2973(12)	5585(12)	39(6)
H(28D)	2178(16)	3296(13)	8539(13)	51(6)
H(28E)	3210(17)	2533(13)	8372(13)	60(7)
H(28F)	1846(15)	2391(12)	8536(12)	41(6)

Table 6. Hydrogen bonds for DCB31 (CCDC 283708) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3A)-H(3A)...O(7A)#1	0.92(2)	1.88(2)	2.7946(17)	173(2)
O(3B)-H(3B)...O(7B)#2	0.98(3)	1.81(3)	2.7910(17)	176(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z
#2 -x,-y+1,-z+1

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Crystal Structure Analysis of:

Bisacetoxyacetal 220 (DCB32)

(CCDC 289914)

Contents:

Figure A6.3 Representation of Bisacetoxyacetal **220**

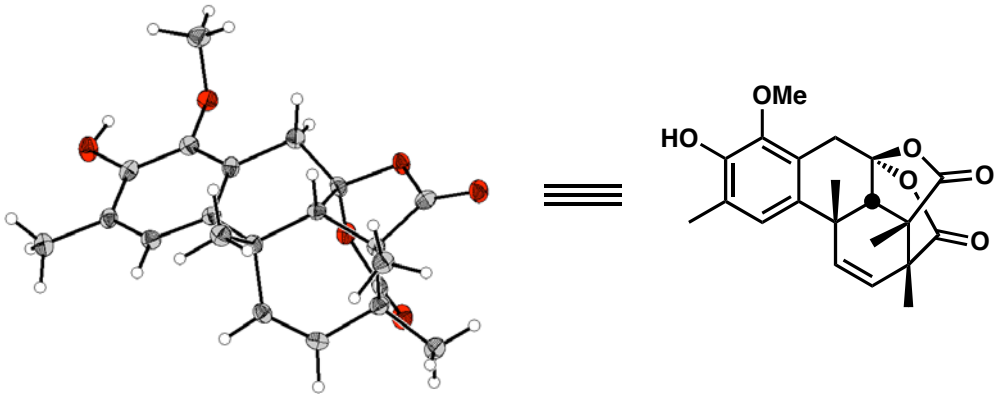

Table 1. Crystal data and structure refinement for DCB32 (CCDC 289914).

Empirical formula	$C_{21}H_{22}O_6$
Formula weight	370.39
Crystallization Solvent	Et_2O/hexanes
Crystal Habit	Needle
Crystal size	0.39 x 0.22 x 0.19 mm^3
Crystal color	Colorless

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 13215 reflections used in lattice determination	2.27 to 28.03°
Unit cell dimensions	a = 21.9617(16) Å b = 8.5236(6) Å c = 19.6358(14) Å
Volume	3675.7(5) $Å^3$
Z	8
Crystal system	Orthorhombic
Space group	Pbcn
Density (calculated)	1.339 Mg/m^3
F(000)	1568
Data collection program	Bruker SMART v5.630
θ range for data collection	1.85 to 28.38°
Completeness to θ = 28.38°	94.2 %
Index ranges	$-28 \le h \le 28$, $-11 \le k \le 11$, $-24 \le l \le 26$
Data collection scan type	ω scans at 5 ϕ settings
Data reduction program	Bruker SAINT v6.45A
Reflections collected	50823
Independent reflections	4344 [R_{int}= 0.0809]
Absorption coefficient	0.098 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9816 and 0.9628

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	Bruker XS v6.12
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	Bruker XL v6.12
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	4344 / 0 / 332
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.880
Final R indices [I>2σ(I), 3001 reflections]	R1 = 0.0466, *w*R2 = 0.0611
R indices (all data)	R1 = 0.0778, *w*R2 = 0.0633
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	0.331 and -0.276 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for DCB32 (CCDC 289914). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
O(1)	2750(1)	8498(1)	11657(1)	20(1)
O(2)	3463(1)	6194(1)	12216(1)	22(1)
O(3)	4347(1)	12923(1)	9814(1)	24(1)
O(4)	3652(1)	11114(1)	10020(1)	19(1)
O(5)	2849(1)	12317(1)	8276(1)	22(1)
O(6)	2812(1)	11335(1)	9329(1)	18(1)
C(1)	3243(1)	8168(2)	10565(1)	16(1)
C(2)	3171(1)	7737(2)	11243(1)	16(1)
C(3)	3539(1)	6609(2)	11548(1)	17(1)
C(4)	3993(1)	5863(2)	11174(1)	17(1)
C(5)	4067(1)	6316(2)	10500(1)	17(1)
C(6)	3705(1)	7443(2)	10182(1)	16(1)
C(7)	3834(1)	7839(2)	9427(1)	15(1)
C(8)	3386(1)	9079(2)	9173(1)	15(1)
C(9)	3172(1)	10217(2)	9710(1)	17(1)
C(10)	2832(1)	9437(2)	10272(1)	18(1)
C(11)	2149(1)	7822(2)	11619(1)	25(1)
C(12)	4388(1)	4633(2)	11498(1)	24(1)
C(13)	3759(1)	6327(2)	8998(1)	20(1)
C(14)	4480(1)	8405(2)	9339(1)	18(1)
C(15)	4634(1)	9789(2)	9089(1)	19(1)
C(16)	4175(1)	11058(2)	8904(1)	18(1)
C(17)	3586(1)	10261(2)	8630(1)	15(1)
C(18)	4452(1)	12247(2)	8416(1)	23(1)
C(19)	3652(1)	9638(2)	7907(1)	21(1)
C(20)	4062(1)	11828(2)	9598(1)	19(1)
C(21)	3057(1)	11422(2)	8689(1)	17(1)

Table 3. Bond lengths [Å] and angles [°] for DCB32 (CCDC 289914).

O(1)-C(2)	1.3917(16)	C(19)-H(19B)	1.006(15)
O(1)-C(11)	1.4405(18)	C(19)-H(19C)	0.974(17)
O(2)-C(3)	1.3695(17)		
O(2)-H(2)	0.887(19)	C(2)-O(1)-C(11)	113.13(12)
O(3)-C(20)	1.2002(16)	C(3)-O(2)-H(2)	108.0(13)
O(4)-C(20)	1.3677(17)	C(20)-O(4)-C(9)	117.64(11)
O(4)-C(9)	1.4373(16)	C(21)-O(6)-C(9)	107.19(11)
O(5)-C(21)	1.2031(16)	C(2)-C(1)-C(6)	118.61(13)
O(6)-C(21)	1.3697(16)	C(2)-C(1)-C(10)	118.79(13)
O(6)-C(9)	1.4462(16)	C(6)-C(1)-C(10)	122.58(13)
C(1)-C(2)	1.3899(19)	C(1)-C(2)-C(3)	121.92(13)
C(1)-C(6)	1.4059(19)	C(1)-C(2)-O(1)	120.79(13)
C(1)-C(10)	1.521(2)	C(3)-C(2)-O(1)	117.17(13)
C(2)-C(3)	1.3915(19)	O(2)-C(3)-C(2)	121.36(13)
C(3)-C(4)	1.3917(19)	O(2)-C(3)-C(4)	118.33(13)
C(4)-C(5)	1.388(2)	C(2)-C(3)-C(4)	120.30(13)
C(4)-C(12)	1.503(2)	C(5)-C(4)-C(3)	117.36(14)
C(5)-C(6)	1.3954(19)	C(5)-C(4)-C(12)	122.04(14)
C(5)-H(5)	0.960(12)	C(3)-C(4)-C(12)	120.60(14)
C(6)-C(7)	1.546(2)	C(4)-C(5)-C(6)	123.54(14)
C(7)-C(14)	1.5080(19)	C(4)-C(5)-H(5)	118.2(7)
C(7)-C(8)	1.5268(19)	C(6)-C(5)-H(5)	118.2(7)
C(7)-C(13)	1.548(2)	C(5)-C(6)-C(1)	118.25(14)
C(8)-C(9)	1.5086(19)	C(5)-C(6)-C(7)	118.43(13)
C(8)-C(17)	1.5300(19)	C(1)-C(6)-C(7)	123.32(13)
C(8)-H(8)	0.966(13)	C(14)-C(7)-C(8)	110.30(12)
C(9)-C(10)	1.490(2)	C(14)-C(7)-C(6)	110.57(12)
C(10)-H(10A)	1.027(14)	C(8)-C(7)-C(6)	110.27(12)
C(10)-H(10B)	0.976(14)	C(14)-C(7)-C(13)	107.68(12)
C(11)-H(11A)	1.018(15)	C(8)-C(7)-C(13)	109.33(12)
C(11)-H(11B)	0.941(14)	C(6)-C(7)-C(13)	108.64(12)
C(11)-H(11C)	1.017(15)	C(9)-C(8)-C(7)	114.69(12)
C(12)-H(12A)	0.965(18)	C(9)-C(8)-C(17)	98.80(11)
C(12)-H(12B)	0.994(18)	C(7)-C(8)-C(17)	119.94(12)
C(12)-H(12C)	0.989(17)	C(9)-C(8)-H(8)	106.2(8)
C(13)-H(13A)	1.003(14)	C(7)-C(8)-H(8)	107.8(8)
C(13)-H(13B)	0.988(15)	C(17)-C(8)-H(8)	108.4(8)
C(13)-H(13C)	0.996(14)	O(4)-C(9)-O(6)	105.61(11)
C(14)-C(15)	1.323(2)	O(4)-C(9)-C(10)	106.90(12)
C(14)-H(14)	0.975(13)	O(6)-C(9)-C(10)	113.83(12)
C(15)-C(16)	1.523(2)	O(4)-C(9)-C(8)	114.14(12)
C(15)-H(15)	0.987(11)	O(6)-C(9)-C(8)	103.46(11)
C(16)-C(18)	1.520(2)	C(10)-C(9)-C(8)	112.83(13)
C(16)-C(20)	1.533(2)	C(9)-C(10)-C(1)	107.47(13)
C(16)-C(17)	1.5582(19)	C(9)-C(10)-H(10A)	107.7(7)
C(17)-C(19)	1.523(2)	C(1)-C(10)-H(10A)	113.2(8)
C(17)-C(21)	1.530(2)	C(9)-C(10)-H(10B)	111.0(8)
C(18)-H(18A)	0.989(14)	C(1)-C(10)-H(10B)	110.6(8)
C(18)-H(18B)	0.977(15)	H(10A)-C(10)-H(10B)	106.9(11)
C(18)-H(18C)	1.001(16)	O(1)-C(11)-H(11A)	111.2(8)
C(19)-H(19A)	0.956(14)	O(1)-C(11)-H(11B)	104.9(8)

H(11A)-C(11)-H(11B)	109.5(11)
O(1)-C(11)-H(11C)	111.2(8)
H(11A)-C(11)-H(11C)	110.5(12)
H(11B)-C(11)-H(11C)	109.4(12)
C(4)-C(12)-H(12A)	112.6(11)
C(4)-C(12)-H(12B)	111.6(10)
H(12A)-C(12)-H(12B)	104.8(14)
C(4)-C(12)-H(12C)	112.2(10)
H(12A)-C(12)-H(12C)	108.5(14)
H(12B)-C(12)-H(12C)	106.7(14)
C(7)-C(13)-H(13A)	109.3(8)
C(7)-C(13)-H(13B)	111.2(8)
H(13A)-C(13)-H(13B)	109.6(11)
C(7)-C(13)-H(13C)	108.8(8)
H(13A)-C(13)-H(13C)	110.4(11)
H(13B)-C(13)-H(13C)	107.5(11)
C(15)-C(14)-C(7)	124.68(14)
C(15)-C(14)-H(14)	118.8(8)
C(7)-C(14)-H(14)	116.5(7)
C(14)-C(15)-C(16)	123.55(14)
C(14)-C(15)-H(15)	119.1(7)
C(16)-C(15)-H(15)	117.2(7)
C(18)-C(16)-C(15)	111.10(13)
C(18)-C(16)-C(20)	109.81(13)
C(15)-C(16)-C(20)	101.49(11)
C(18)-C(16)-C(17)	113.92(13)
C(15)-C(16)-C(17)	108.83(12)
C(20)-C(16)-C(17)	111.00(12)
C(19)-C(17)-C(21)	111.62(12)
C(19)-C(17)-C(8)	116.54(13)
C(21)-C(17)-C(8)	99.01(11)
C(19)-C(17)-C(16)	113.21(12)
C(21)-C(17)-C(16)	108.81(12)
C(8)-C(17)-C(16)	106.55(11)
C(16)-C(18)-H(18A)	107.5(8)
C(16)-C(18)-H(18B)	111.6(8)
H(18A)-C(18)-H(18B)	110.3(12)
C(16)-C(18)-H(18C)	108.8(9)
H(18A)-C(18)-H(18C)	111.5(12)
H(18B)-C(18)-H(18C)	107.2(12)
C(17)-C(19)-H(19A)	107.7(8)
C(17)-C(19)-H(19B)	110.6(8)
H(19A)-C(19)-H(19B)	111.7(12)
C(17)-C(19)-H(19C)	113.5(9)
H(19A)-C(19)-H(19C)	104.7(12)
H(19B)-C(19)-H(19C)	108.6(12)
O(3)-C(20)-O(4)	118.39(14)
O(3)-C(20)-C(16)	124.22(14)
O(4)-C(20)-C(16)	117.06(13)
O(5)-C(21)-O(6)	120.27(13)
O(5)-C(21)-C(17)	130.33(14)
O(6)-C(21)-C(17)	109.40(12)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for DCB32 (CCDC 289914). The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2 a^{*2} U^{11}$ + ... + 2 h k a* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	219(6)	189(6)	191(6)	-17(5)	52(5)	31(5)
O(2)	300(7)	204(6)	154(6)	14(5)	13(5)	46(5)
O(3)	273(6)	157(6)	288(7)	-25(5)	-80(5)	-20(5)
O(4)	233(6)	155(6)	172(6)	-15(5)	-14(5)	-8(5)
O(5)	248(6)	236(6)	179(6)	56(5)	-2(5)	32(5)
O(6)	215(6)	187(6)	141(6)	24(5)	18(5)	52(5)
C(1)	198(9)	125(8)	164(8)	-5(7)	-11(7)	-4(7)
C(2)	186(8)	133(8)	168(9)	-39(7)	23(7)	0(7)
C(3)	227(9)	148(9)	130(9)	-8(7)	-8(7)	-46(7)
C(4)	201(9)	112(8)	200(9)	-4(7)	-20(7)	-16(7)
C(5)	172(9)	147(8)	204(9)	-35(7)	31(7)	20(7)
C(6)	172(8)	139(8)	166(8)	-26(7)	1(7)	-13(7)
C(7)	156(8)	139(8)	161(8)	-18(7)	3(7)	18(7)
C(8)	136(8)	152(8)	162(9)	-18(7)	-2(7)	-18(7)
C(9)	166(8)	156(8)	183(8)	15(7)	-40(7)	20(7)
C(10)	211(9)	175(9)	157(9)	1(7)	36(8)	24(7)
C(11)	232(10)	239(10)	269(11)	-6(9)	92(9)	14(8)
C(12)	245(10)	208(10)	272(11)	45(8)	2(8)	35(8)
C(13)	221(10)	182(9)	205(10)	-34(8)	4(8)	11(8)
C(14)	179(9)	198(9)	159(9)	-11(7)	3(7)	40(7)
C(15)	141(8)	234(9)	180(9)	-23(7)	3(7)	0(7)
C(16)	168(8)	170(8)	188(9)	-1(7)	3(7)	-14(7)
C(17)	167(8)	146(8)	148(8)	-11(7)	10(7)	7(7)
C(18)	228(10)	218(10)	249(10)	30(8)	2(8)	-26(8)
C(19)	239(10)	241(10)	159(9)	7(8)	3(8)	-8(9)
C(20)	178(9)	154(9)	228(9)	32(7)	-44(7)	41(7)
C(21)	188(9)	169(8)	159(9)	-30(7)	-2(7)	-52(7)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for DCB32 (CCDC 289914).

	x	y	z	U_{iso}
H(2)	3183(9)	6820(20)	12395(10)	66(7)
H(5)	4383(6)	5822(14)	10239(6)	7(3)
H(8)	3027(6)	8542(15)	9011(6)	11(4)
H(10A)	2434(6)	9003(15)	10073(7)	16(4)
H(10B)	2719(6)	10191(17)	10624(7)	21(4)
H(11A)	1959(6)	8003(17)	11152(8)	27(4)
H(11B)	1921(6)	8358(16)	11952(7)	15(4)
H(11C)	2158(6)	6658(19)	11731(7)	26(4)
H(12A)	4187(8)	3630(20)	11532(9)	59(6)
H(12B)	4495(7)	4910(20)	11975(9)	56(6)
H(12C)	4777(8)	4488(19)	11252(8)	49(5)
H(13A)	4066(6)	5529(17)	9151(7)	26(4)
H(13B)	3815(6)	6542(16)	8508(8)	22(4)
H(13C)	3338(7)	5917(15)	9061(7)	22(4)
H(14)	4801(6)	7679(15)	9475(6)	12(4)
H(15)	5070(5)	10055(15)	9044(6)	9(4)
H(18A)	4804(6)	12732(16)	8649(7)	23(4)
H(18B)	4157(7)	13051(17)	8286(7)	29(4)
H(18C)	4578(6)	11692(17)	7990(8)	32(5)
H(19A)	3300(6)	9017(16)	7809(7)	20(4)
H(19B)	4038(7)	9014(17)	7859(7)	30(5)
H(19C)	3650(6)	10458(19)	7561(8)	36(5)

Table 6. Hydrogen bonds for DCB32 (CCDC 289914) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(5)#1	0.887(19)	2.02(2)	2.7848(15)	144.2(17)
O(2)-H(2)...O(1)	0.887(19)	2.248(19)	2.7418(14)	114.8(15)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+2,z+1/2

CALIFORNIA INSTITUTE OF TECHNOLOGY

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X-RAY CRYSTALLOGRAPHY LABORATORY

Crystal Structure Analysis of:

Alcohol 255 (DCB34)

Contents:

Figure A6.4 Representation of Alcohol **255**

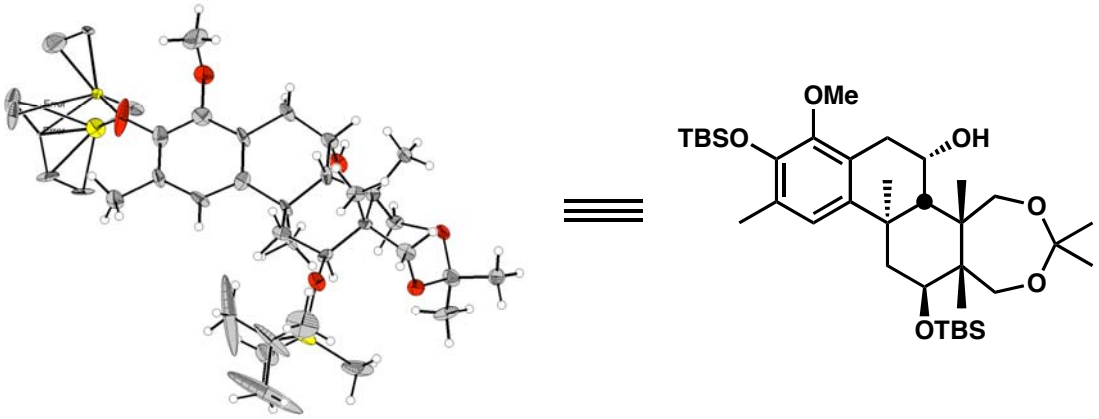

Table 1. Crystal data and structure refinement for dcb34.

Empirical formula	C36 H49 O6 Si2
Formula weight	633.93
Crystallization Solvent	Methylene Chloride
Crystal Habit	Fragment
Crystal size	0.45 x 0.20 x 0.19 mm^3
Crystal color	Colorless

Data Collection

Preliminary Photos		
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	100(2) K	
θ range for 2391 reflections used in lattice determination	2.25 to 25.75°	
Unit cell dimensions	a = 8.012(3) Å b = 12.103(5) Å c = 21.064(8) Å	α= 104.652(5)° β= 92.405(7)° γ = 98.610(6)°
Volume	1947.0(12) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.081 Mg/m^3	
F(000)	682	
θ range for data collection	1.76 to 27.12°	
Completeness to θ = 27.12°	78.9 %	
Index ranges	-10<=h<=8, -15<=k<=15, -26<=l<=12	
Data collection scan type	scans at 3 settings	
Reflections collected	8155	
Independent reflections	6807 [R_{int}= 0.0961; GOF_{merge}=]	
Absorption coefficient	0.129 mm^{-1}	
Absorption correction	None	

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	direct
Secondary solution method	difmap
Hydrogen placement	geom
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6807 / 0 / 456
Treatment of hydrogen atoms	mixed
Goodness-of-fit on F^2	2.722
Final R indices [I>2σ(I), 4077 reflections]	R1 = 0.1484, wR2 = 0.1836
R indices (all data)	R1 = 0.2120, wR2 = 0.1890
Type of weighting scheme used	calc
Weighting scheme used	calc w=1/[^2^(Fo^2^)+(0.0000P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3
Max shift/error	1.254
Average shift/error	0.004
Largest diff. peak and hole	0.655 and -0.594 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for dcb34. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Si(2A)	11898(6)	1267(5)	4132(2)	15(2)	0.480(9)
Si(2B)	12395(6)	2036(5)	4004(2)	32(2)	0.520(9)
O(6)	2561(6)	4434(4)	2066(2)	26(1)	1
O(4)	3040(6)	1577(4)	-102(2)	21(1)	1
O(3)	7053(6)	620(4)	947(2)	27(1)	1
O(5)	2281(6)	3355(4)	432(2)	24(1)	1
O(1A)	10070(40)	1775(16)	4115(16)	23(7)	0.480(9)
C(1)	2380(8)	2466(5)	1362(3)	16(2)	1
O(2)	8803(7)	-67(4)	2989(3)	41(2)	1
C(2)	4738(9)	3387(6)	2278(3)	23(2)	1
C(3)	4299(8)	1754(6)	459(3)	21(2)	1
C(4)	4798(8)	1409(6)	1584(3)	20(2)	1
C(5)	5795(9)	384(6)	1376(3)	23(2)	1
C(6)	5952(8)	2528(5)	1996(3)	19(2)	1
C(7)	7591(9)	3162(6)	3129(4)	25(2)	1
C(8)	7268(8)	3098(6)	1588(3)	21(2)	1
C(9)	3425(8)	1492(6)	1051(3)	16(2)	1
C(10)	3552(8)	3555(5)	1752(3)	19(2)	1
C(11)	8602(9)	3023(6)	3647(3)	24(2)	1
C(12)	6986(9)	2280(7)	2562(3)	24(2)	1
C(13)	7315(8)	1161(6)	2542(3)	22(2)	1
C(14)	1097(8)	2053(6)	1829(3)	20(2)	1
C(15)	1296(8)	2793(6)	853(3)	22(2)	1
C(16)	8395(9)	1028(6)	3049(4)	30(2)	1
C(17)	9097(10)	1930(7)	3580(4)	30(2)	1
C(18)	976(8)	2272(6)	-653(3)	25(2)	1
C(19)	2236(8)	320(5)	817(3)	23(2)	1
C(20)	6564(9)	111(6)	1978(3)	24(2)	1
C(21)	9165(10)	4017(6)	4246(3)	38(2)	1
C(22)	2536(10)	2627(6)	-208(4)	28(2)	1
C(23)	5312(9)	6404(7)	2242(4)	45(2)	1
C(24)	3956(9)	3325(6)	-466(4)	34(2)	1
C(25)	2088(11)	6074(7)	1347(5)	71(3)	1
C(26)	26(11)	6041(8)	2774(4)	64(3)	1
C(27)	2062(17)	7851(9)	2892(9)	241(12)	1
C(28)	1911(11)	6533(7)	2886(6)	80(4)	1
C(29)	2709(15)	6347(16)	3472(5)	225(13)	1
C(30)	7871(15)	-666(8)	3383(5)	95(5)	1
C(34)	15112(10)	2027(7)	4889(4)	39(2)	1
C(33)	12570(10)	2764(7)	5392(3)	43(2)	1
C(32)	13620(60)	2710(70)	4690(20)	330(60)	0.480(9)
O(1B)	10270(40)	1780(20)	4019(18)	67(10)	0.520(9)
C(37)	13940(30)	3570(18)	4427(13)	49(8)	0.480(9)
C(38)	12530(30)	502(17)	4794(9)	62(7)	0.520(9)
C(39)	13340(30)	2090(30)	4776(15)	42(7)	0.520(9)
C(42)	12884(10)	1006(6)	3290(3)	33(2)	1
C(40)	11720(20)	-94(12)	4414(8)	21(4)	0.480(9)

C(41)	13220(20)	3598(12)	3960(8)	30(4)	0.520(9)
Si(1)	2960(3)	5826(2)	2116(1)	36(1)	1

Table 3. Bond lengths [Å] and angles [°] for dcb34.

Si(2A)-O(1A)	1.68(3)	C(14)-H(14A)	0.9800
Si(2A)-C(40)	1.876(15)	C(14)-H(14B)	0.9800
Si(2A)-C(42)	1.943(8)	C(14)-H(14C)	0.9800
Si(2A)-C(32)	2.11(7)	C(15)-H(15A)	0.9900
Si(2B)-O(1B)	1.69(3)	C(15)-H(15B)	0.9900
Si(2B)-C(39)	1.75(3)	C(16)-C(17)	1.381(10)
Si(2B)-C(42)	1.793(8)	C(17)-O(1B)	1.35(3)
Si(2B)-C(41)	1.934(15)	C(18)-C(22)	1.470(9)
O(6)-C(10)	1.464(7)	C(18)-H(18A)	0.9800
O(6)-Si(1)	1.643(5)	C(18)-H(18B)	0.9800
O(4)-C(22)	1.456(8)	C(18)-H(18C)	0.9800
O(4)-C(3)	1.471(7)	C(19)-H(19A)	0.9800
O(3)-C(5)	1.426(8)	C(19)-H(19B)	0.9800
O(3)-H(3)	0.8400	C(19)-H(19C)	0.9800
O(5)-C(15)	1.441(7)	C(20)-H(20A)	0.9900
O(5)-C(22)	1.454(8)	C(20)-H(20B)	0.9900
O(1A)-C(17)	1.41(3)	C(21)-H(21A)	0.9800
C(1)-C(15)	1.516(9)	C(21)-H(21B)	0.9800
C(1)-C(10)	1.520(9)	C(21)-H(21C)	0.9800
C(1)-C(14)	1.567(9)	C(22)-C(24)	1.516(9)
C(1)-C(9)	1.572(8)	C(23)-Si(1)	1.892(8)
O(2)-C(16)	1.388(8)	C(23)-H(23A)	0.9800
O(2)-C(30)	1.403(11)	C(23)-H(23B)	0.9800
C(2)-C(10)	1.502(8)	C(23)-H(23C)	0.9800
C(2)-C(6)	1.554(8)	C(24)-H(24A)	0.9800
C(2)-H(2A)	0.9900	C(24)-H(24B)	0.9800
C(2)-H(2B)	0.9900	C(24)-H(24C)	0.9800
C(3)-C(9)	1.535(9)	C(25)-Si(1)	1.847(8)
C(3)-H(3A)	0.9900	C(25)-H(25A)	0.9800
C(3)-H(3B)	0.9900	C(25)-H(25B)	0.9800
C(4)-C(6)	1.551(9)	C(25)-H(25C)	0.9800
C(4)-C(5)	1.556(8)	C(26)-C(28)	1.523(11)
C(4)-C(9)	1.570(9)	C(26)-H(26A)	0.9800
C(4)-H(4)	1.0000	C(26)-H(26B)	0.9800
C(5)-C(20)	1.519(9)	C(26)-H(26C)	0.9800
C(5)-H(5)	1.0000	C(27)-C(28)	1.578(15)
C(6)-C(12)	1.540(9)	C(27)-H(27A)	0.9800
C(6)-C(8)	1.576(9)	C(27)-H(27B)	0.9800
C(7)-C(11)	1.391(9)	C(27)-H(27C)	0.9800
C(7)-C(12)	1.397(9)	C(28)-C(29)	1.449(17)
C(7)-H(7)	0.9500	C(28)-Si(1)	1.923(9)
C(8)-H(8A)	0.9800	C(29)-H(29A)	0.9800
C(8)-H(8B)	0.9800	C(29)-H(29B)	0.9800
C(8)-H(8C)	0.9800	C(29)-H(29C)	0.9800
C(9)-C(19)	1.537(9)	C(30)-H(30A)	0.9800
C(10)-H(10)	1.0000	C(30)-H(30B)	0.9800
C(11)-C(17)	1.412(10)	C(30)-H(30C)	0.9800
C(11)-C(21)	1.505(9)	C(34)-C(39)	1.45(3)
C(12)-C(13)	1.410(9)	C(34)-C(32)	1.65(5)
C(13)-C(16)	1.402(9)	C(33)-C(39)	1.55(3)
C(13)-C(20)	1.528(8)	C(33)-C(32)	1.73(5)

C(32)-C(37)	1.29(9)
C(38)-C(39)	1.94(4)
O(1A)-Si(2A)-C(40)	113.4(11)
O(1A)-Si(2A)-C(42)	112.9(13)
C(40)-Si(2A)-C(42)	108.8(5)
O(1A)-Si(2A)-C(32)	103.6(15)
C(40)-Si(2A)-C(32)	117(2)
C(42)-Si(2A)-C(32)	100.4(15)
O(1B)-Si(2B)-C(39)	109.1(16)
O(1B)-Si(2B)-C(42)	106.2(11)
C(39)-Si(2B)-C(42)	119.3(11)
O(1B)-Si(2B)-C(41)	112.0(12)
C(39)-Si(2B)-C(41)	99.8(12)
C(42)-Si(2B)-C(41)	110.5(6)
C(10)-O(6)-Si(1)	126.8(4)
C(22)-O(4)-C(3)	115.3(5)
C(5)-O(3)-H(3)	109.5
C(15)-O(5)-C(22)	116.3(5)
C(17)-O(1A)-Si(2A)	130(2)
C(15)-C(1)-C(10)	107.9(5)
C(15)-C(1)-C(14)	104.9(5)
C(10)-C(1)-C(14)	108.9(5)
C(15)-C(1)-C(9)	113.1(6)
C(10)-C(1)-C(9)	110.7(5)
C(14)-C(1)-C(9)	111.1(5)
C(16)-O(2)-C(30)	112.3(6)
C(10)-C(2)-C(6)	112.6(5)
C(10)-C(2)-H(2A)	109.1
C(6)-C(2)-H(2A)	109.1
C(10)-C(2)-H(2B)	109.1
C(6)-C(2)-H(2B)	109.1
H(2A)-C(2)-H(2B)	107.8
O(4)-C(3)-C(9)	110.2(5)
O(4)-C(3)-H(3A)	109.6
C(9)-C(3)-H(3A)	109.6
O(4)-C(3)-H(3B)	109.6
C(9)-C(3)-H(3B)	109.6
H(3A)-C(3)-H(3B)	108.1
C(6)-C(4)-C(5)	112.0(5)
C(6)-C(4)-C(9)	119.5(6)
C(5)-C(4)-C(9)	115.5(5)
C(6)-C(4)-H(4)	102.2
C(5)-C(4)-H(4)	102.2
C(9)-C(4)-H(4)	102.2
O(3)-C(5)-C(20)	111.5(6)
O(3)-C(5)-C(4)	111.1(6)
C(20)-C(5)-C(4)	110.5(6)
O(3)-C(5)-H(5)	107.9
C(20)-C(5)-H(5)	107.9
C(4)-C(5)-H(5)	107.9
C(12)-C(6)-C(4)	110.9(6)
C(12)-C(6)-C(2)	110.1(5)
C(4)-C(6)-C(2)	105.8(5)
C(12)-C(6)-C(8)	106.6(6)
C(4)-C(6)-C(8)	113.9(5)
C(2)-C(6)-C(8)	109.6(5)
C(11)-C(7)-C(12)	124.2(7)
C(11)-C(7)-H(7)	117.9
C(12)-C(7)-H(7)	117.9
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(3)-C(9)-C(19)	108.6(5)
C(3)-C(9)-C(4)	109.4(5)
C(19)-C(9)-C(4)	108.9(5)
C(3)-C(9)-C(1)	110.8(5)
C(19)-C(9)-C(1)	109.7(5)
C(4)-C(9)-C(1)	109.4(5)
O(6)-C(10)-C(2)	107.6(5)
O(6)-C(10)-C(1)	110.2(5)
C(2)-C(10)-C(1)	115.2(6)
O(6)-C(10)-H(10)	107.9
C(2)-C(10)-H(10)	107.9
C(1)-C(10)-H(10)	107.9
C(7)-C(11)-C(17)	117.5(7)
C(7)-C(11)-C(21)	120.5(6)
C(17)-C(11)-C(21)	122.0(7)
C(7)-C(12)-C(13)	117.3(6)
C(7)-C(12)-C(6)	120.7(6)
C(13)-C(12)-C(6)	121.9(6)
C(16)-C(13)-C(12)	118.3(6)
C(16)-C(13)-C(20)	120.0(6)
C(12)-C(13)-C(20)	121.7(6)
C(1)-C(14)-H(14A)	109.5
C(1)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(1)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(5)-C(15)-C(1)	113.0(6)
O(5)-C(15)-H(15A)	109.0
C(1)-C(15)-H(15A)	109.0
O(5)-C(15)-H(15B)	109.0
C(1)-C(15)-H(15B)	109.0
H(15A)-C(15)-H(15B)	107.8
C(17)-C(16)-O(2)	119.7(7)
C(17)-C(16)-C(13)	123.3(7)
O(2)-C(16)-C(13)	117.0(7)
O(1B)-C(17)-C(16)	120.7(14)
O(1B)-C(17)-O(1A)	11(3)
C(16)-C(17)-O(1A)	123.0(10)
O(1B)-C(17)-C(11)	120.6(14)
C(16)-C(17)-C(11)	118.6(7)
O(1A)-C(17)-C(11)	117.5(11)

C(22)-C(18)-H(18A)	109.5	H(26A)-C(26)-H(26B)	109.5
C(22)-C(18)-H(18B)	109.5	C(28)-C(26)-H(26C)	109.5
H(18A)-C(18)-H(18B)	109.5	H(26A)-C(26)-H(26C)	109.5
C(22)-C(18)-H(18C)	109.5	H(26B)-C(26)-H(26C)	109.5
H(18A)-C(18)-H(18C)	109.5	C(28)-C(27)-H(27A)	109.5
H(18B)-C(18)-H(18C)	109.5	C(28)-C(27)-H(27B)	109.5
C(9)-C(19)-H(19A)	109.5	H(27A)-C(27)-H(27B)	109.5
C(9)-C(19)-H(19B)	109.5	C(28)-C(27)-H(27C)	109.5
H(19A)-C(19)-H(19B)	109.5	H(27A)-C(27)-H(27C)	109.5
C(9)-C(19)-H(19C)	109.5	H(27B)-C(27)-H(27C)	109.5
H(19A)-C(19)-H(19C)	109.5	C(29)-C(28)-C(26)	112.9(11)
H(19B)-C(19)-H(19C)	109.5	C(29)-C(28)-C(27)	113.7(11)
C(5)-C(20)-C(13)	115.6(6)	C(26)-C(28)-C(27)	106.1(9)
C(5)-C(20)-H(20A)	108.4	C(29)-C(28)-Si(1)	110.7(7)
C(13)-C(20)-H(20A)	108.4	C(26)-C(28)-Si(1)	107.6(6)
C(5)-C(20)-H(20B)	108.4	C(27)-C(28)-Si(1)	105.4(8)
C(13)-C(20)-H(20B)	108.4	C(28)-C(29)-H(29A)	109.5
H(20A)-C(20)-H(20B)	107.5	C(28)-C(29)-H(29B)	109.5
C(11)-C(21)-H(21A)	109.5	H(29A)-C(29)-H(29B)	109.5
C(11)-C(21)-H(21B)	109.5	C(28)-C(29)-H(29C)	109.5
H(21A)-C(21)-H(21B)	109.5	H(29A)-C(29)-H(29C)	109.5
C(11)-C(21)-H(21C)	109.5	H(29B)-C(29)-H(29C)	109.5
H(21A)-C(21)-H(21C)	109.5	O(2)-C(30)-H(30A)	109.5
H(21B)-C(21)-H(21C)	109.5	O(2)-C(30)-H(30B)	109.5
O(5)-C(22)-O(4)	107.4(5)	H(30A)-C(30)-H(30B)	109.5
O(5)-C(22)-C(18)	112.5(6)	O(2)-C(30)-H(30C)	109.5
O(4)-C(22)-C(18)	107.1(6)	H(30A)-C(30)-H(30C)	109.5
O(5)-C(22)-C(24)	105.3(6)	H(30B)-C(30)-H(30C)	109.5
O(4)-C(22)-C(24)	111.1(6)	C(39)-C(34)-C(32)	30(4)
C(18)-C(22)-C(24)	113.4(7)	C(39)-C(33)-C(32)	28(3)
Si(1)-C(23)-H(23A)	109.5	C(37)-C(32)-C(34)	123(4)
Si(1)-C(23)-H(23B)	109.5	C(37)-C(32)-C(33)	124(4)
H(23A)-C(23)-H(23B)	109.5	C(34)-C(32)-C(33)	96(4)
Si(1)-C(23)-H(23C)	109.5	C(37)-C(32)-Si(2A)	116(3)
H(23A)-C(23)-H(23C)	109.5	C(34)-C(32)-Si(2A)	99(4)
H(23B)-C(23)-H(23C)	109.5	C(33)-C(32)-Si(2A)	93(3)
C(22)-C(24)-H(24A)	109.5	C(17)-O(1B)-Si(2B)	127(3)
C(22)-C(24)-H(24B)	109.5	C(34)-C(39)-C(33)	113.8(18)
H(24A)-C(24)-H(24B)	109.5	C(34)-C(39)-Si(2B)	123(2)
C(22)-C(24)-H(24C)	109.5	C(33)-C(39)-Si(2B)	117(2)
H(24A)-C(24)-H(24C)	109.5	C(34)-C(39)-C(38)	95.0(19)
H(24B)-C(24)-H(24C)	109.5	C(33)-C(39)-C(38)	100.8(16)
Si(1)-C(25)-H(25A)	109.5	Si(2B)-C(39)-C(38)	98.6(14)
Si(1)-C(25)-H(25B)	109.5	Si(2B)-C(42)-Si(2A)	32.6(2)
H(25A)-C(25)-H(25B)	109.5	O(6)-Si(1)-C(25)	108.9(3)
Si(1)-C(25)-H(25C)	109.5	O(6)-Si(1)-C(23)	111.8(3)
H(25A)-C(25)-H(25C)	109.5	C(25)-Si(1)-C(23)	109.2(4)
H(25B)-C(25)-H(25C)	109.5	O(6)-Si(1)-C(28)	104.3(4)
C(28)-C(26)-H(26A)	109.5	C(25)-Si(1)-C(28)	113.9(5)
C(28)-C(26)-H(26B)	109.5	C(23)-Si(1)-C(28)	108.8(4)