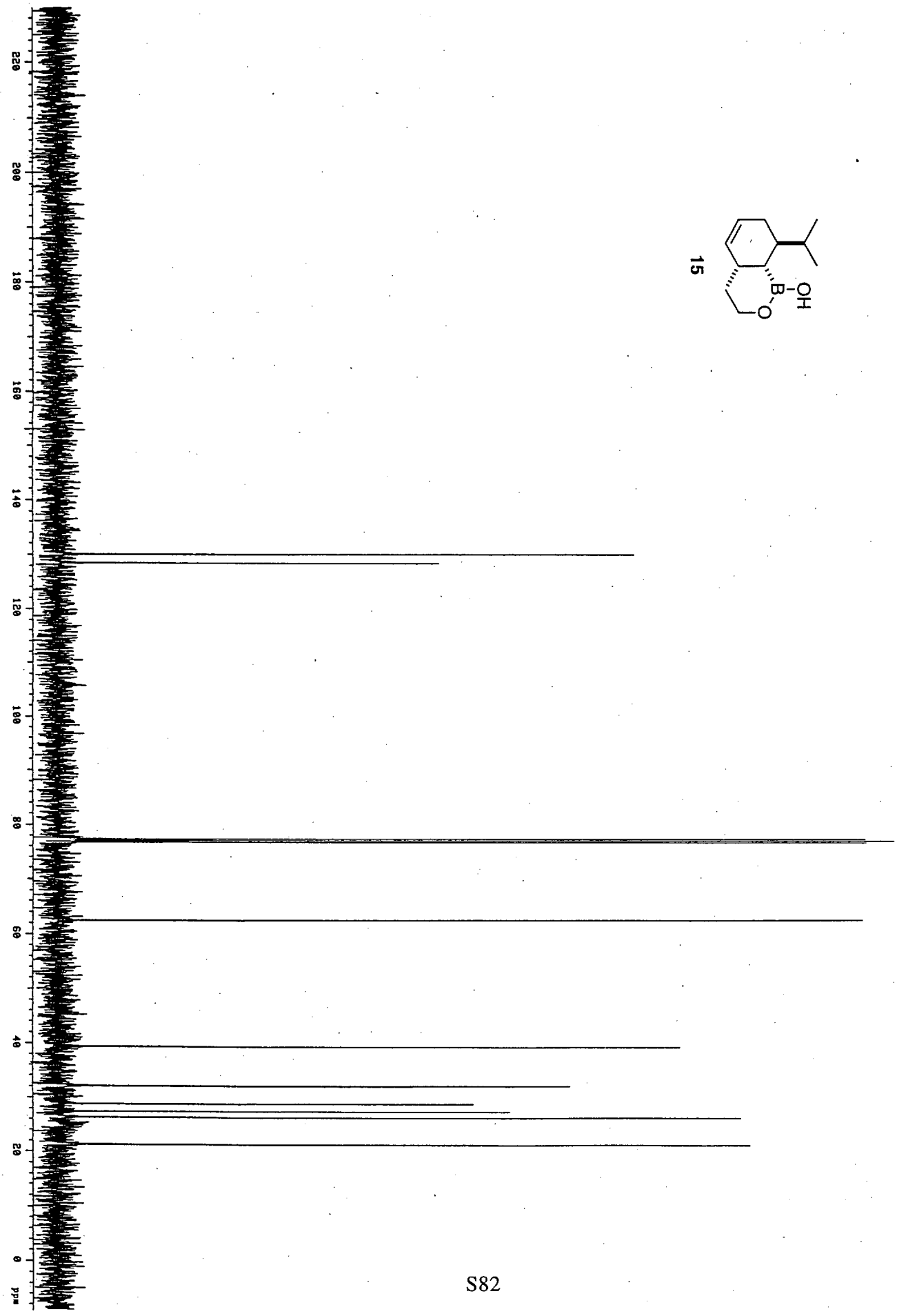

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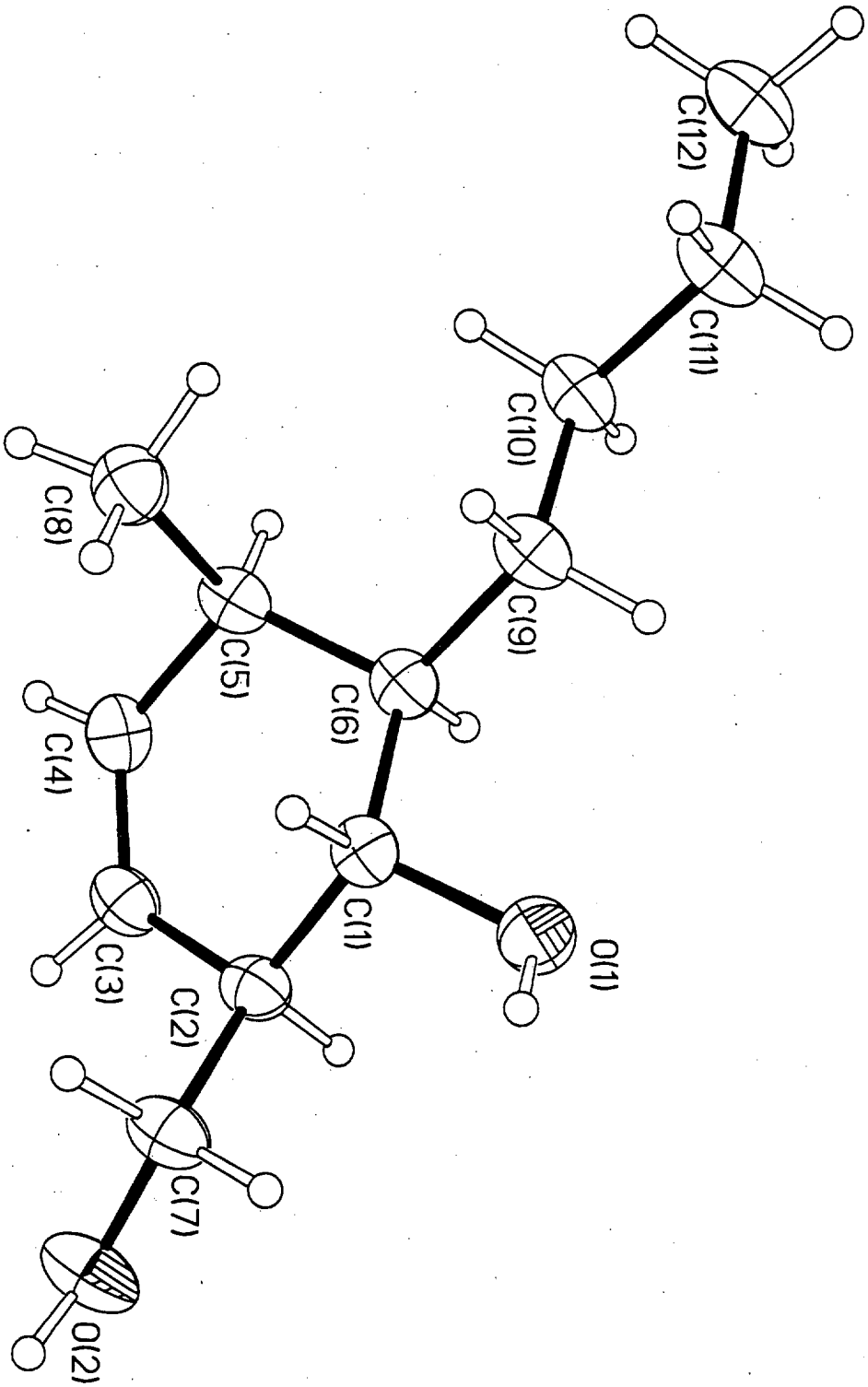

Table 1. Crystal data and structure refinement for k9717a.

Identification code	k9717a
Empirical formula	$C_{12}H_{22}O_2$
Formula weight	198.30
Temperature	150.0(1) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 12.8590(10) Å alpha = 90° b = 4.999(4) Å beta = 104.12(3)° c = 19.429(5) Å gamma = 90°
Volume, Z	1211.2(10) Å^3, 4
Density (calculated)	1.087 Mg/m^3
Absorption coefficient	0.072 mm^{-1}
F(000)	440
Crystal size	0.32 x 0.30 x 0.24 mm
θ range for data collection	3.01 to 22.50°
Limiting indices	$-13 \le h \le 13$, $-5 \le k \le 5$, $-20 \le l \le 20$
Reflections collected	7373
Independent reflections	1587 (R_{int} = 0.085)
Completeness to θ = 22.50°	99.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1587 / 0 / 132
Goodness-of-fit on F^2	0.895
Final R indices [I>2σ(I)]	R1 = 0.0492, wR2 = 0.1151
R indices (all data)	R1 = 0.0998, wR2 = 0.1269
Extinction coefficient	0.012(3)
Largest diff. peak and hole	0.198 and -0.180 eÅ^{-3}

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for k9717a. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	404(2)	2480(4)	4993(1)	58(1)
O(2)	235(2)	2111(4)	2806(1)	68(1)
C(1)	1383(2)	2287(5)	4768(1)	43(1)
C(2)	1145(2)	1118(6)	4020(1)	45(1)
C(3)	2124(3)	12(6)	3843(2)	50(1)
C(4)	3055(3)	-303(6)	4309(2)	52(1)
C(5)	3259(2)	455(5)	5079(1)	46(1)
C(6)	2199(2)	640(6)	5307(1)	46(1)
C(7)	609(2)	3230(6)	3497(1)	54(1)
C(8)	3937(2)	3004(6)	5201(2)	59(1)
C(9)	2332(2)	1728(6)	6058(1)	54(1)
C(10)	3118(3)	204(6)	6643(1)	55(1)
C(11)	3157(3)	1277(7)	7381(1)	70(1)
C(12)	4001(3)	-51(7)	7965(1)	76(1)

Table 3. Bond lengths [Å] and angles [°] for k9717a.

O(1)-C(1)	1.433(3)	O(2)-C(7)	1.425(3)
C(1)-C(2)	1.527(4)	C(1)-C(6)	1.529(4)
C(2)-C(3)	1.491(4)	C(2)-C(7)	1.511(4)
C(3)-C(4)	1.323(4)	C(4)-C(5)	1.503(4)
C(5)-C(8)	1.530(4)	C(5)-C(6)	1.534(4)
C(6)-C(9)	1.529(4)	C(9)-C(10)	1.527(4)
C(10)-C(11)	1.519(4)	C(11)-C(12)	1.518(4)
O(1)-C(1)-C(2)	109.2(2)	O(1)-C(1)-C(6)	109.6(2)
C(2)-C(1)-C(6)	112.9(2)	C(3)-C(2)-C(7)	112.1(2)
C(3)-C(2)-C(1)	112.2(2)	C(7)-C(2)-C(1)	109.0(2)
C(4)-C(3)-C(2)	124.0(3)	C(3)-C(4)-C(5)	124.1(3)
C(4)-C(5)-C(8)	108.5(2)	C(4)-C(5)-C(6)	110.5(2)
C(8)-C(5)-C(6)	114.7(2)	C(9)-C(6)-C(1)	111.1(2)
C(9)-C(6)-C(5)	113.4(2)	C(1)-C(6)-C(5)	110.2(2)
O(2)-C(7)-C(2)	110.7(2)	C(10)-C(9)-C(6)	115.6(2)
C(11)-C(10)-C(9)	112.9(3)	C(12)-C(11)-C(10)	113.8(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for k9717a.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(1)	52(1)	66(2)	56(1)	5(1)	15(1)	13(1)
O(2)	98(2)	51(1)	42(1)	-1(1)	-6(1)	3(1)
C(1)	49(2)	36(2)	44(2)	0(1)	12(2)	0(2)
C(2)	50(2)	41(2)	42(2)	1(1)	5(2)	-5(2)
C(3)	64(2)	45(2)	41(2)	-2(1)	11(2)	0(2)
C(4)	61(2)	44(2)	54(2)	0(2)	23(2)	5(2)
C(5)	57(2)	37(2)	41(2)	0(1)	7(2)	3(2)
C(6)	53(2)	39(2)	45(2)	0(1)	12(2)	-2(2)
C(7)	68(2)	50(2)	40(2)	-2(2)	2(2)	-2(2)
C(8)	63(2)	56(2)	58(2)	0(2)	16(2)	-2(2)
C(9)	67(2)	54(2)	41(2)	-3(2)	11(2)	2(2)
C(10)	75(2)	51(2)	41(2)	1(2)	15(2)	0(2)
C(11)	91(3)	74(2)	42(2)	-3(2)	11(2)	6(2)
C(12)	97(3)	82(3)	43(2)	6(2)	8(2)	7(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for k9717a.

	x	y	z	U(eq)
H(1A)	54	3816	4801	87
H(2)	0	3337	2514	101
H(1B)	1678	4132	4754	52
H(2B)	625	-385	3998	54
H(3A)	2077	-498	3365	60
H(4A)	3631	-1054	4147	62
H(5A)	3694	-1007	5363	55
H(6A)	1907	-1217	5299	55
H(7A)	-2	4011	3653	65
H(7B)	1127	4683	3481	65
H(8A)	4574	2755	5016	88
H(8B)	4157	3389	5711	88
H(8C)	3513	4503	4954	88
H(9A)	2573	3611	6066	65
H(9B)	1621	1726	6170	65
H(10A)	2907	-1705	6622	66
H(10B)	3844	314	6556	66
H(11A)	3301	3223	7387	84
H(11B)	2446	1021	7482	84
H(12A)	3959	671	8426	113
H(12B)	4715	306	7889	113
H(12C)	3876	-1985	7956	113

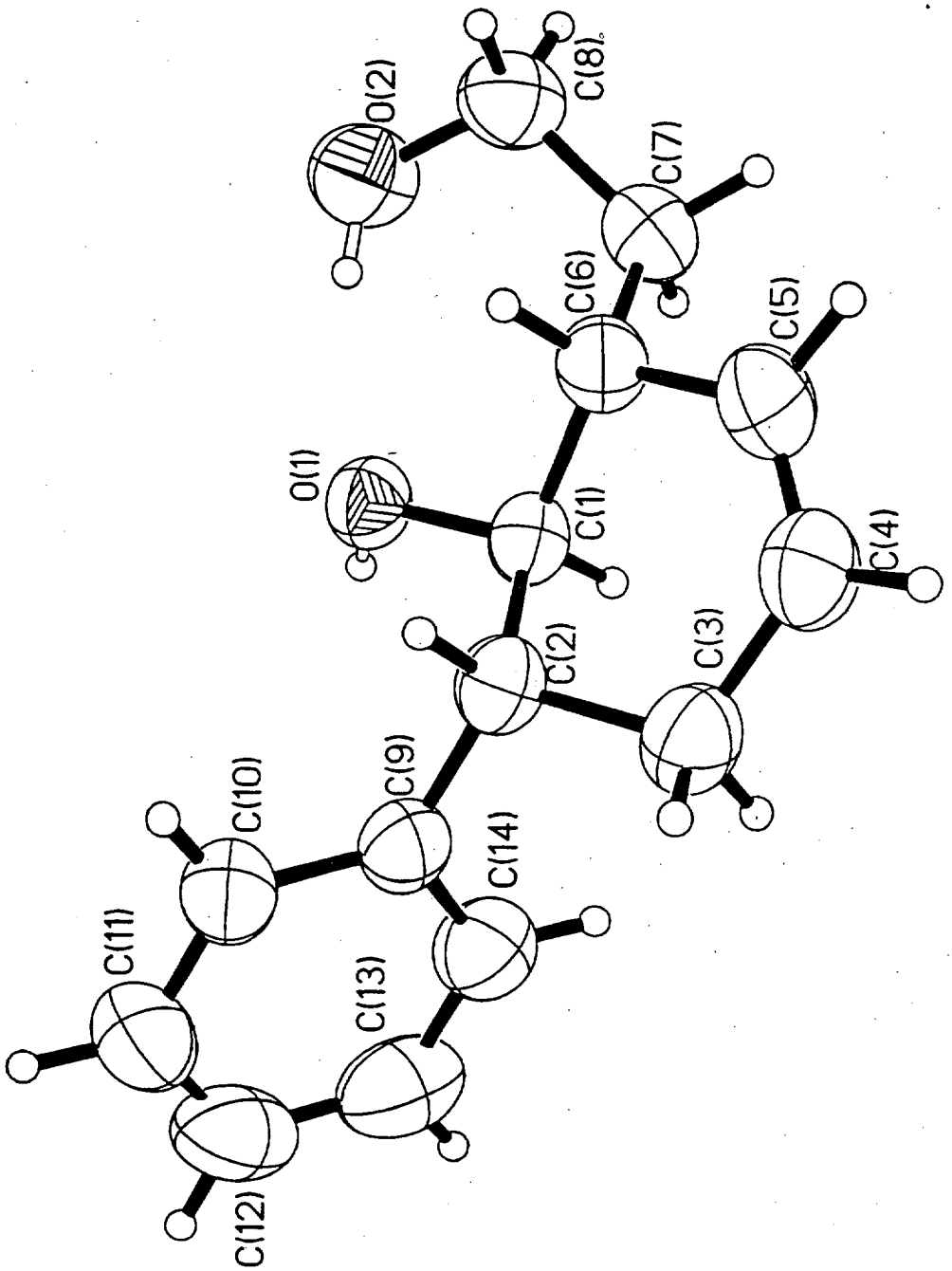

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Table 1. Crystal data and structure refinement for 1.

Identification code	k9732
Empirical formula	$C_{14}H_2H_{16}O_2$
Formula weight	218.28
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 11.2670(10) Å alpha = 90° b = 5.4800(10) Å beta = 94.15(3)° c = 19.5220(10) Å gamma = 90°
Volume, Z	1202.2(3) $Å^3$, 4
Density (calculated)	1.206 Mg/m^3
Absorption coefficient	0.079 mm^{-1}
F(000)	472
Crystal size	0.35 x 0.26 x 0.14 mm
θ range for data collection	5.20 to 26.42°
Limiting indices	$-14 \le h \le 13$, $-6 \le k \le 6$, $-24 \le l \le 24$
Reflections collected	4574
Independent reflections	2411 (R_{int} = 0.0288)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2411 / 0 / 154
Goodness-of-fit on F^2	1.049
Final R indices [I>2σ(I)]	R1 = 0.0543, wR2 = 0.1513
R indices (all data)	R1 = 0.0698, wR2 = 0.1647
Extinction coefficient	0.025(15)
Largest diff. peak and hole	0.226 and -0.233 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	6883(1)	322(2)	8267(1)	52(1)
O(2)	8724(1)	3054(3)	7927(1)	75(1)
C(1)	7314(1)	-1563(3)	8733(1)	47(1)
C(2)	6392(1)	-2113(3)	9250(1)	51(1)
C(3)	6831(2)	-4238(3)	9712(1)	63(1)
C(4)	8112(2)	-3978(3)	9950(1)	68(1)
C(5)	8841(2)	-2439(3)	9679(1)	65(1)
C(6)	8493(1)	-742(3)	9088(1)	53(1)
C(7)	9499(2)	-468(3)	8595(1)	64(1)
C(8)	9693(2)	2095(4)	8337(1)	66(1)
C(9)	5162(1)	-2578(3)	8916(1)	53(1)
C(10)	4249(2)	-945(3)	9010(1)	67(1)
C(11)	3111(2)	-1331(5)	8730(1)	88(1)
C(12)	2851(2)	-3385(5)	8346(1)	92(1)
C(13)	3753(2)	-5029(4)	8237(1)	85(1)
C(14)	4898(2)	-4628(3)	8519(1)	67(1)

Table 3. Bond lengths [Å] and angles [°] for 1.

O(1)-H(1O)	0.82(2)	O(1)-C(1)	1.437(2)
O(2)-H(2O)	0.81(2)	O(2)-C(8)	1.408(2)
C(1)-C(6)	1.522(2)	C(1)-C(2)	1.530(2)
C(2)-C(9)	1.510(2)	C(2)-C(3)	1.532(2)
C(3)-C(4)	1.491(2)	C(4)-C(5)	1.315(3)
C(5)-C(6)	1.512(2)	C(6)-C(7)	1.546(2)
C(7)-C(8)	1.513(3)	C(9)-C(10)	1.385(2)
C(9)-C(14)	1.386(2)	C(10)-C(11)	1.374(3)
C(11)-C(12)	1.372(4)	C(12)-C(13)	1.386(4)
C(13)-C(14)	1.383(3)		

H(1O)-O(1)-C(1)	110(2)	H(2O)-O(2)-C(8)	113(2)
O(1)-C(1)-C(6)	108.61(12)	O(1)-C(1)-C(2)	110.21(11)
C(6)-C(1)-C(2)	111.72(12)	C(9)-C(2)-C(1)	113.22(12)
C(9)-C(2)-C(3)	111.88(13)	C(1)-C(2)-C(3)	109.41(13)
C(4)-C(3)-C(2)	112.00(14)	C(5)-C(4)-C(3)	123.7(2)
C(4)-C(5)-C(6)	124.5(2)	C(5)-C(6)-C(1)	109.60(13)
C(5)-C(6)-C(7)	111.91(13)	C(1)-C(6)-C(7)	113.64(13)
C(8)-C(7)-C(6)	115.3(2)	O(2)-C(8)-C(7)	114.3(2)
C(10)-C(9)-C(14)	117.8(2)	C(10)-C(9)-C(2)	120.0(2)
C(14)-C(9)-C(2)	122.11(14)	C(11)-C(10)-C(9)	121.8(2)
C(12)-C(11)-C(10)	120.0(2)	C(11)-C(12)-C(13)	119.2(2)
C(14)-C(13)-C(12)	120.6(2)	C(13)-C(14)-C(9)	120.5(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

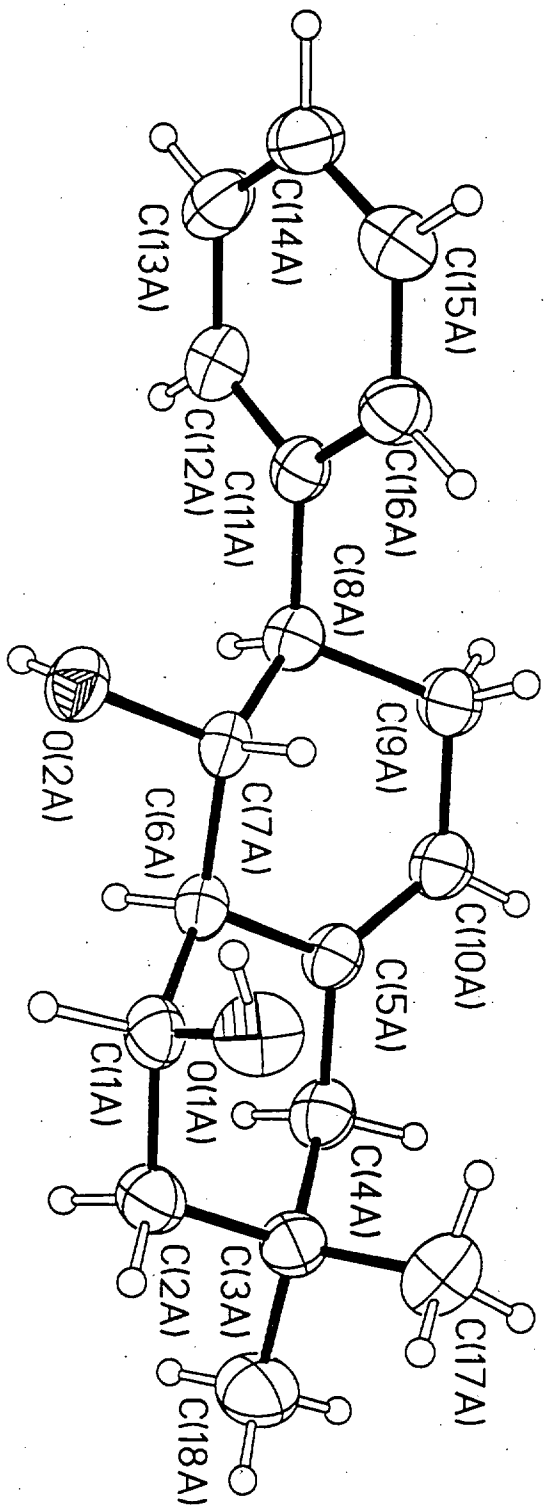
The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(1)	55(1)	48(1)	51(1)	4(1)	-1(1)	3(1)
O(2)	72(1)	84(1)	70(1)	23(1)	-2(1)	-9(1)
C(1)	52(1)	41(1)	49(1)	-1(1)	2(1)	6(1)
C(2)	57(1)	45(1)	51(1)	-2(1)	5(1)	4(1)
C(3)	70(1)	57(1)	61(1)	10(1)	6(1)	3(1)
C(4)	72(1)	66(1)	63(1)	16(1)	-4(1)	8(1)
C(5)	59(1)	69(1)	64(1)	6(1)	-9(1)	7(1)
C(6)	53(1)	50(1)	56(1)	0(1)	1(1)	3(1)
C(7)	50(1)	66(1)	78(1)	5(1)	5(1)	4(1)
C(8)	61(1)	73(1)	64(1)	7(1)	3(1)	-8(1)
C(9)	55(1)	49(1)	55(1)	9(1)	11(1)	0(1)
C(10)	61(1)	58(1)	84(1)	11(1)	14(1)	7(1)
C(11)	57(1)	86(2)	121(2)	30(1)	9(1)	10(1)
C(12)	62(1)	110(2)	100(2)	45(1)	-15(1)	-19(1)
C(13)	97(2)	79(1)	76(1)	9(1)	-10(1)	-28(1)
C(14)	72(1)	61(1)	68(1)	-2(1)	2(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(1B)	7448(1)	-3046(3)	8469(1)	57
H(2B)	6342(1)	-672(3)	9544(1)	61
H(3A)	6360(2)	-4313(3)	10108(1)	75
H(3B)	6717(2)	-5757(3)	9460(1)	75
H(4A)	8413(2)	-4960(3)	10310(1)	81
H(5A)	9625(2)	-2391(3)	9864(1)	78
H(6A)	8362(1)	873(3)	9284(1)	64
H(7A)	10236(2)	-1039(3)	8829(1)	77
H(7B)	9322(2)	-1523(3)	8202(1)	77
H(8A)	9858(2)	3160(4)	8730(1)	80
H(8B)	10389(2)	2098(4)	8073(1)	80
H(10A)	4412(2)	452(3)	9271(1)	81
H(11A)	2517(2)	-199(5)	8800(1)	105
H(12A)	2079(2)	-3670(5)	8161(1)	110
H(13A)	3587(2)	-6413(4)	7972(1)	102
H(14A)	5495(2)	-5743(3)	8441(1)	81
H(2O)	8095(21)	2432(41)	8009(12)	79(7)
H(1O)	6506(19)	-282(37)	7935(12)	76(6)



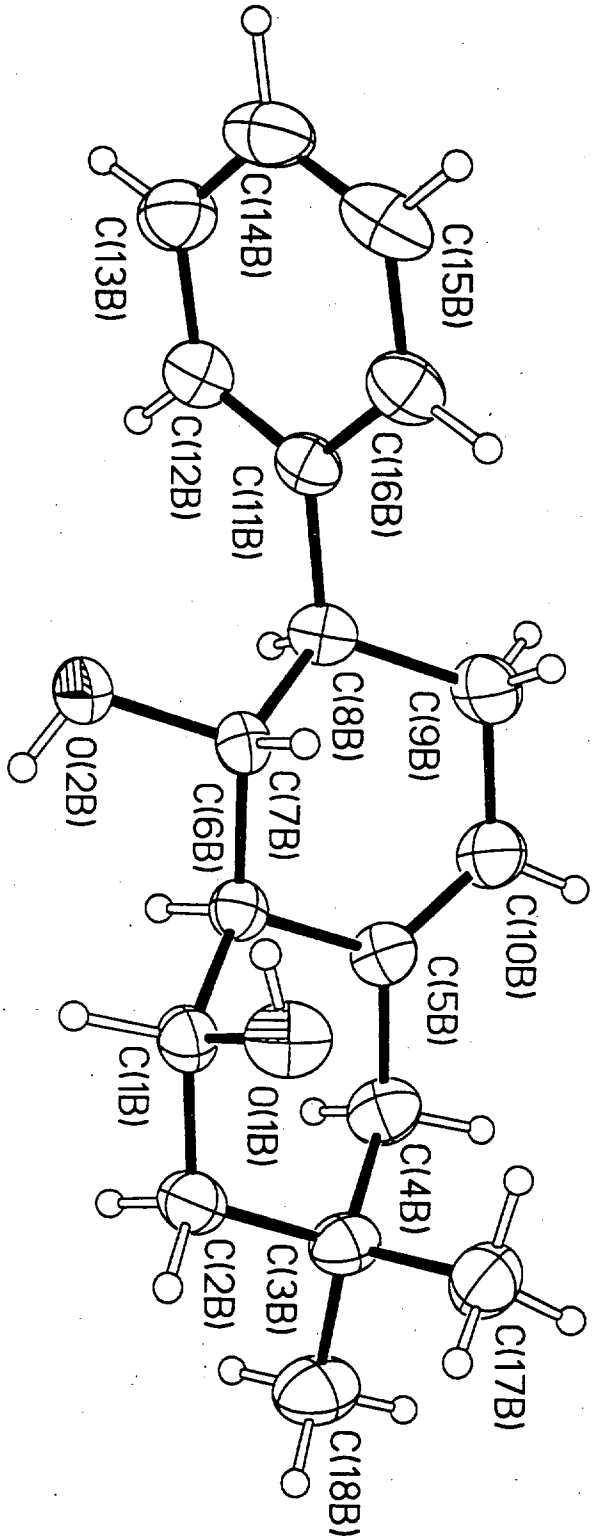


Table 1. Crystal data and structure refinement for k9820.

Identification code	k9820	
Empirical formula	C18 H24 O2	
Formula weight	272.37	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.079(1) Å	α= 70.43(1)°.
	b = 11.954(1) Å	β= 80.85(1)°.
	c = 13.802(1) Å	γ = 83.42(1)°.
Volume	1543.6(5) Å^3	
Z	4	
Density (calculated)	1.172 Mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	592	
Crystal size	0.13 x 0.12 x 0.08 mm^3	
Theta range for data collection	2.42 to 20.86°.	
Index ranges	0<=h<=10, -11<=k<=11, -13<=l<=13	
Reflections collected	7967	
Independent reflections	3214 [R(int) = 0.040]	
Completeness to theta = 20.86°	99.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3214 / 0 / 371	
Goodness-of-fit on F^2	1.061	
Final R indices [I>2sigma(I)]	R1 = 0.0442, wR2 = 0.1129	
R indices (all data)	R1 = 0.0531, wR2 = 0.1200	
Extinction coefficient	0.048(5)	
Largest diff. peak and hole	0.173 and -0.222 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for k9820. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1A)	3048(2)	7275(2)	7794(2)	74(1)
O(2A)	917(2)	5822(1)	9893(1)	59(1)
C(1A)	2003(2)	6640(2)	7667(2)	56(1)
C(2A)	2031(3)	6786(2)	6527(2)	65(1)
C(3A)	1504(3)	7995(2)	5840(2)	60(1)
C(4A)	96(3)	8269(2)	6337(2)	62(1)
C(5A)	8(2)	8162(2)	7462(2)	52(1)
C(6A)	609(2)	7006(2)	8147(2)	48(1)
C(7A)	609(2)	7007(2)	9244(2)	46(1)
C(8A)	-708(2)	7566(2)	9654(2)	53(1)
C(9A)	-851(3)	8868(2)	8969(2)	64(1)
C(10A)	-616(3)	8987(2)	7843(2)	63(1)
C(11A)	-797(2)	7432(2)	10786(2)	50(1)
C(12A)	-1761(3)	6768(2)	11509(2)	63(1)
C(13A)	-1825(3)	6622(2)	12555(2)	73(1)
C(14A)	-928(3)	7130(3)	12895(2)	70(1)
C(15A)	25(3)	7795(2)	12198(2)	66(1)
C(16A)	88(2)	7952(2)	11156(2)	59(1)
C(17A)	2397(3)	8991(3)	5714(2)	84(1)
C(18A)	1425(4)	7911(3)	4767(2)	91(1)
O(1B)	-8282(2)	5172(2)	11885(1)	65(1)
O(2B)	-5810(2)	6134(1)	9706(1)	65(1)
C(1B)	-6916(2)	4687(2)	11859(2)	51(1)
C(2B)	-6712(3)	3770(2)	12901(2)	58(1)
C(3B)	-6708(2)	4249(2)	13797(2)	57(1)
C(4B)	-5698(3)	5215(2)	13453(2)	65(1)
C(5B)	-5854(2)	6144(2)	12421(2)	52(1)
C(7B)	-6147(2)	6625(2)	10535(2)	44(1)
C(6B)	-5910(2)	5660(2)	11554(2)	46(1)
C(8B)	-5367(2)	7716(2)	10339(2)	52(1)
C(9B)	-5860(3)	8230(2)	11219(2)	70(1)

C(10B)	-5859(3)	7299(2)	12254(2)	66(1)
C(11B)	-5443(2)	8596(2)	9263(2)	49(1)
C(12B)	-4407(3)	8627(2)	8475(2)	62(1)
C(13B)	-4465(3)	9398(3)	7481(2)	77(1)
C(14B)	-5577(4)	10162(3)	7253(2)	79(1)
C(15B)	-6624(3)	10144(2)	8020(3)	78(1)
C(16B)	-6562(3)	9376(2)	9011(2)	64(1)
C(17B)	-8093(3)	4765(3)	14136(2)	71(1)
C(18B)	-6262(3)	3222(3)	14730(2)	82(1)

Table 3. Bond lengths [Å] and angles [°] for k9820.

O(1A)-C(1A)	1.431(3)
O(2A)-C(7A)	1.430(3)
C(1A)-C(2A)	1.520(3)
C(1A)-C(6A)	1.537(3)
C(2A)-C(3A)	1.529(3)
C(3A)-C(17A)	1.522(4)
C(3A)-C(4A)	1.525(4)
C(3A)-C(18A)	1.532(4)
C(4A)-C(5A)	1.505(3)
C(5A)-C(10A)	1.321(3)
C(5A)-C(6A)	1.511(3)
C(6A)-C(7A)	1.514(3)
C(7A)-C(8A)	1.529(3)
C(8A)-C(11A)	1.506(3)
C(8A)-C(9A)	1.531(3)
C(9A)-C(10A)	1.496(4)
C(11A)-C(12A)	1.382(3)
C(11A)-C(16A)	1.387(3)
C(12A)-C(13A)	1.386(4)
C(13A)-C(14A)	1.364(4)
C(14A)-C(15A)	1.360(4)
C(15A)-C(16A)	1.379(3)
O(1B)-C(1B)	1.431(3)
O(2B)-C(7B)	1.432(3)
C(1B)-C(2B)	1.516(3)
C(1B)-C(6B)	1.537(3)
C(2B)-C(3B)	1.528(3)
C(3B)-C(17B)	1.529(3)
C(3B)-C(4B)	1.531(4)
C(3B)-C(18B)	1.539(3)
C(4B)-C(5B)	1.503(3)
C(5B)-C(10B)	1.320(3)
C(5B)-C(6B)	1.504(3)
C(7B)-C(6B)	1.524(3)

C(7B)-C(8B)	1.525(3)
C(8B)-C(11B)	1.513(3)
C(8B)-C(9B)	1.528(3)
C(9B)-C(10B)	1.489(4)
C(11B)-C(12B)	1.376(3)
C(11B)-C(16B)	1.388(3)
C(12B)-C(13B)	1.379(4)
C(13B)-C(14B)	1.369(4)
C(14B)-C(15B)	1.367(4)
C(15B)-C(16B)	1.375(4)

O(1A)-C(1A)-C(2A)	110.0(2)
O(1A)-C(1A)-C(6A)	112.33(19)
C(2A)-C(1A)-C(6A)	111.85(19)
C(1A)-C(2A)-C(3A)	116.4(2)
C(17A)-C(3A)-C(4A)	109.5(2)
C(17A)-C(3A)-C(2A)	112.8(2)
C(4A)-C(3A)-C(2A)	107.6(2)
C(17A)-C(3A)-C(18A)	108.7(2)
C(4A)-C(3A)-C(18A)	109.6(2)
C(2A)-C(3A)-C(18A)	108.6(2)
C(5A)-C(4A)-C(3A)	114.4(2)
C(10A)-C(5A)-C(4A)	122.6(2)
C(10A)-C(5A)-C(6A)	121.9(2)
C(4A)-C(5A)-C(6A)	115.4(2)
C(5A)-C(6A)-C(7A)	112.47(19)
C(5A)-C(6A)-C(1A)	112.6(2)
C(7A)-C(6A)-C(1A)	112.42(18)
O(2A)-C(7A)-C(6A)	109.23(18)
O(2A)-C(7A)-C(8A)	112.61(19)
C(6A)-C(7A)-C(8A)	112.29(18)
C(11A)-C(8A)-C(7A)	112.91(18)
C(11A)-C(8A)-C(9A)	112.5(2)
C(7A)-C(8A)-C(9A)	107.9(2)
C(10A)-C(9A)-C(8A)	111.5(2)
C(5A)-C(10A)-C(9A)	124.6(2)

C(12A)-C(11A)-C(16A)	116.9(2)
C(12A)-C(11A)-C(8A)	121.1(2)
C(16A)-C(11A)-C(8A)	122.0(2)
C(11A)-C(12A)-C(13A)	121.2(3)
C(14A)-C(13A)-C(12A)	120.5(3)
C(15A)-C(14A)-C(13A)	119.4(3)
C(14A)-C(15A)-C(16A)	120.3(3)
C(15A)-C(16A)-C(11A)	121.7(2)
O(1B)-C(1B)-C(2B)	109.64(19)
O(1B)-C(1B)-C(6B)	111.96(18)
C(2B)-C(1B)-C(6B)	111.16(19)
C(1B)-C(2B)-C(3B)	116.28(19)
C(2B)-C(3B)-C(17B)	112.8(2)
C(2B)-C(3B)-C(4B)	108.3(2)
C(17B)-C(3B)-C(4B)	109.5(2)
C(2B)-C(3B)-C(18B)	108.6(2)
C(17B)-C(3B)-C(18B)	108.1(2)
C(4B)-C(3B)-C(18B)	109.5(2)
C(5B)-C(4B)-C(3B)	114.7(2)
C(10B)-C(5B)-C(4B)	123.6(2)
C(10B)-C(5B)-C(6B)	121.5(2)
C(4B)-C(5B)-C(6B)	114.8(2)
O(2B)-C(7B)-C(6B)	109.14(17)
O(2B)-C(7B)-C(8B)	111.38(18)
C(6B)-C(7B)-C(8B)	112.29(18)
C(5B)-C(6B)-C(7B)	113.28(18)
C(5B)-C(6B)-C(1B)	112.21(19)
C(7B)-C(6B)-C(1B)	111.88(18)
C(11B)-C(8B)-C(7B)	112.13(18)
C(11B)-C(8B)-C(9B)	114.5(2)
C(7B)-C(8B)-C(9B)	107.81(19)
C(10B)-C(9B)-C(8B)	111.7(2)
C(5B)-C(10B)-C(9B)	124.7(2)
C(12B)-C(11B)-C(16B)	116.9(2)
C(12B)-C(11B)-C(8B)	120.8(2)
C(16B)-C(11B)-C(8B)	122.3(2)

C(11B)-C(12B)-C(13B)	122.0(3)
C(14B)-C(13B)-C(12B)	120.0(3)
C(15B)-C(14B)-C(13B)	119.2(3)
C(14B)-C(15B)-C(16B)	120.6(3)
C(15B)-C(16B)-C(11B)	121.3(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for k9820. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

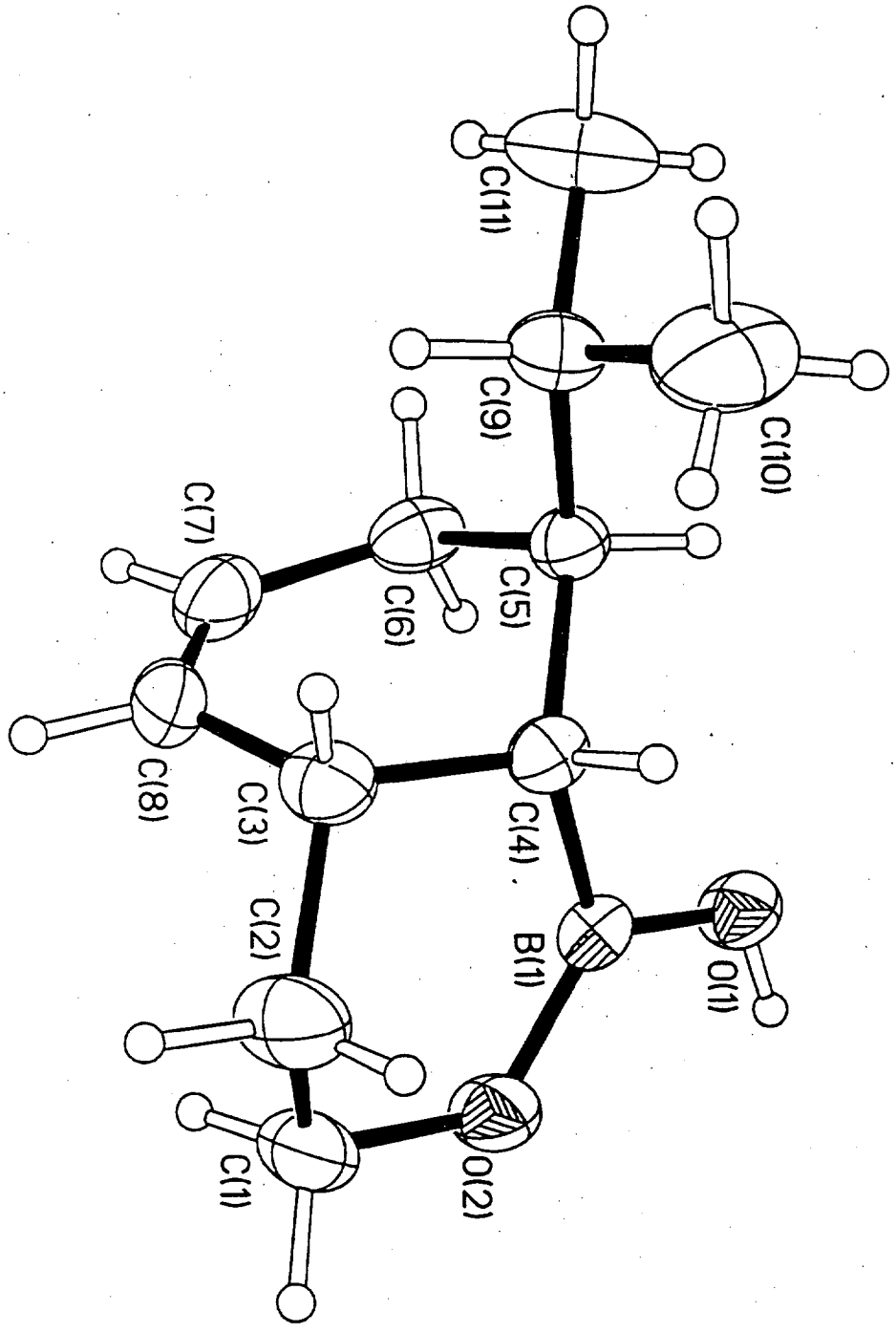
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1A)	55(1)	94(1)	76(1)	-27(1)	-14(1)	-6(1)
O(2A)	67(1)	46(1)	59(1)	-6(1)	-18(1)	2(1)
C(1A)	62(2)	46(1)	59(2)	-15(1)	-15(1)	4(1)
C(2A)	75(2)	62(2)	57(2)	-22(1)	-13(1)	7(1)
C(3A)	71(2)	58(2)	51(2)	-16(1)	-13(1)	-1(1)
C(4A)	67(2)	58(2)	57(2)	-10(1)	-20(1)	-1(1)
C(5A)	52(2)	49(2)	52(2)	-8(1)	-15(1)	-2(1)
C(6A)	54(2)	40(1)	52(2)	-11(1)	-16(1)	-6(1)
C(7A)	50(1)	36(1)	51(1)	-7(1)	-14(1)	-5(1)
C(8A)	51(2)	51(2)	55(2)	-13(1)	-12(1)	-3(1)
C(9A)	75(2)	52(2)	61(2)	-14(1)	-14(1)	12(1)
C(10A)	74(2)	50(2)	57(2)	-6(1)	-16(1)	12(1)
C(11A)	47(1)	45(1)	54(2)	-12(1)	-9(1)	2(1)
C(12A)	57(2)	55(2)	70(2)	-9(1)	-11(1)	-7(1)
C(13A)	77(2)	68(2)	58(2)	-3(2)	3(2)	-9(2)
C(14A)	80(2)	70(2)	53(2)	-16(2)	-7(2)	4(2)
C(15A)	66(2)	72(2)	67(2)	-30(2)	-12(2)	2(2)
C(16A)	54(2)	65(2)	58(2)	-21(1)	0(1)	-10(1)
C(17A)	84(2)	76(2)	79(2)	-6(2)	-10(2)	-13(2)
C(18A)	120(3)	94(2)	58(2)	-24(2)	-20(2)	12(2)
O(1B)	52(1)	72(1)	69(1)	-14(1)	-15(1)	-10(1)
O(2B)	99(1)	47(1)	52(1)	-21(1)	-8(1)	-2(1)
C(1B)	57(2)	48(1)	52(2)	-20(1)	-8(1)	-3(1)
C(2B)	58(2)	48(1)	61(2)	-11(1)	-3(1)	-4(1)
C(3B)	58(2)	61(2)	48(2)	-9(1)	-8(1)	-3(1)
C(4B)	65(2)	76(2)	54(2)	-18(1)	-16(1)	-8(1)
C(5B)	51(2)	60(2)	50(2)	-18(1)	-11(1)	-10(1)
C(7B)	45(1)	43(1)	47(1)	-19(1)	-8(1)	0(1)
C(6B)	42(1)	46(1)	48(1)	-15(1)	-6(1)	0(1)
C(8B)	45(1)	55(2)	56(2)	-13(1)	-12(1)	-8(1)
C(9B)	97(2)	55(2)	67(2)	-25(1)	-14(2)	-24(2)

C(10B)	89(2)	66(2)	54(2)	-26(1)	-12(1)	-23(2)
C(11B)	49(2)	43(1)	57(2)	-13(1)	-10(1)	-12(1)
C(12B)	62(2)	56(2)	65(2)	-14(1)	-10(1)	-4(1)
C(13B)	90(2)	69(2)	65(2)	-14(2)	-4(2)	-17(2)
C(14B)	108(3)	59(2)	67(2)	-2(2)	-28(2)	-24(2)
C(15B)	82(2)	50(2)	96(2)	-5(2)	-36(2)	-3(2)
C(16B)	55(2)	55(2)	79(2)	-14(2)	-11(1)	-8(1)
C(17B)	69(2)	78(2)	62(2)	-22(2)	-2(1)	1(2)
C(18B)	81(2)	84(2)	63(2)	-1(2)	-14(2)	2(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for k9820.

	x	y	z	U(eq)
H(1A)	3235	6990	8389	111
H(2A)	250	5436	10030	89
H(1AB)	2196	5793	8032	67
H(2AB)	1504	6180	6479	78
H(2AC)	2953	6633	6247	78
H(4AA)	-212	9073	5955	74
H(4AB)	-511	7732	6272	74
H(6AA)	14	6390	8196	58
H(7AA)	1335	7492	9232	55
H(8AA)	-1451	7158	9570	63
H(9AA)	-1748	9202	9134	77
H(9AB)	-208	9317	9115	77
H(10A)	-932	9692	7377	76
H(12A)	-2379	6412	11291	75
H(13A)	-2484	6174	13028	88
H(14A)	-967	7023	13598	84
H(15A)	638	8146	12425	80
H(16A)	739	8417	10689	71
H(17A)	2335	9141	6362	126
H(17B)	2106	9700	5194	126
H(17C)	3314	8761	5506	126
H(18A)	1011	8639	4349	137
H(18B)	899	7261	4840	137
H(18C)	2317	7781	4440	137
H(1B)	-8450	5518	11291	98
H(2B)	-5705	5408	9946	97
H(1BB)	-6752	4283	11336	62
H(2BB)	-5862	3319	12820	70
H(2BC)	-7420	3220	13092	70
H(4BA)	-5790	5606	13975	78

H(4BB)	-4794	4838	13421	78
H(7BA)	-7109	6875	10573	53
H(6BA)	-5018	5273	11430	55
H(8BB)	-4419	7442	10389	62
H(9BA)	-5282	8847	11172	84
H(9BB)	-6765	8592	11143	84
H(10B)	-5861	7548	12824	80
H(12B)	-3645	8113	8618	74
H(13B)	-3748	9399	6965	92
H(14B)	-5620	10687	6585	95
H(15B)	-7386	10656	7870	94
H(16B)	-7282	9380	9523	77
H(17D)	-8067	4945	14760	107
H(17E)	-8750	4195	14261	107
H(17F)	-8331	5479	13599	107
H(18D)	-5408	2865	14526	123
H(18E)	-6920	2636	14967	123
H(18F)	-6181	3524	15279	123



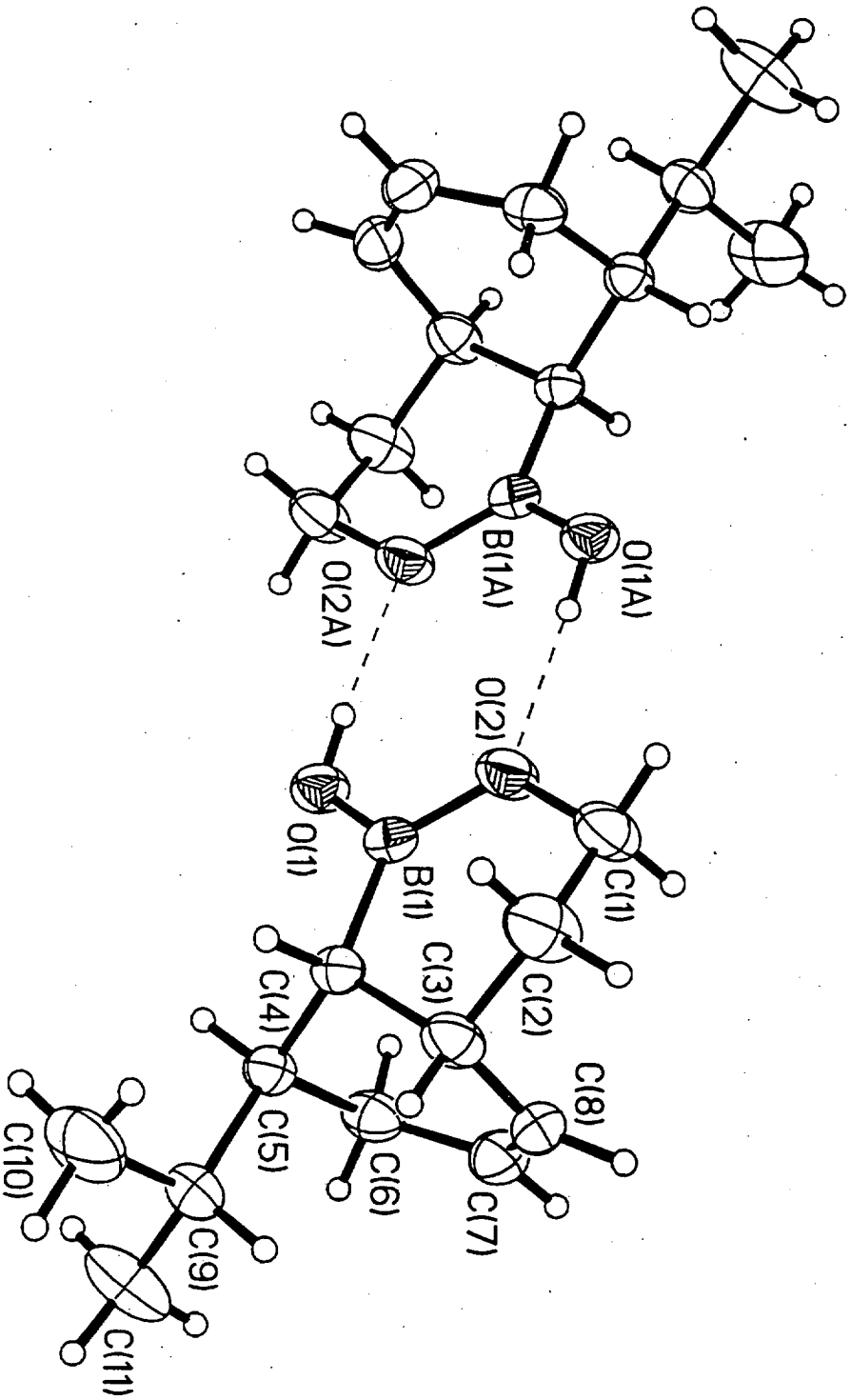

O(1A)
B(1A)
O(2A)
O(2)
O(1)
B(1)
C(1)
C(3)
C(2)
C(4)
C(8)
C(5)
C(6)
C(7)
C(10)
C(9)
C(11)

Table 1. Crystal data and structure refinement for 1.

Identification code	k9811
Empirical formula	$C_{11}H_{19}BO_2$
Formula weight	194.07
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 10.3504(4) Å alpha = 90° b = 10.9465(3) Å beta = 113.698(2)° c = 10.9959(4) Å gamma = 90°
Volume, Z	1140.79(7) Å^3, 4
Density (calculated)	1.130 Mg/m^3
Absorption coefficient	0.074 mm^{-1}
F(000)	424
Crystal size	0.35 x 0.38 x 0.21 mm
θ range for data collection	2.75 to 26.38°
Limiting indices	$0 \le h \le 12$, $0 \le k \le 13$, $-13 \le l \le 12$
Reflections collected	12437
Independent reflections	2328 (R_{int} = 0.0490)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2328 / 0 / 134
Goodness-of-fit on F^2	1.094
Final R indices [I>2σ(I)]	R1 = 0.0503, wR2 = 0.1446
R indices (all data)	R1 = 0.0719, wR2 = 0.1575
Extinction coefficient	0.072(11)
Largest diff. peak and hole	0.221 and -0.165 eÅ^{-3}

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	6894(1)	410(1)	304(1)	56(1)
O(2)	4729(1)	863(1)	-1400(1)	62(1)
B(1)	6164(2)	1015(2)	-838(2)	46(1)
C(1)	3883(2)	1343(2)	-2691(2)	78(1)
C(2)	4520(2)	2464(2)	-3017(2)	79(1)
C(3)	6030(2)	2246(2)	-2868(2)	57(1)
C(4)	6948(2)	1917(1)	-1430(1)	45(1)
C(5)	8416(2)	1464(1)	-1275(2)	47(1)
C(6)	8215(2)	283(1)	-2073(2)	59(1)
C(7)	7083(2)	397(2)	-3414(2)	72(1)
C(8)	6127(2)	1262(2)	-3781(2)	68(1)
C(9)	9268(2)	2438(2)	-1656(2)	57(1)
C(10)	9403(3)	3617(2)	-901(3)	114(1)
C(11)	10721(2)	1995(2)	-1465(3)	105(1)

Table 3. Bond lengths [Å] and angles [°] for 1.

O(1)-B(1)	1.351(2)	O(2)-B(1)	1.370(2)
O(2)-C(1)	1.435(2)	B(1)-C(4)	1.576(2)
C(1)-C(2)	1.503(3)	C(2)-C(3)	1.523(2)
C(3)-C(8)	1.504(3)	C(3)-C(4)	1.525(2)
C(4)-C(5)	1.541(2)	C(5)-C(6)	1.529(2)
C(5)-C(9)	1.545(2)	C(6)-C(7)	1.475(3)
C(7)-C(8)	1.310(3)	C(9)-C(10)	1.510(3)
C(9)-C(11)	1.512(3)		

B(1)-O(2)-C(1)	121.41(12)	O(1)-B(1)-O(2)	117.36(14)
O(1)-B(1)-C(4)	120.18(14)	O(2)-B(1)-C(4)	122.35(14)
O(2)-C(1)-C(2)	112.56(14)	C(1)-C(2)-C(3)	112.1(2)
C(8)-C(3)-C(2)	112.4(2)	C(8)-C(3)-C(4)	110.01(13)
C(2)-C(3)-C(4)	109.54(12)	C(3)-C(4)-C(5)	111.52(11)
C(3)-C(4)-B(1)	111.48(12)	C(5)-C(4)-B(1)	113.68(11)
C(6)-C(5)-C(4)	107.96(12)	C(6)-C(5)-C(9)	112.89(12)
C(4)-C(5)-C(9)	113.11(12)	C(7)-C(6)-C(5)	111.85(14)
C(8)-C(7)-C(6)	124.6(2)	C(7)-C(8)-C(3)	123.8(2)
C(10)-C(9)-C(11)	109.3(2)	C(10)-C(9)-C(5)	112.2(2)
C(11)-C(9)-C(5)	112.66(14)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(1)	57(1)	65(1)	51(1)	11(1)	27(1)	2(1)
O(2)	50(1)	84(1)	58(1)	17(1)	27(1)	-2(1)
B(1)	50(1)	48(1)	44(1)	-2(1)	25(1)	2(1)
C(1)	44(1)	120(2)	67(1)	31(1)	20(1)	2(1)
C(2)	58(1)	98(2)	80(1)	39(1)	27(1)	19(1)
C(3)	52(1)	62(1)	60(1)	19(1)	25(1)	-1(1)
C(4)	50(1)	42(1)	48(1)	0(1)	24(1)	-1(1)
C(5)	47(1)	48(1)	48(1)	2(1)	22(1)	-2(1)
C(6)	66(1)	50(1)	77(1)	-5(1)	44(1)	-1(1)
C(7)	80(1)	82(1)	67(1)	-26(1)	43(1)	-24(1)
C(8)	62(1)	101(2)	42(1)	0(1)	20(1)	-22(1)
C(9)	52(1)	56(1)	67(1)	1(1)	28(1)	-9(1)
C(10)	133(2)	79(2)	166(2)	-47(2)	98(2)	-58(2)
C(11)	64(1)	93(2)	171(2)	22(2)	62(2)	-4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(1B)	2954(2)	1543(2)	-2731(2)	93
H(1C)	3770(2)	720(2)	-3353(2)	93
H(2A)	4510(2)	3125(2)	-2433(2)	95
H(2B)	3950(2)	2711(2)	-3923(2)	95
H(3A)	6389(2)	3007(2)	-3084(2)	68
H(4A)	7102(2)	2676(1)	-918(1)	54
H(5A)	8948(2)	1260(1)	-337(2)	56
H(6A)	9092(2)	77(1)	-2148(2)	71
H(6B)	7987(2)	-376(1)	-1604(2)	71
H(7A)	7046(2)	-185(2)	-4044(2)	86
H(8A)	5470(2)	1267(2)	-4658(2)	82
H(9A)	8751(2)	2620(2)	-2602(2)	69
H(10A)	9961(19)	4186(7)	-1148(16)	171
H(10B)	9851(20)	3458(4)	35(3)	171
H(10C)	8482(3)	3955(10)	-1112(16)	171
H(11A)	11242(8)	2657(5)	-1624(19)	157
H(11B)	10634(2)	1344(12)	-2077(13)	157
H(11C)	11209(8)	1704(16)	-572(6)	157
H(1O)	6410(24)	52(21)	663(22)	105(8)