Table 1. Crystal data and structure refinement for compound 1.

Crystal data

Empirical formula	C25 H26 O5
Formula weight	406.46
Temperature	290(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 10.044(2) Å α= 90 °.
	b = 10.216(2) Å β = 90 °.
	c = 21.784(4) Å γ = 90 °.
Volume	2235.3 (5) Å3,
Z	4
Density (calculated)	1.208 Mg/m3
radiation_type	MoKa
cell parameters from 29 reflections	
θ	2.85 to 12.08 °
Absorption coefficient	0.083 mm-1
F(000)	864

Crystal size	0.60 × 0.50 × 0.20 mm

Data collection

Siemens P4 diffractometer	
ω scans	
θ range for data collection	1.87 to 27.00°.
Limiting indices	
h	0 to 12,
k	0 to 13,
l	-1 to 27
Reflections collected	3050
Independent reflections	2771
1120 reflections with I > 2σ (I)	
R(int)	0.0143
Absorption correction	None
3 standard reflections every 97 reflections	
intensity decay:	3.39%

Refinement

Refinement method	Full-matrix least-squares on F2

Data / restraints / parameters	2771 / 0 / 280
Goodness-of-fit on F2	0.801
Final R indices [I>2sigma(I)]	R1 = 0.0365, wR2 = 0.0606
R indices (all data)	R1 = 0.1146, wR2 = 0.0700
Absolute structure parameter	0 (10)
H-atom parameters constrained	
w=1/[s2(Fo2)+(0.0232P)2+0.0000P]	
where P=(Fo2+2Fc2)/3	
(Δ/σ)max = 0.000	
$\Delta\rho$max = 0.112 e.A-3	
$\Delta\rho$min = -0.115 e.A-3	
Extinction correlation	SHELXL-97
Extinction coefficient	0.0048 (4)
Data collection:	XSCANS (Siemens, 1994);
cell refinement:	XSCANS;
data reduction:	SHELXTL (Siemens, 1998);
program(s) used to solve structure:	SHELXS-97 (Sheldrick, 1990);
program(s) used to refine structure:	SHELXL-97 (Sheldrick, 1997);
molecular_graphics:	SHELXTL;
software used to prepare material	

for publication: SHELXTL.

Table 2. Atomic coordinates (× 104) and equivalent isotropic displacement parameters (A2 × 103) for compound 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	7028(2)	5197(2)	5724(1)	66(1)
O(7)	7832(2)	5541(2)	3585(1)	71(1)
O(19)	4335(2)	2254(2)	5443(1)	84(1)
O(20)	4766(2)	2409(2)	4283(1)	80(1)
O(22)	9408(3)	6795(3)	3213(1)	108(1)
C(2)	6660(4)	4318(3)	6221(1)	74(1)
C(3)	5268(4)	3793(4)	6147(2)	75(1)
C(4)	5111(3)	3181(3)	5525(2)	64(1)

C(4A)	5867(3)	3755(3)	5027(2)	54(1)
C(5)	5663(3)	3367(3)	4412(2)	60(1)
C(6)	6296(3)	3982(3)	3934(1)	62(1)
C(6A)	7209(3)	4940(3)	4082(2)	56(1)
C(8)	8991(4)	6247(4)	3655(2)	76(1)
C(9)	9586(3)	6241(3)	4283(1)	67(1)
C(10)	8545(3)	6357(3)	4797(1)	57(1)
C(10A)	7481(3)	5367(3)	4680(1)	51(1)
C(10B)	6782(3)	4754(3)	5143(1)	52(1)
C(1')	5978(3)	3631(3)	3274(1)	81(1)
C(2')	4866(4)	4474(4)	3027(2)	104(2)
C(3')	3922(5)	4167(5)	2668(2)	103(1)
C(4')	3853(9)	2898(7)	2409(5)	320(6)
C(5')	2861(4)	5098(5)	2470(2)	182(2)
C(11)	8053(3)	7743(3)	4877(2)	58(1)
C(12)	7280(4)	8329(4)	4433(2)	82(1)
C(13)	6888(4)	9626(4)	4483(2)	99(2)
C(14)	7252(4)	10324(4)	4990(2)	106(2)
C(15)	7991(4)	9763(4)	5448(2)	103(2)
C(16)	8407(3)	8461(4)	5388(2)	79(1)

C(17)	6892(4)	5150(3)	6796(1)	108(1)
C(18)	4866(4)	2843(4)	6656(2)	128(2)

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

O(1)-C(10B)	1.366(3)
O(1)-C(2)	1.455(3)
O(7)-C(8)	1.377(4)
O(7)-C(6A)	1.395(3)
O(19)-C(4)	1.239(3)
O(20)-C(5)	1.360(3)
O(20)-H(20O)	0.8200
O(22)-C(8)	1.189(4)
C(2)-C(3)	1.506(4)
C(2)-C(17)	1.531(4)
C(2)-H(2)	0.9800
C(3)-C(4)	1.501(4)

C(3)-C(18)	1.528(4)
C(3)-H(3)	0.9800
C(4)-C(4A)	1.449(4)
C(4A)-C(10B)	1.396(3)
C(4A)-C(5)	1.411(4)
C(5)-C(6)	1.374(4)
C(6)-C(6A)	1.380(4)
C(6)-C(1')	1.514(4)
C(6A)-C(10A)	1.399(4)
C(8)-C(9)	1.493(4)
C(9)-C(10)	1.538(3)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(10)-C(10A)	1.493(4)
C(10)-C(11)	1.509(4)
C(10)-H(10)	0.9800
C(10A)-C(10B)	1.381(4)
C(1')-C(2')	1.510(4)
C(1')-H(1'A)	0.9700
C(1')-H(1'B)	0.9700

C(2')-C(3')	1.268(4)
C(2')-H(2')	0.9300
C(3')-C(4')	1.416(6)
C(3')-C(5')	1.493(5)
C(4')-H(4'A)	0.9600
C(4')-H(4'B)	0.9600
C(4')-H(4'C)	0.9600
C(5')-H(5'A)	0.9600
C(5')-H(5'B)	0.9600
C(5')-H(5'C)	0.9600
C(11)-C(16)	1.379(4)
C(11)-C(12)	1.379(4)
C(12)-C(13)	1.386(4)
C(12)-H(12)	0.9300
C(13)-C(14)	1.365(5)
C(13)-H(13)	0.9300
C(14)-C(15)	1.369(5)
C(14)-H(14)	0.9300
C(15)-C(16)	1.400(4)
C(15)-H(15)	0.9300

C(16)-H(16)	0.9300
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600

C(10B)-O(1)-C(2)	116.0(2)
C(8)-O(7)-C(6A)	121.6(3)
C(5)-O(20)-H(20O)	109.5
O(1)-C(2)-C(3)	112.1(3)
O(1)-C(2)-C(17)	103.1(3)
C(3)-C(2)-C(17)	115.2(3)
O(1)-C(2)-H(2)	108.7
C(3)-C(2)-H(2)	108.7
C(17)-C(2)-H(2)	108.7
C(4)-C(3)-C(2)	110.0(3)
C(4)-C(3)-C(18)	111.3(3)
C(2)-C(3)-C(18)	113.2(3)

C(4)-C(3)-H(3)	107.4
C(2)-C(3)-H(3)	107.4
C(18)-C(3)-H(3)	107.4
O(19)-C(4)-C(4A)	122.1(3)
O(19)-C(4)-C(3)	121.0(3)
C(4A)-C(4)-C(3)	116.9(3)
C(10B)-C(4A)-C(5)	118.3(3)
C(10B)-C(4A)-C(4)	120.3(3)
C(5)-C(4A)-C(4)	121.4(3)
O(20)-C(5)-C(6)	118.6(3)
O(20)-C(5)-C(4A)	119.7(3)
C(6)-C(5)-C(4A)	121.6(3)
C(5)-C(6)-C(6A)	117.0(3)
C(5)-C(6)-C(1')	120.9(3)
C(6A)-C(6)-C(1')	122.1(3)
C(6)-C(6A)-O(7)	115.3(3)
C(6)-C(6A)-C(10A)	124.8(3)
O(7)-C(6A)-C(10A)	119.8(3)
O(22)-C(8)-O(7)	117.1(4)
O(22)-C(8)-C(9)	127.0(4)

O(7)-C(8)-C(9)	116.0(3)
C(8)-C(9)-C(10)	113.3(3)
C(8)-C(9)-H(9A)	108.9
C(10)-C(9)-H(9A)	108.9
C(8)-C(9)-H(9B)	108.9
C(10)-C(9)-H(9B)	108.9
H(9A)-C(9)-H(9B)	107.7
C(10A)-C(10)-C(11)	114.9(2)
C(10A)-C(10)-C(9)	108.0(3)
C(11)-C(10)-C(9)	112.3(3)
C(10A)-C(10)-H(10)	107.1
C(11)-C(10)-H(10)	107.1
C(9)-C(10)-H(10)	107.1
C(10B)-C(10A)-C(6A)	116.0(3)
C(10B)-C(10A)-C(10)	123.1(3)
C(6A)-C(10A)-C(10)	120.7(3)
O(1)-C(10B)-C(10A)	115.8(3)
O(1)-C(10B)-C(4A)	122.0(3)
C(10A)-C(10B)-C(4A)	122.2(3)
C(2')-C(1')-C(6)	111.0(3)

C(2')-C(1')-H(1'A)	109.4
C(6)-C(1')-H(1'A)	109.4
C(2')-C(1')-H(1'B)	109.4
C(6)-C(1')-H(1'B)	109.4
H(1'A)-C(1')-H(1'B)	108.0
C(3')-C(2')-C(1')	129.2(4)
C(3')-C(2')-H(2')	115.4
C(1')-C(2')-H(2')	115.4
C(2')-C(3')-C(4')	120.6(5)
C(2')-C(3')-C(5')	123.7(5)
C(4')-C(3')-C(5')	115.7(5)
C(3')-C(4')-H(4'A)	109.5
C(3')-C(4')-H(4'B)	109.5
H(4'A)-C(4')-H(4'B)	109.5
C(3')-C(4')-H(4'C)	109.5
H(4'A)-C(4')-H(4'C)	109.5
H(4'B)-C(4')-H(4'C)	109.5
C(3')-C(5')-H(5'A)	109.5
C(3')-C(5')-H(5'B)	109.5
H(5'A)-C(5')-H(5'B)	109.5

C(3')-C(5')-H(5'C)	109.5
H(5'A)-C(5')-H(5'C)	109.5
H(5'B)-C(5')-H(5'C)	109.5
C(16)-C(11)-C(12)	118.7(3)
C(16)-C(11)-C(10)	120.6(3)
C(12)-C(11)-C(10)	120.7(3)
C(11)-C(12)-C(13)	121.3(4)
C(11)-C(12)-H(12)	119.3
C(13)-C(12)-H(12)	119.3
C(14)-C(13)-C(12)	119.2(4)
C(14)-C(13)-H(13)	120.4
C(12)-C(13)-H(13)	120.4
C(13)-C(14)-C(15)	121.1(4)
C(13)-C(14)-H(14)	119.5
C(15)-C(14)-H(14)	119.5
C(14)-C(15)-C(16)	119.4(4)
C(14)-C(15)-H(15)	120.3
C(16)-C(15)-H(15)	120.3
C(11)-C(16)-C(15)	120.3(4)
C(11)-C(16)-H(16)	119.8

C(15)-C(16)-H(16)	119.8
C(2)-C(17)-H(17A)	109.5
C(2)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(2)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(3)-C(18)-H(18A)	109.5
C(3)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(3)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A2 × 103) for compound 1.

The anisotropic displacement factor exponent takes the form:

-2 pi2 [h2 a*2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	82(2)	61(2)	53(1)	-3(1)	-9(1)	-11(1)
O(7)	72(2)	84(2)	56(2)	4(1)	-8(1)	-1(2)
O(19)	79(2)	73(2)	100(2)	4(2)	-6(2)	-23(2)
O(20)	83(2)	61(2)	95(2)	-14(2)	-19(2)	-12(1)
O(22)	104(2)	145(2)	74(2)	23(2)	5(2)	-25(2)
C(2)	91(3)	75(2)	56(2)	4(2)	-2(2)	-4(2)
C(3)	74(3)	76(3)	74(3)	-2(2)	4(2)	-3(2)
C(4)	55(2)	52(2)	84(3)	-2(2)	-12(2)	0(2)
C(4A)	58(2)	41(2)	64(2)	2(2)	-9(2)	0(2)
C(5)	61(2)	39(2)	79(3)	-5(2)	-19(2)	-1(2)
C(6)	64(2)	60(2)	61(2)	-8(2)	-21(2)	8(2)
C(6A)	56(2)	49(2)	62(2)	4(2)	-7(2)	7(2)

C(8)	70(3)	84(3)	75(3)	3(3)	1(3)	17(2)
C(9)	49(2)	80(2)	73(2)	5(2)	-4(2)	11(2)
C(10)	55(2)	58(2)	57(2)	2(2)	-10(2)	4(2)
C(10A)	51(2)	49(2)	51(2)	-6(2)	-14(2)	9(2)
C(10B)	55(2)	50(2)	50(2)	-3(2)	-6(2)	6(2)
C(1')	90(3)	86(3)	66(3)	-18(2)	-15(2)	0(3)
C(2')	119(4)	111(3)	83(3)	-12(3)	-44(3)	6(3)
C(3')	102(4)	112(4)	94(3)	16(3)	-38(3)	-22(3)
C(4')	367(12)	173(7)	421(12)	-55(7)	-306(11)	-35(6)
C(5')	145(5)	232(6)	168(5)	80(4)	-79(4)	-3(5)
C(11)	49(2)	52(2)	74(2)	3(2)	0(2)	-7(2)
C(12)	94(3)	68(3)	82(3)	14(2)	12(2)	23(2)
C(13)	87(3)	87(4)	123(4)	24(3)	32(3)	13(3)
C(14)	77(3)	59(3)	183(6)	17(4)	47(4)	4(3)
C(15)	68(3)	76(3)	165(5)	-49(3)	19(3)	-18(3)
C(16)	57(2)	75(3)	103(3)	-20(2)	-9(2)	-15(2)
C(17)	142(3)	127(3)	55(2)	-6(3)	5(3)	-29(4)
C(18)	143(4)	154(4)	87(3)	10(3)	14(3)	-62(4)

Table 5. Hydrogen coordinates (× 104) and isotropic displacement parameters (A2 × 103) for compound 1.

	x	y	z	U(eq)
H(20O)	4444	2131	4603	96
H(2)	7284	3580	6226	89
H(3)	4658	4541	6167	90
H(9A)	10208	6963	4316	81
H(9B)	10083	5435	4338	81
H(10)	8986	6107	5181	68
H(1'A)	6767	3749	3023	97
H(1'B)	5720	2717	3251	97
H(2')	4874	5341	3156	125
H(4'A)	4437	2848	2061	560(90)
H(4'B)	2956	2722	2281	165(19)

H(4'C)	4119	2263	2710	440(70)
H(5'A)	2903	5875	2717	218
H(5'B)	2005	4694	2518	218
H(5'C)	2994	5326	2047	218
H(12)	7017	7846	4092	98
H(13)	6383	10015	4175	119
H(14)	6994	11195	5025	128
H(15)	8214	10241	5797	124
H(16)	8925	8080	5693	94
H(17A)	7795	5457	6800	130
H(17B)	6729	4630	7155	130
H(17C)	6296	5885	6792	130
H(18A)	3995	2501	6572	153
H(18B)	4856	3296	7043	153
H(18C)	5495	2137	6674	153

H-bond:

O20 H20O O19 0.82 1.84 2.570(3) 147.9 .