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

Crystal data	
Empirical formula	C24 H32 O6
Formula weight	416.50
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 7.806(1) Å α = 90 °.
	b = 15.010(3) Å β = 90 °.
	c = 18.893(3) Å γ = 90 °.
Volume,	2213.7(5) Å3,
Z	4
Density (calculated)	1.250 Mg/m3
radiation_type	MoKa
cell parameters from 33 reflections	
θ	4.97 to 14.94°
Absorption coefficient	0.089 mm-1
F(000)	896
Crystal size	0.58 x 0.56 x 0.52 mm
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	1.73 to 28.00°.
Limiting indices	
h	0 to 10,
k	0 to 19,
l	-1 to 24
Reflections collected	3371
Independent reflections	3035
1120 reflections with I > 2σ (I)	
R(int)	0.0064
Absorption correction	None
3 standard reflections every 97 reflections	
intensity decay:	1.71%
Refinement	
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	3035 / 0 / 277

Goodness-of-fit on F2	0.879
Final R indices [I>2sigma(I)]	R1 = 0.0370, wR2 = 0.0845
R indices (all data)	R1 = 0.0561, wR2 = 0.0892
Absolute structure parameter	0 (10)
H-atom parameters constrained	
w=1/[s2(Fo2)+(0.0549P)2+0.0000P]	
where P=(Fo2+2Fc2)/3	
(Δ/σ)max = 0.000	
Δρmax = 0.144 e.A-3	
Δρmin = -0.129 e.A-3	
Extinction correlation	SHELXL-97
Extinction coefficient	0.0242(16)
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(12)	2594(2)	5834(1)	5384(1)	53(1)
O(14)	3491(2)	2764(1)	5547(1)	47(1)
O(16)	2117(2)	5823(1)	4217(1)	62(1)
O(19)	7316(2)	3334(1)	9062(1)	49(1)
O(2')	1379(4)	1934(2)	5989(1)	101(1)
O(2")	7172(3)	4194(1)	10012(1)	82(1)
C(1)	7922(3)	5196(2)	6978(1)	50(1)
C(2)	9414(3)	5261(2)	7495(1)	55(1)
C(3)	10139(3)	4356(2)	7667(1)	58(1)
C(4)	8823(3)	3688(2)	7967(1)	48(1)
C(5)	7240(3)	3680(1)	7468(1)	43(1)
C(6)	5798(3)	3028(2)	7655(1)	48(1)
C(7)	4729(3)	2835(1)	7002(1)	49(1)
C(8)	4374(3)	3657(1)	6563(1)	39(1)
C(9)	5117(3)	4449(1)	6677(1)	39(1)

C(10)	6455(3)	4596(1)	7260(1)	39(1)
C(11)	4651(3)	5265(1)	6247(1)	47(1)
C(12)	2894(3)	5176(1)	5921(1)	45(1)
C(13)	2755(3)	4305(1)	5548(1)	40(1)
C(14)	3024(3)	3508(1)	6001(1)	40(1)
C(15)	2499(3)	4436(1)	4861(1)	44(1)
C(16)	2371(3)	5413(2)	4751(1)	48(1)
C(17)	2351(4)	3830(2)	4238(1)	60(1)
C(18)	9651(4)	2766(2)	7975(1)	66(1)
C(19)	8484(3)	3959(2)	8738(1)	50(1)
C(20)	5529(3)	5084(2)	7874(1)	48(1)
C(1')	2929(5)	1396(2)	4998(2)	82(1)
C(2')	2478(4)	2038(2)	5562(1)	59(1)
C(1")	5684(4)	2812(2)	10009(1)	64(1)
C(2")	6781(3)	3527(2)	9714(1)	49(1)

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

O(12)-C(16)	1.363(3)
O(12)-C(12)	1.436(2)
O(14)-C(2')	1.347(3)
O(14)-C(14)	1.454(2)
O(16)-C(16)	1.199(2)
O(19)-C(2")	1.332(3)
O(19)-C(19)	1.445(3)
O(2')-C(2')	1.188(3)
O(2")-C(2")	1.189(3)
C(1)-C(2)	1.523(3)
C(1)-C(10)	1.550(3)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(3)	1.507(4)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.543(3)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(18)	1.527(3)
C(4)-C(19)	1.536(3)
C(4)-C(5)	1.554(3)
C(5)-C(6)	1.532(3)

C(5)-C(10)	1.556(3)
C(5)-H(5)	0.9800
C(6)-C(7)	1.518(3)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-C(8)	1.511(3)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-C(9)	1.340(3)
C(8)-C(14)	1.513(3)
C(9)-C(11)	1.514(3)
C(9)-C(10)	1.534(3)
C(10)-C(20)	1.551(3)
C(11)-C(12)	1.510(3)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.488(3)
C(12)-H(12)	0.9800
C(13)-C(15)	1.327(3)
C(13)-C(14)	1.485(3)
C(14)-H(14)	0.9800
C(15)-C(16)	1.484(3)
C(15)-C(17)	1.492(3)
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(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(1')-C(2')	1.480(4)
C(1')-H(1'A)	0.9600
C(1')-H(1'B)	0.9600
C(1')-H(1'C)	0.9600
C(1")-C(2")	1.483(4)
C(1")-H(1"A)	0.9600
C(1")-H(1"B)	0.9600
C(1")-H(1"C)	0.9600

C(16)-O(12)-C(12)	108.68(16)

C(2')-O(14)-C(14)	117.49(19)
C(2")-O(19)-C(19)	116.57(18)
C(2)-C(1)-C(10)	112.46(17)
C(2)-C(1)-H(1A)	109.1
C(10)-C(1)-H(1A)	109.1
C(2)-C(1)-H(1B)	109.1
C(10)-C(1)-H(1B)	109.1
H(1A)-C(1)-H(1B)	107.8
C(3)-C(2)-C(1)	111.57(19)
C(3)-C(2)-H(2A)	109.3
C(1)-C(2)-H(2A)	109.3
C(3)-C(2)-H(2B)	109.3
C(1)-C(2)-H(2B)	109.3
H(2A)-C(2)-H(2B)	108.0
C(2)-C(3)-C(4)	114.5(2)
C(2)-C(3)-H(3A)	108.6
C(4)-C(3)-H(3A)	108.6
C(2)-C(3)-H(3B)	108.6
C(4)-C(3)-H(3B)	108.6
H(3A)-C(3)-H(3B)	107.6
C(18)-C(4)-C(19)	107.69(19)
C(18)-C(4)-C(3)	108.1(2)
C(19)-C(4)-C(3)	106.89(19)
C(18)-C(4)-C(5)	109.59(19)
C(19)-C(4)-C(5)	116.14(19)
C(3)-C(4)-C(5)	108.12(17)
C(6)-C(5)-C(4)	116.66(17)
C(6)-C(5)-C(10)	109.47(19)
C(4)-C(5)-C(10)	117.35(17)
C(6)-C(5)-H(5)	103.8
C(4)-C(5)-H(5)	103.8
C(10)-C(5)-H(5)	103.8
C(7)-C(6)-C(5)	109.75(17)
C(7)-C(6)-H(6A)	109.7
C(5)-C(6)-H(6A)	109.7
C(7)-C(6)-H(6B)	109.7
C(5)-C(6)-H(6B)	109.7
H(6A)-C(6)-H(6B)	108.2
C(8)-C(7)-C(6)	113.05(17)
C(8)-C(7)-H(7A)	109.0
C(6)-C(7)-H(7A)	109.0
C(8)-C(7)-H(7B)	109.0
C(6)-C(7)-H(7B)	109.0
H(7A)-C(7)-H(7B)	107.8

C(9)-C(8)-C(7)	123.78(19)
C(9)-C(8)-C(14)	123.00(18)
C(7)-C(8)-C(14)	113.16(18)
C(8)-C(9)-C(11)	121.84(19)
C(8)-C(9)-C(10)	122.54(18)
C(11)-C(9)-C(10)	115.61(17)
C(9)-C(10)-C(1)	109.91(15)
C(9)-C(10)-C(20)	106.71(18)
C(1)-C(10)-C(20)	109.04(17)
C(9)-C(10)-C(5)	108.80(16)
C(1)-C(10)-C(5)	108.03(18)
C(20)-C(10)-C(5)	114.31(16)
C(12)-C(11)-C(9)	111.45(18)
C(12)-C(11)-H(11A)	109.3
C(9)-C(11)-H(11A)	109.3
C(12)-C(11)-H(11B)	109.3
C(9)-C(11)-H(11B)	109.3
H(11A)-C(11)-H(11B)	108.0
O(12)-C(12)-C(13)	104.98(16)
O(12)-C(12)-C(11)	112.06(18)
C(13)-C(12)-C(11)	109.70(18)
O(12)-C(12)-H(12)	110.0
C(13)-C(12)-H(12)	110.0
C(11)-C(12)-H(12)	110.0
C(15)-C(13)-C(14)	134.69(19)
C(15)-C(13)-C(12)	110.09(19)
C(14)-C(13)-C(12)	115.11(17)
O(14)-C(14)-C(13)	108.35(15)
O(14)-C(14)-C(8)	110.59(17)
C(13)-C(14)-C(8)	112.61(17)
O(14)-C(14)-H(14)	108.4
C(13)-C(14)-H(14)	108.4
C(8)-C(14)-H(14)	108.4
C(13)-C(15)-C(16)	107.04(19)
C(13)-C(15)-C(17)	133.9(2)
C(16)-C(15)-C(17)	119.11(19)
O(16)-C(16)-O(12)	121.4(2)
O(16)-C(16)-C(15)	129.5(2)
O(12)-C(16)-C(15)	109.12(18)
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5

H(17B)-C(17)-H(17C)	109.5
C(4)-C(18)-H(18A)	109.5
C(4)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(4)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
O(19)-C(19)-C(4)	109.72(18)
O(19)-C(19)-H(19A)	109.7
C(4)-C(19)-H(19A)	109.7
O(19)-C(19)-H(19B)	109.7
C(4)-C(19)-H(19B)	109.7
H(19A)-C(19)-H(19B)	108.2
C(10)-C(20)-H(20A)	109.5
C(10)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(10)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(2')-C(1')-H(1'A)	109.5
C(2')-C(1')-H(1'B)	109.5
H(1'A)-C(1')-H(1'B)	109.5
C(2')-C(1')-H(1'C)	109.5
H(1'A)-C(1')-H(1'C)	109.5
H(1'B)-C(1')-H(1'C)	109.5
O(2')-C(2')-O(14)	123.0(2)
O(2')-C(2')-C(1')	125.1(3)
O(14)-C(2')-C(1')	111.9(3)
C(2")-C(1")-H(1"A)	109.5
C(2")-C(1")-H(1"B)	109.5
H(1"A)-C(1")-H(1"B)	109.5
C(2")-C(1")-H(1"C)	109.5
H(1"A)-C(1")-H(1"C)	109.5
H(1"B)-C(1")-H(1"C)	109.5
O(2")-C(2")-O(19)	122.7(2)
O(2")-C(2")-C(1")	125.4(2)
O(19)-C(2")-C(1")	111.8(2)

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(12)	66(1)	40(1)	53(1)	5(1)	-7(1)	8(1)
O(14)	57(1)	37(1)	46(1)	-7(1)	-3(1)	-6(1)
O(16)	67(1)	64(1)	57(1)	17(1)	-7(1)	3(1)
O(19)	59(1)	48(1)	38(1)	-1(1)	3(1)	-4(1)
O(2')	109(2)	85(1)	110(2)	-7(1)	14(2)	-55(2)
O(2")	130(2)	65(1)	51(1)	-15(1)	15(1)	-21(1)
C(1)	61(2)	50(1)	40(1)	2(1)	5(1)	-14(1)
C(2)	56(1)	64(2)	46(1)	-1(1)	9(1)	-18(1)
C(3)	48(1)	80(2)	46(1)	-3(1)	9(1)	-5(1)
C(4)	50(1)	53(1)	40(1)	-1(1)	2(1)	3(1)
C(5)	53(1)	43(1)	31(1)	-4(1)	7(1)	1(1)
C(6)	63(1)	40(1)	40(1)	7(1)	-2(1)	-5(1)
C(7)	67(2)	36(1)	44(1)	2(1)	-3(1)	-11(1)
C(8)	51(1)	36(1)	31(1)	-1(1)	4(1)	-2(1)
C(9)	51(1)	37(1)	30(1)	0(1)	7(1)	-1(1)
C(10)	49(1)	36(1)	31(1)	-2(1)	6(1)	-4(1)
C(11)	64(2)	33(1)	43(1)	-1(1)	-4(1)	-3(1)
C(12)	52(1)	39(1)	45(1)	3(1)	5(1)	3(1)
C(13)	36(1)	41(1)	43(1)	-1(1)	1(1)	-2(1)
C(14)	46(1)	36(1)	39(1)	-2(1)	6(1)	-5(1)
C(15)	39(1)	48(1)	45(1)	1(1)	-3(1)	2(1)
C(16)	40(1)	54(1)	49(1)	6(1)	-1(1)	6(1)
C(17)	70(2)	62(1)	47(1)	-3(1)	-9(1)	6(1)
C(18)	68(2)	72(2)	59(1)	2(1)	0(2)	19(2)
C(19)	56(1)	57(1)	38(1)	2(1)	-1(1)	-7(1)
C(20)	57(1)	46(1)	41(1)	-9(1)	3(1)	2(1)
C(1')	100(2)	49(1)	97(2)	-20(2)	-34(2)	1(2)
C(2')	68(2)	43(1)	64(2)	3(1)	-21(2)	-14(1)
C(1")	69(2)	55(1)	68(2)	12(1)	19(2)	10(1)
C(2")	60(2)	49(1)	38(1)	2(1)	1(1)	10(1)

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

	x	y	z	U(eq)
H(1A)	8333	4957	6532	60
H(1B)	7476	5789	6889	60
H(2A)	10306	5630	7291	66
H(2B)	9028	5544	7928	66
H(3A)	11056	4428	8008	70
H(3B)	10634	4106	7240	70
H(5)	7694	3448	7021	51
H(6A)	6284	2478	7835	57
H(6B)	5079	3283	8021	57
H(7A)	5324	2401	6711	59
H(7B)	3648	2574	7147	59
H(11A)	4677	5786	6550	56
H(11B)	5492	5349	5875	56
H(12)	2013	5218	6289	54
H(14)	1939	3365	6236	48
H(17A)	3461	3746	4030	72
H(17B)	1592	4089	3895	72
H(17C)	1903	3265	4389	72
H(18A)	9846	2571	7498	80
H(18B)	8903	2352	8210	80
H(18C)	10723	2794	8223	80
H(19A)	9554	3969	8999	60
H(19B)	7995	4553	8752	60
H(20A)	4739	5511	7683	57
H(20B)	6359	5385	8163	57
H(20C)	4916	4658	8156	57
H(1'A)	3451	879	5205	98
H(1'B)	3716	1669	4674	98
H(1'C)	1910	1222	4749	98
H(1"A)	6392	2363	10223	77
H(1"B)	5017	2549	9636	77
H(1"C)	4931	3059	10360	77