X-ray data for Chettaphanin I · $CHCl_3$; $C_{22}H_{29}Cl_3O_6$, M = 495.80 gmol^{-1}, Orthorhombic, $P\ 2_12_12_1$, a = 7.338(3), b = 11.777(5), c = 26.354(12) Å, U = 2277.5(18) Å^3, T = 173 K, Z = 4, μ (Mo-Kα) = 0.439 mm^{-1}, 5438 reflections measured, 2094 unique (R_{int} = 0.1894) which were used in all calculations. The final wR (F^2) was 0.3330 (all data). The data were measured using a Bruker SMART CCD diffractometer, using Mo-Kα graphite monochromated radiation (λ = 0.71073 Å). The structures were solved by direct methods using the program SHELXS-97.[1] The refinement and all further calculations were carried out using SHELXL-97.[2] The H-atoms were included in calculated positions and treated as riding atoms using the SHELXL default parameters. The non-H atoms were refined anisotropically, using weighted full-matrix least-square on F^2. Figure X is drawn with ORTEP.[3]

CCDC-232426 (chettaphanin I) · $CHCl_3$, contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

[1] G. M. Sheldrick, *SHELXS-97-Program for crystal structure solution*, University of Göttingen, Göttingen, Germany (1997).

[2] G. M. Sheldrick, *SHELXL-97-Program for crystal structure refinement*, University of Göttingen, Göttingen, Germany (1997).

[3] L. J. Farrugia, *J. Appl. Cryst.* **1997**, *30*, 565.

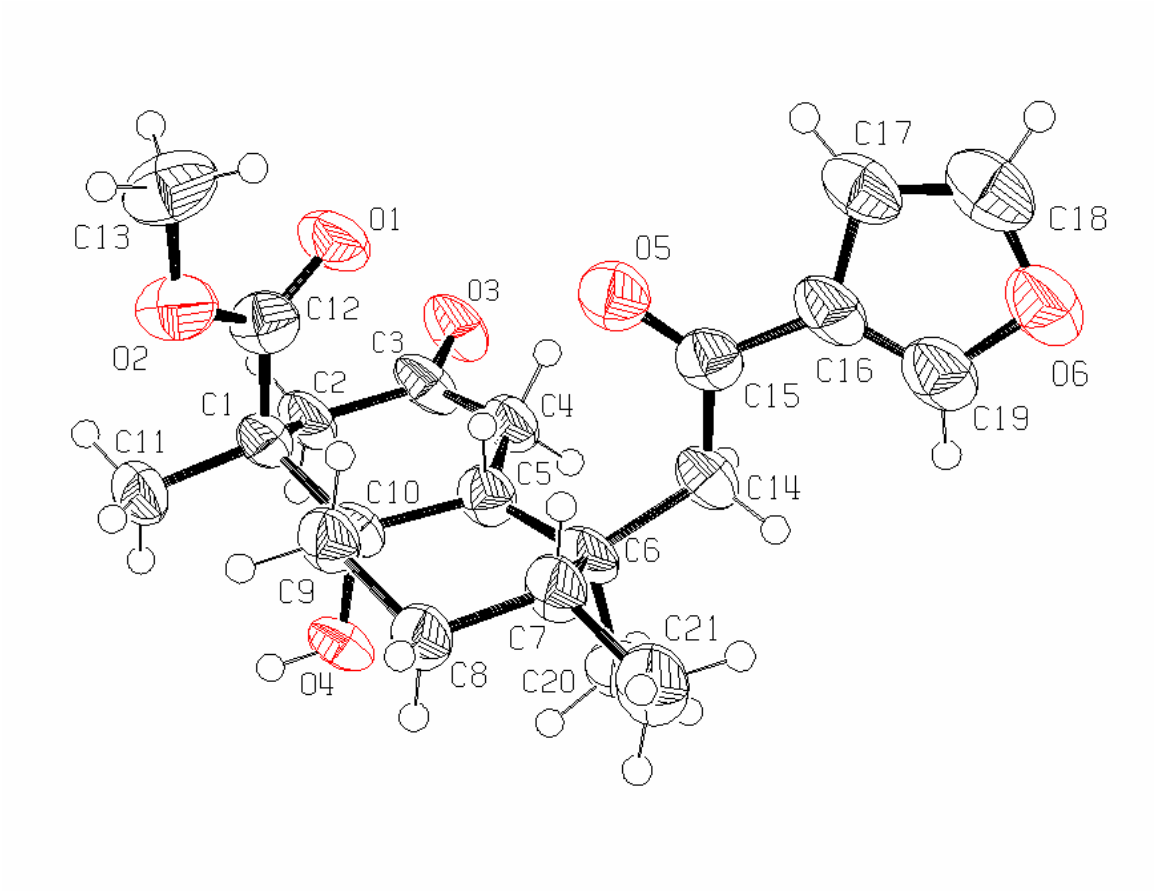

Figure 1. Displacement ellipsoids are drawn at the 50% probability level. The chloroform molecule is omitted for clarity.

Table 1. Crystal data and structure refinement for 4101.

Chemical formula	$C_{22}H_{29}Cl_3O_6$
Formula weight	495.80
Crystal system	Orthorhombic
Space group	P 2_1 2_1 2_1
Crystal colour and shape	colourless block
Crystal size	0.20 x 0.20 x 0.10
a (Å)	7.338(3)
b (Å)	11.777(5)
c (Å)	26.354(12)
V (Å^3)	2277.5(18)
Z	4
T (K)	173(2)
D_c (g·cm^{-3})	1.446
μ (mm^{-1})	0.439
Scan range (°)	$1.55 < \theta < 28.67$
Unique reflections	5438
Reflections used [I>2σ(I)]	2094
Absolute structure parameters	0.15(19)
R_{int}	0.1894
Final *R* indices [I>2σ(I)]	0.1195, wR_2 0.2671
R indices (all data)	0.2263, wR_2 0.3330
Goodness-of-fit	0.905
Max, Min Δρ/e (Å^{-3})	1.048, -0.669

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 4101. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	683(11)	-481(7)	-1085(3)	45(2)
C(2)	2206(11)	139(8)	-1339(3)	52(2)
C(3)	3640(11)	-581(7)	-1565(4)	54(2)
C(4)	3092(11)	-1696(7)	-1753(3)	49(2)
C(5)	1376(11)	-2093(7)	-1742(3)	46(2)
C(6)	862(10)	-3173(7)	-2025(3)	46(2)
C(7)	-757(10)	-3826(8)	-1780(3)	51(2)
C(8)	-2220(11)	-3062(7)	-1579(3)	50(2)
C(9)	-1447(11)	-2220(8)	-1193(3)	50(2)
C(10)	-120(10)	-1399(7)	-1472(3)	46(2)
C(11)	-813(12)	347(8)	-922(3)	57(2)
C(12)	1472(13)	-1061(8)	-639(3)	55(2)
C(13)	963(15)	-1767(10)	193(3)	78(3)
C(14)	2458(11)	-4023(7)	-2081(3)	50(2)
C(15)	3148(11)	-4577(7)	-1622(3)	48(2)
C(16)	3982(11)	-5696(8)	-1669(4)	58(2)
C(17)	4874(12)	-6359(8)	-1298(4)	63(2)
C(18)	5311(13)	-7332(10)	-1520(4)	73(3)
C(19)	4026(12)	-6314(8)	-2092(4)	65(3)
C(20)	373(11)	-2789(8)	-2569(3)	51(2)
C(21)	-1591(13)	-4725(9)	-2133(4)	70(3)
C(22)	6194(13)	1054(9)	470(4)	64(3)
O(1)	3063(8)	-1403(6)	-607(2)	64(2)
O(2)	287(8)	-1209(6)	-246(2)	67(2)
O(3)	5249(7)	-244(5)	-1612(2)	63(2)
O(4)	-1073(7)	-814(5)	-1866(2)	52(2)
O(5)	3017(8)	-4175(6)	-1186(2)	61(2)
O(6)	4825(9)	-7359(6)	-2019(3)	71(2)
Cl(1)	7211(4)	2204(3)	169(1)	81(1)
Cl(2)	5054(4)	194(3)	35(1)	86(1)
Cl(3)	4754(4)	1493(3)	952(1)	86(1)

Table 3. Bond lengths [Å] and angles [°] for 4101.

C(1)-C(12)	1.477(12)
C(1)-C(2)	1.494(11)
C(1)-C(11)	1.530(11)
C(1)-C(10)	1.599(11)
C(2)-C(3)	1.477(11)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-O(3)	1.252(10)
C(3)-C(4)	1.461(12)
C(4)-C(5)	1.343(11)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.522(11)
C(5)-C(10)	1.543(11)
C(5)-H(5)	1.0000
C(6)-C(20)	1.546(11)
C(6)-C(14)	1.548(11)
C(6)-C(7)	1.555(11)
C(7)-C(8)	1.498(11)
C(7)-C(21)	1.537(12)
C(7)-H(7)	1.0000
C(8)-C(9)	1.530(11)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.556(11)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-O(4)	1.430(9)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-O(1)	1.237(11)
C(12)-O(2)	1.362(10)
C(13)-O(2)	1.421(11)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(15)	1.465(12)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-O(5)	1.244(10)
C(15)-C(16)	1.458(12)
C(16)-C(19)	1.333(13)
C(16)-C(17)	1.413(13)
C(17)-C(18)	1.327(14)
C(17)-H(17)	0.9500
C(18)-O(6)	1.363(12)
C(18)-H(18)	0.9500
C(19)-O(6)	1.377(11)
C(19)-H(19)	0.9500
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800

C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-Cl(3)	1.732(10)
C(22)-Cl(1)	1.737(10)
C(22)-Cl(2)	1.744(10)
C(22)-H(22)	1.0000
O(4)-H(4)	0.8400

C(12)-C(1)-C(2)	106.8(7)
C(12)-C(1)-C(11)	110.7(7)
C(2)-C(1)-C(11)	110.5(7)
C(12)-C(1)-C(10)	109.8(7)
C(2)-C(1)-C(10)	108.7(6)
C(11)-C(1)-C(10)	110.2(6)
C(3)-C(2)-C(1)	115.7(7)
C(3)-C(2)-H(2A)	108.4
C(1)-C(2)-H(2A)	108.4
C(3)-C(2)-H(2B)	108.4
C(1)-C(2)-H(2B)	108.4
H(2A)-C(2)-H(2B)	107.4
O(3)-C(3)-C(4)	120.8(8)
O(3)-C(3)-C(2)	122.0(8)
C(4)-C(3)-C(2)	117.2(7)
C(5)-C(4)-C(3)	124.3(7)
C(5)-C(4)-H(4A)	106.3
C(3)-C(4)-H(4A)	106.3
C(5)-C(4)-H(4B)	106.3
C(3)-C(4)-H(4B)	106.3
H(4A)-C(4)-H(4B)	106.4
C(4)-C(5)-C(6)	120.8(7)
C(4)-C(5)-C(10)	119.6(7)
C(6)-C(5)-C(10)	119.5(7)
C(4)-C(5)-H(5)	91.3
C(6)-C(5)-H(5)	91.3
C(10)-C(5)-H(5)	91.3
C(5)-C(6)-C(20)	105.5(7)
C(5)-C(6)-C(14)	113.6(6)
C(20)-C(6)-C(14)	106.1(6)
C(5)-C(6)-C(7)	113.6(7)
C(20)-C(6)-C(7)	110.6(7)
C(14)-C(6)-C(7)	107.3(6)
C(8)-C(7)-C(21)	110.1(7)
C(8)-C(7)-C(6)	113.4(7)
C(21)-C(7)-C(6)	113.2(7)
C(8)-C(7)-H(7)	106.5
C(21)-C(7)-H(7)	106.5
C(6)-C(7)-H(7)	106.5
C(7)-C(8)-C(9)	111.1(7)
C(7)-C(8)-H(8A)	109.4
C(9)-C(8)-H(8A)	109.4
C(7)-C(8)-H(8B)	109.4
C(9)-C(8)-H(8B)	109.4
H(8A)-C(8)-H(8B)	108.0
C(8)-C(9)-C(10)	108.7(6)

C(8)-C(9)-H(9A)	110.0
C(10)-C(9)-H(9A)	110.0
C(8)-C(9)-H(9B)	110.0
C(10)-C(9)-H(9B)	110.0
H(9A)-C(9)-H(9B)	108.3
O(4)-C(10)-C(5)	105.5(6)
O(4)-C(10)-C(9)	109.7(6)
C(5)-C(10)-C(9)	109.5(7)
O(4)-C(10)-C(1)	108.5(6)
C(5)-C(10)-C(1)	112.9(6)
C(9)-C(10)-C(1)	110.4(6)
C(1)-C(11)-H(11A)	109.5
C(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(1)-C(12)-O(2)	120.7(8)
O(1)-C(12)-C(1)	124.9(8)
O(2)-C(12)-C(1)	114.4(8)
O(2)-C(13)-H(13A)	109.5
O(2)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
O(2)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(6)	118.1(7)
C(15)-C(14)-H(14A)	107.8
C(6)-C(14)-H(14A)	107.8
C(15)-C(14)-H(14B)	107.8
C(6)-C(14)-H(14B)	107.8
H(14A)-C(14)-H(14B)	107.1
O(5)-C(15)-C(16)	117.1(8)
O(5)-C(15)-C(14)	124.4(8)
C(16)-C(15)-C(14)	118.5(8)
C(19)-C(16)-C(17)	105.5(8)
C(19)-C(16)-C(15)	125.2(9)
C(17)-C(16)-C(15)	129.4(9)
C(18)-C(17)-C(16)	106.5(9)
C(18)-C(17)-H(17)	126.8
C(16)-C(17)-H(17)	126.8
C(17)-C(18)-O(6)	112.5(9)
C(17)-C(18)-H(18)	123.8
O(6)-C(18)-H(18)	123.8
C(16)-C(19)-O(6)	112.4(9)
C(16)-C(19)-H(19)	123.8
O(6)-C(19)-H(19)	123.8
C(6)-C(20)-H(20A)	109.5
C(6)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(6)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(7)-C(21)-H(21A)	109.5
C(7)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5

C(7)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
Cl(3)-C(22)-Cl(1)	111.3(6)
Cl(3)-C(22)-Cl(2)	111.3(5)
Cl(1)-C(22)-Cl(2)	111.0(5)
Cl(3)-C(22)-H(22)	107.7
Cl(1)-C(22)-H(22)	107.7
Cl(2)-C(22)-H(22)	107.7
C(12)-O(2)-C(13)	117.0(7)
C(10)-O(4)-H(4)	109.5
C(18)-O(6)-C(19)	103.1(8)

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for 4101.
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}
C(1)	30(4)	54(5)	50(5)	-1(4)	1(3)	4(3)
C(2)	24(4)	60(5)	74(6)	-4(4)	2(4)	4(4)
C(3)	25(4)	50(5)	87(6)	8(4)	0(4)	4(3)
C(4)	30(4)	53(5)	63(5)	-6(4)	-1(4)	5(3)
C(5)	34(4)	49(5)	55(5)	-2(4)	5(3)	-1(4)
C(6)	17(4)	58(5)	62(5)	-3(4)	3(3)	3(3)
C(7)	27(4)	61(5)	64(5)	-11(4)	9(3)	-5(4)
C(8)	30(4)	59(5)	61(5)	-12(4)	5(4)	-4(4)
C(9)	32(4)	55(5)	63(5)	-8(4)	3(4)	-3(4)
C(10)	24(4)	61(5)	54(4)	-3(4)	2(3)	2(4)
C(11)	36(4)	67(5)	68(5)	-12(5)	4(4)	7(4)
C(12)	49(5)	62(5)	54(5)	4(4)	0(4)	-8(4)
C(13)	78(7)	103(8)	52(5)	16(6)	0(5)	-25(6)
C(14)	30(4)	57(5)	64(5)	3(4)	6(4)	6(4)
C(15)	30(4)	53(5)	62(5)	-1(4)	-1(4)	-8(3)
C(16)	25(4)	58(5)	91(7)	0(5)	-1(4)	2(4)
C(17)	35(5)	76(6)	78(6)	13(5)	4(4)	12(5)
C(18)	37(5)	87(7)	94(8)	18(6)	14(5)	10(5)
C(19)	39(5)	65(6)	93(7)	-1(6)	-2(5)	2(5)
C(20)	37(5)	59(5)	56(5)	4(4)	0(3)	-4(4)
C(21)	37(5)	74(6)	98(7)	-23(6)	8(5)	-11(5)
C(22)	40(5)	74(6)	79(6)	9(5)	2(4)	1(5)
O(1)	35(3)	84(5)	74(4)	6(3)	-4(3)	9(3)
O(2)	51(4)	99(5)	52(3)	11(3)	1(3)	-9(4)
O(3)	22(3)	63(4)	103(5)	-2(3)	5(3)	-4(3)
O(4)	26(3)	60(3)	68(4)	5(3)	-5(2)	5(3)
O(5)	42(4)	70(4)	72(4)	-7(3)	-2(3)	-2(3)
O(6)	47(4)	64(4)	103(5)	-1(4)	0(4)	9(3)
Cl(1)	55(2)	84(2)	104(2)	12(2)	9(1)	-9(1)
Cl(2)	53(2)	95(2)	109(2)	-5(2)	-10(1)	-11(2)
Cl(3)	72(2)	85(2)	102(2)	16(2)	21(2)	14(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 4101.

	x	y	z	U(eq)
H(2A)	1685	622	-1610	63
H(2B)	2782	649	-1087	63
H(4A)	3483	-1729	-2113	59
H(4B)	3845	-2258	-1569	59
H(5)	1632	-2532	-1425	56
H(7)	-249	-4244	-1482	61
H(8A)	-3180	-3526	-1415	60
H(8B)	-2783	-2640	-1863	60
H(9A)	-789	-2634	-922	60
H(9B)	-2450	-1783	-1034	60
H(11A)	-1874	-80	-802	85
H(11B)	-1167	818	-1213	85
H(11C)	-356	834	-649	85
H(13A)	1443	-2514	98	116
H(13B)	-26	-1861	439	116
H(13C)	1939	-1311	344	116
H(14A)	2068	-4626	-2319	60
H(14B)	3487	-3617	-2242	60
H(17)	5114	-6149	-956	76
H(18)	5898	-7942	-1350	87
H(19)	3558	-6062	-2409	79
H(20A)	-690	-2285	-2557	76
H(20B)	90	-3456	-2777	76
H(20C)	1409	-2382	-2717	76
H(21A)	-2379	-5232	-1935	105
H(21B)	-614	-5168	-2291	105
H(21C)	-2313	-4349	-2397	105
H(22)	7185	589	627	77
H(4)	-1915	-423	-1739	77

Table 6. Torsion angles [deg] for 4101.

C(12)-C(1)-C(2)-C(3)	66.1(10)
C(11)-C(1)-C(2)-C(3)	-173.3(7)
C(10)-C(1)-C(2)-C(3)	-52.3(10)
C(1)-C(2)-C(3)-O(3)	-152.1(8)
C(1)-C(2)-C(3)-C(4)	30.4(12)
O(3)-C(3)-C(4)-C(5)	-176.3(9)
C(2)-C(3)-C(4)-C(5)	1.3(14)
C(3)-C(4)-C(5)-C(6)	169.6(8)
C(3)-C(4)-C(5)-C(10)	-5.9(14)
C(4)-C(5)-C(6)-C(20)	-87.1(9)
C(10)-C(5)-C(6)-C(20)	88.4(8)
C(4)-C(5)-C(6)-C(14)	28.6(11)
C(10)-C(5)-C(6)-C(14)	-155.9(7)
C(4)-C(5)-C(6)-C(7)	151.6(8)
C(10)-C(5)-C(6)-C(7)	-32.9(10)
C(5)-C(6)-C(7)-C(8)	38.6(10)
C(20)-C(6)-C(7)-C(8)	-79.7(9)
C(14)-C(6)-C(7)-C(8)	165.0(7)
C(5)-C(6)-C(7)-C(21)	165.0(8)
C(20)-C(6)-C(7)-C(21)	46.6(10)
C(14)-C(6)-C(7)-C(21)	-68.6(10)
C(21)-C(7)-C(8)-C(9)	175.4(7)
C(6)-C(7)-C(8)-C(9)	-56.6(10)
C(7)-C(8)-C(9)-C(10)	66.1(9)
C(4)-C(5)-C(10)-O(4)	99.8(9)
C(6)-C(5)-C(10)-O(4)	-75.8(9)
C(4)-C(5)-C(10)-C(9)	-142.2(8)
C(6)-C(5)-C(10)-C(9)	42.2(9)
C(4)-C(5)-C(10)-C(1)	-18.7(11)
C(6)-C(5)-C(10)-C(1)	165.8(7)
C(8)-C(9)-C(10)-O(4)	59.0(9)
C(8)-C(9)-C(10)-C(5)	-56.5(8)
C(8)-C(9)-C(10)-C(1)	178.5(6)
C(12)-C(1)-C(10)-O(4)	172.8(6)
C(2)-C(1)-C(10)-O(4)	-70.6(7)
C(11)-C(1)-C(10)-O(4)	50.6(8)
C(12)-C(1)-C(10)-C(5)	-70.5(9)
C(2)-C(1)-C(10)-C(5)	46.0(9)
C(11)-C(1)-C(10)-C(5)	167.2(7)
C(12)-C(1)-C(10)-C(9)	52.5(9)
C(2)-C(1)-C(10)-C(9)	169.1(7)
C(11)-C(1)-C(10)-C(9)	-69.7(8)
C(2)-C(1)-C(12)-O(1)	-29.5(12)
C(11)-C(1)-C(12)-O(1)	-149.9(9)
C(10)-C(1)-C(12)-O(1)	88.3(11)
C(2)-C(1)-C(12)-O(2)	150.8(7)
C(11)-C(1)-C(12)-O(2)	30.4(10)
C(10)-C(1)-C(12)-O(2)	-91.5(9)
C(5)-C(6)-C(14)-C(15)	67.7(10)
C(20)-C(6)-C(14)-C(15)	-176.9(7)
C(7)-C(6)-C(14)-C(15)	-58.6(10)
C(6)-C(14)-C(15)-O(5)	-25.2(12)
C(6)-C(14)-C(15)-C(16)	152.2(7)

O(5)-C(15)-C(16)-C(19)	171.0(9)
C(14)-C(15)-C(16)-C(19)	-6.5(13)
O(5)-C(15)-C(16)-C(17)	-8.3(13)
C(14)-C(15)-C(16)-C(17)	174.2(8)
C(19)-C(16)-C(17)-C(18)	-2.5(10)
C(15)-C(16)-C(17)-C(18)	176.9(9)
C(16)-C(17)-C(18)-O(6)	1.8(11)
C(17)-C(16)-C(19)-O(6)	2.4(10)
C(15)-C(16)-C(19)-O(6)	-177.1(8)
O(1)-C(12)-O(2)-C(13)	0.0(13)
C(1)-C(12)-O(2)-C(13)	179.7(8)
C(17)-C(18)-O(6)-C(19)	-0.4(10)
C(16)-C(19)-O(6)-C(18)	-1.3(10)