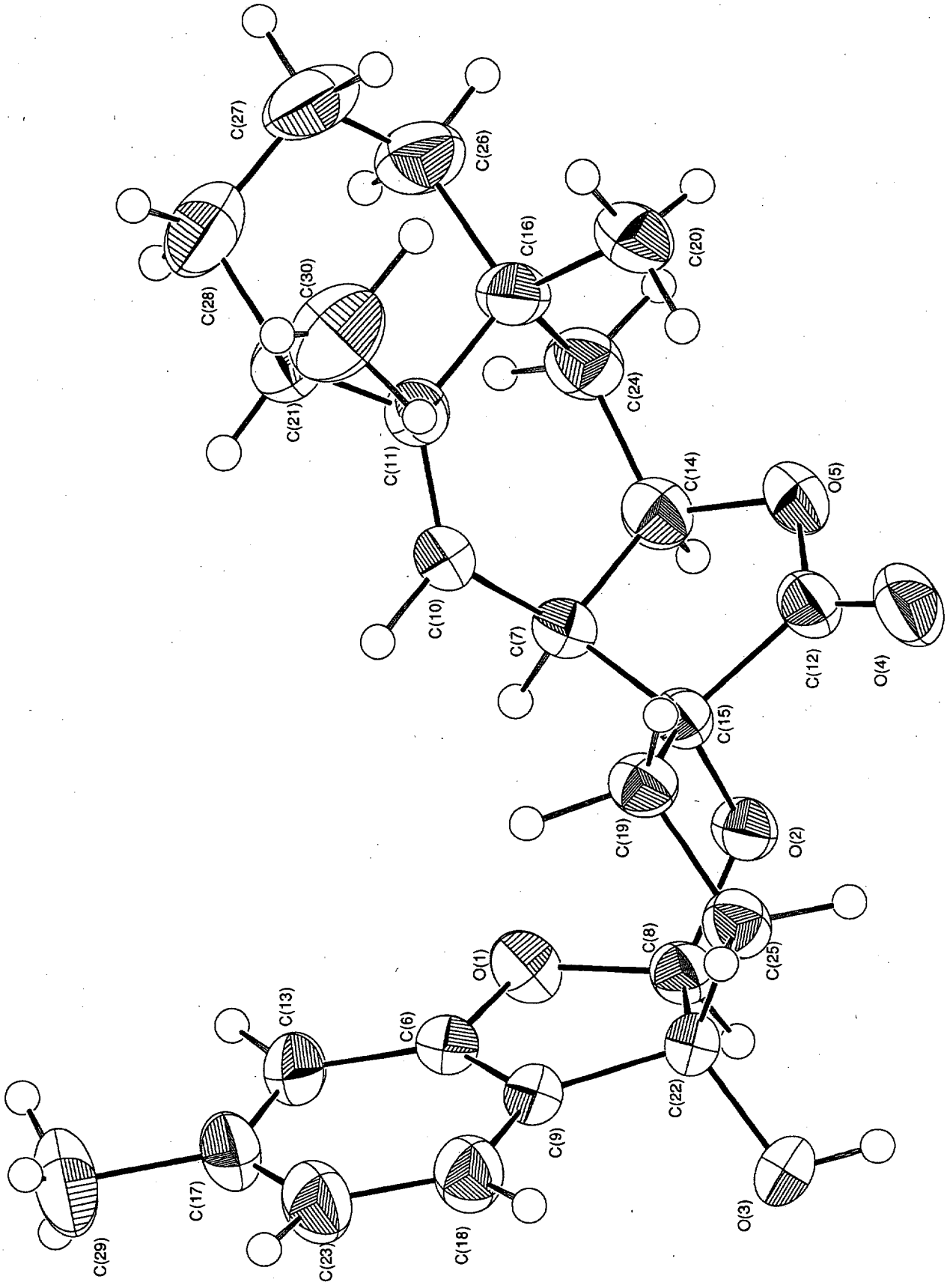
C(27)
C(26)
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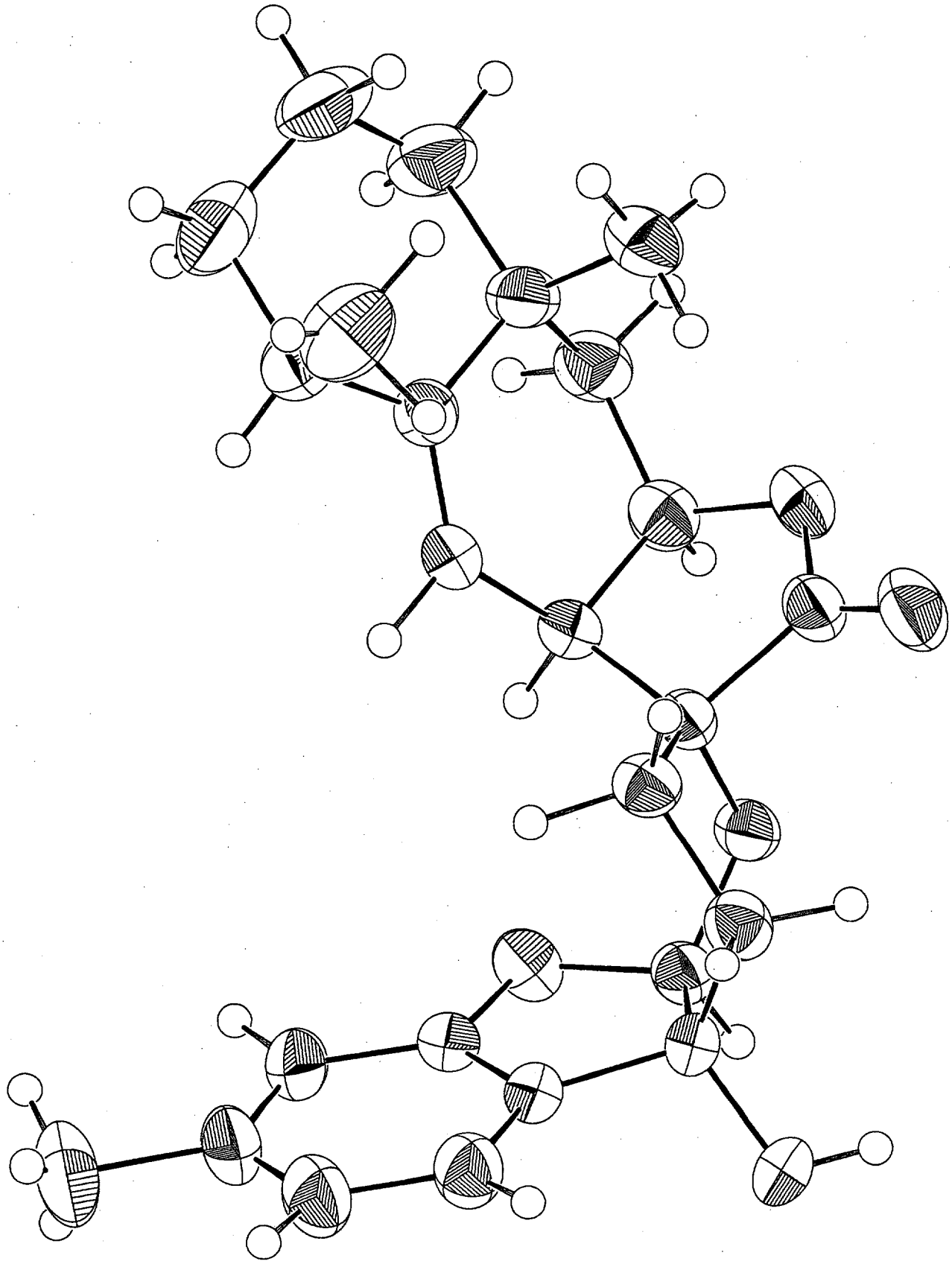

Crystal and molecular structure of MAC06061

Abstract

We present the crystal and molecular structure of MAC06061.

Comment

The study of the titled structure was undertaken to establish its three dimensional structure. Geometries are tabulated below. All Diagrams and calculations were performed using maXus (MacScience, Japan).

Experimental

Compound MAC06061

Crystal data

$C_{25}H_{30}O_5$	X-ray radiation
$M_r = 410.00$	$\lambda = 0.71073$ Å
Orthorhombic	Cell parameters from 150 reflections
$P2_12_12_1$	$\theta = 1$–$25°$
$a = 6.448000$ (0) Å	$\mu = 0.87$ mm^{-1}
$b = 11.490000$ (0) Å	$T = 298$ K
$c = 28.976999$ (0) Å	Cube
$V = 2146.800049$ (0) Å^3	0.35 × 0.2 × 0.15 mm
$Z = 4$	Colourless
$D_x = 1.530$ Mg m^{-3}	Crystal source: Local laboratory
$D_m = 1.500$ Mg m^{-3}	

Data collection

DIP Image plate diffractometer [$I > 3.00$ sigma(I)]

Absorption correction:	$\theta_{max} = 25.34°$
spherical	$h = 0 \rightarrow 7$
2173 measured reflections	$k = 0 \rightarrow 13$
2152 independent reflections	$l = 0 \rightarrow 35$
2017 observed reflections	

Refinement

Refinement on F	$(\Delta/\sigma)_{max} = 3.8469$
$R = 0.044$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
$wR = 0.193$	$\Delta\rho_{min} = -0.23$ e Å^{-3}
$S = 1.974$	Extinction correction: None
2017 reflections	Atomic scattering factors from
358 parameters	*D.* Waasmaier&*A.* Kirfel,*Acta*
Only coordinates of H atoms refined	*Cryst.*1995,*A*51, 416-431
Count statistics	

Data collection: DIP Image plate. Data reduction: maXus. Program(s) used to solve structure: maXus *SIR*92. Program(s) used to refine structure: maXus. Molecular graphics: maXus. Software used to prepare material for publication: maXus.

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* MAC06061

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
O1	0.9635 (1)	0.3375 (1)	0.37420 (3)	0.0426 (5)
O2	0.8547 (1)	0.26250 (9)	0.30310 (2)	0.0378 (4)
O3	0.5484 (2)	0.4986 (1)	0.33240 (3)	0.0530 (6)
O4	0.5562 (2)	0.0862 (1)	0.25640 (3)	0.0569 (6)
O5	0.8769 (2)	0.0197 (1)	0.26410 (3)	0.0484 (5)
C6	0.8446 (2)	0.3671 (1)	0.41180 (4)	0.0349 (6)
C7	0.9532 (2)	0.0826 (1)	0.34100 (4)	0.0366 (6)

C9	0.6468 (2)	0.3996 (1)	0.40070 (4)	0.0363 (6)
C10	0.8953 (2)	−0.0035 (1)	0.37810 (4)	0.0402 (6)
C11	0.9124 (2)	−0.1187 (1)	0.37640 (4)	0.0400 (6)
C12	0.7185 (2)	0.0853 (1)	0.27710 (4)	0.0411 (7)
C13	0.9167 (2)	0.3640 (2)	0.45700 (4)	0.0463 (7)
C14	1.0473 (2)	0.0240 (1)	0.29800 (4)	0.0435 (7)
C15	0.7726 (2)	0.1542 (1)	0.32100 (4)	0.0338 (6)
C16	0.9913 (2)	−0.1798 (1)	0.33320 (4)	0.0438 (6)
C17	0.7794 (3)	0.3984 (2)	0.49160 (4)	0.0532 (8)
C18	0.5104 (2)	0.4319 (2)	0.43510 (4)	0.0483 (7)
C19	0.5789 (2)	0.1740 (1)	0.35040 (4)	0.0375 (6)
C20	0.8064 (3)	−0.2215 (2)	0.30350 (6)	0.0536 (8)
C21	0.8498 (3)	−0.1896 (2)	0.41840 (5)	0.0528 (8)
C22	0.6156 (2)	0.3887 (1)	0.34920 (4)	0.0363 (6)
C23	0.5799 (3)	0.4311 (2)	0.48060 (5)	0.0551 (8)
C24	1.1301 (2)	−0.0953 (2)	0.30610 (5)	0.0475 (7)
C25	0.4724 (2)	0.2880 (1)	0.33660 (4)	0.0414 (6)
C26	1.1246 (3)	−0.2866 (2)	0.34550 (6)	0.062 (1)
C27	1.0319 (3)	−0.3625 (2)	0.38270 (7)	0.071 (1)
C28	0.9976 (3)	−0.2921 (2)	0.42650 (7)	0.069 (1)
C29	0.8499 (4)	0.3978 (2)	0.54110 (6)	0.077 (1)
C30	0.6235 (3)	−0.2315 (2)	0.41550 (8)	0.072 (1)
H24A	1.263 (2)	−0.089 (2)	0.3246 (5)	0.05000
H25A	0.349 (3)	0.300 (2)	0.3522 (5)	0.05000
H24B	1.167 (2)	−0.135 (2)	0.2752 (5)	0.05000
H26A	1.259 (3)	−0.259 (2)	0.3561 (5)	0.05000
H18	0.370 (2)	0.451 (2)	0.4271 (5)	0.05000
H20A	0.702 (3)	−0.156 (2)	0.3007 (5)	0.05000
H20B	0.845 (2)	−0.243 (2)	0.2776 (6)	0.05000
H10	0.841 (2)	0.041 (2)	0.4083 (5)	0.05000
H14	1.164 (2)	0.079 (2)	0.2818 (5)	0.05000

H27A	1.115 (3)	0.428 (2)	0.5333 (5)	0.05000
H8	0.902 (2)	0.430 (2)	0.3159 (5)	0.05000
H19A	0.628 (2)	0.186 (2)	0.3866 (5)	0.05000
H13	1.067 (2)	0.336 (2)	0.4643 (5)	0.05000
H25B	0.456 (2)	0.292 (2)	0.3006 (5)	0.05000
H23	0.488 (2)	0.446 (2)	0.5062 (5)	0.05000
H7	1.058 (2)	0.142 (2)	0.3543 (5)	0.05000
H27B	0.881 (2)	−0.393 (2)	0.3700 (5)	0.05000
H26B	1.167 (2)	−0.332 (2)	0.3177 (5)	0.05000
H28A	1.128 (3)	−0.261 (2)	0.4353 (5)	0.05000
H3	0.504 (2)	0.493 (2)	0.3043 (5)	0.05000
H19B	0.488 (2)	0.113 (2)	0.3464 (5)	0.05000
H30A	0.585 (3)	−0.246 (2)	0.4371 (6)	0.05000
H20C	0.741 (2)	−0.286 (2)	0.3202 (5)	0.05000
H29A	0.956 (3)	0.447 (2)	0.5405 (5)	0.05000
H29B	0.765 (3)	0.374 (2)	0.5589 (6)	0.05000
H29C	0.960 (2)	0.336 (2)	0.5423 (5)	0.05000
H30B	0.529 (2)	−0.162 (2)	0.4009 (5)	0.05000
H21	0.853 (2)	−0.135 (2)	0.4441 (6)	0.05000
H30C	0.607 (3)	−0.291 (2)	0.3854 (5)	0.05000
H28B	0.930 (2)	−0.333 (2)	0.4519 (6)	0.05000

Table 2. *Geometric parameters* (Å, °) *for* MAC06061

O1—C6	1.375 (2)	C12—C15	1.538 (2)
O1—C8	1.451 (2)	C13—C17	1.395 (3)
O2—C8	1.411 (2)	C14—C24	1.490 (3)
O2—C15	1.448 (2)	C15—C19	1.529 (2)
O3—C22	1.421 (2)	C16—C20	1.546 (3)
O4—C12	1.206 (2)	C16—C24	1.536 (3)
O5—C12	1.324 (2)	C16—C26	1.540 (3)
O5—C14	1.475 (2)	C17—C23	1.378 (3)
C6—C9	1.367 (2)	C17—C29	1.505 (3)
C6—C13	1.390 (2)	C18—C23	1.393 (2)
C7—C10	1.508 (2)	C19—C25	1.532 (3)
C7—C14	1.541 (2)	C21—C28	1.533 (3)
C7—C15	1.539 (2)	C21—C30	1.539 (3)
C8—C22	1.562 (2)	C22—C25	1.525 (3)
C9—C18	1.380 (2)	C26—C27	1.510 (3)
C9—C22	1.511 (2)	C27—C28	1.521 (4)
C10—C11	1.329 (3)	C19—H19A	1.11 (2)
C11—C16	1.523 (2)	C30—H30C	1.11 (2)
C11—C21	1.519 (3)		

C6—O1—C8	107.7 (1)	C12—C15—C19	110.6 (2)
C8—O2—C15	115.5 (1)	C11—C16—C20	110.0 (2)
C12—O5—C14	111.5 (2)	C11—C16—C24	108.9 (2)
O1—C6—C9	113.7 (2)	C11—C16—C26	111.3 (2)
O1—C6—C13	123.6 (2)	C20—C16—C24	111.1 (2)
C9—C6—C13	122.7 (2)	C20—C16—C26	108.2 (2)
C10—C7—C14	112.8 (2)	C24—C16—C26	107.3 (2)
C10—C7—C15	115.6 (2)	C13—C17—C23	120.2 (2)
C14—C7—C15	103.1 (1)	C13—C17—C29	119.5 (2)
O1—C8—O2	109.7 (2)	C23—C17—C29	120.3 (2)
O1—C8—C22	107.4 (1)	C9—C18—C23	118.5 (2)
O2—C8—C22	114.6 (2)	C15—C19—C25	110.4 (2)
C6—C9—C18	119.9 (2)	C11—C21—C28	111.7 (2)
C6—C9—C22	109.5 (2)	C11—C21—C30	112.1 (2)
C18—C9—C22	130.6 (2)	C28—C21—C30	110.9 (2)
C7—C10—C11	127.3 (2)	O3—C22—C8	112.1 (2)
C10—C11—C16	121.2 (2)	O3—C22—C9	107.8 (2)
C10—C11—C21	118.8 (2)	O3—C22—C25	114.1 (2)
C16—C11—C21	120.0 (2)	C8—C22—C9	100.9 (1)
O4—C12—O5	122.2 (2)	C8—C22—C25	108.9 (2)
O4—C12—C15	127.1 (2)	C9—C22—C25	112.3 (2)
O5—C12—C15	110.7 (2)	C17—C23—C18	121.4 (2)
C6—C13—C17	117.2 (2)	C14—C24—C16	117.0 (2)
O5—C14—C7	105.1 (2)	C19—C25—C22	108.4 (2)
O5—C14—C24	109.9 (2)	C16—C26—C27	113.9 (2)
C7—C14—C24	114.6 (2)	C26—C27—C28	110.2 (2)
O2—C15—C7	108.5 (1)	C21—C28—C27	111.8 (2)
O2—C15—C12	103.2 (1)	C15—C19—H19A	108.2 (9)
O2—C15—C19	111.7 (2)	C25—C19—H19A	105.4 (10)
C7—C15—C12	102.0 (2)	C21—C30—H30C	109.0 (9)
C7—C15—C19	119.2 (2)		

C6—O1—C8—O2	−133.4 (2)	C15—O2—C8—C22	−57.8 (2)
C8—O1—C6—C9	4.1 (2)	C14—O5—C12—O4	−173.4 (2)
C8—O1—C6—C13	−176.3 (2)	C12—O5—C14—C7	12.4 (2)
C6—O1—C8—C22	−8.2 (1)	C14—O5—C12—C15	5.6 (2)
C15—O2—C8—O1	63.1 (2)	C12—O5—C14—C24	136.1 (2)
C8—O2—C15—C7	−96.7 (2)	O1—C6—C9—C18	−179.8 (2)
C8—O2—C15—C12	155.6 (2)	O1—C6—C9—C22	2.1 (2)
C8—O2—C15—C19	36.7 (2)	O1—C6—C13—C17	178.9 (3)

C13—C6—C9—C18	0.5 (2)	C16—C11—C21—C30	−85.7 (2)
C13—C6—C9—C22	−177.6 (2)	O4—C12—C15—O2	−89.5 (2)
C10—C7—C14—O5	100.9 (2)	O4—C12—C15—C7	157.9 (2)
C14—C7—C10—C11	−1.9 (2)	O4—C12—C15—C19	30.1 (2)
C10—C7—C14—C24	−19.9 (2)	O5—C12—C15—O2	91.5 (2)
C10—C7—C15—O2	154.6 (2)	O5—C12—C15—C7	−21.0 (2)
C15—C7—C10—C11	116.4 (2)	O5—C12—C15—C19	−148.8 (2)
C10—C7—C15—C12	−96.9 (2)	C6—C13—C17—C23	1.5 (2)
C10—C7—C15—C19	25.2 (2)	C6—C13—C17—C29	−179.4 (3)
C14—C7—C15—O2	−81.9 (2)	O5—C14—C24—C16	−71.2 (2)
C15—C7—C14—O5	−24.5 (1)	C7—C14—C24—C16	46.8 (2)
C14—C7—C15—C12	26.6 (2)	O2—C15—C19—C25	24.4 (2)
C14—C7—C15—C19	148.7 (2)	C7—C15—C19—C25	152.3 (2)
C15—C7—C14—C24	−145.3 (2)	C12—C15—C19—C25	−90.0 (2)
O1—C8—C22—O3	123.3 (2)	C11—C16—C24—C14	−48.3 (2)
O1—C8—C22—C9	8.9 (1)	C11—C16—C26—C27	45.2 (2)
O1—C8—C22—C25	−109.5 (2)	C20—C16—C24—C14	73.1 (2)
O2—C8—C22—O3	−114.5 (2)	C20—C16—C26—C27	−75.8 (2)
O2—C8—C22—C9	131.0 (2)	C26—C16—C24—C14	−168.9 (2)
O2—C8—C22—C25	12.6 (2)	C24—C16—C26—C27	164.2 (2)
C6—C9—C18—C23	0.4 (2)	C13—C17—C23—C18	−0.6 (2)
C6—C9—C22—O3	−124.3 (2)	C29—C17—C23—C18	−179.7 (3)
C6—C9—C22—C8	−6.7 (2)	C9—C18—C23—C17	−0.4 (2)
C6—C9—C22—C25	109.2 (2)	C15—C19—C25—C22	−66.3 (2)
C18—C9—C22—O3	57.9 (2)	C11—C21—C28—C27	−49.6 (2)
C18—C9—C22—C8	175.5 (2)	C30—C21—C28—C27	76.2 (2)
C22—C9—C18—C23	178.1 (3)	O3—C22—C25—C19	171.6 (2)
C18—C9—C22—C25	−68.6 (2)	C8—C22—C25—C19	45.6 (2)
C7—C10—C11—C16	−2.1 (2)	C9—C22—C25—C19	−65.3 (2)
C7—C10—C11—C21	178.4 (3)	C16—C26—C27—C28	−58.2 (2)
C10—C11—C16—C20	−96.3 (2)	C26—C27—C28—C21	60.0 (2)
C10—C11—C16—C24	25.7 (2)	O2—C15—C19—H19A	−90.5 (10)
C10—C11—C16—C26	143.8 (2)	C7—C15—C19—H19A	37.4 (10)
C10—C11—C21—C28	−141.0 (2)	C12—C15—C19—H19A	155.1 (10)
C10—C11—C21—C30	93.8 (2)	H19A—C19—C25—C22	50.3 (9)
C21—C11—C16—C20	83.2 (2)	C11—C21—C30—H30C	63.1 (10)
C21—C11—C16—C24	−154.8 (2)	C28—C21—C30—H30C	−62.5 (10)
C21—C11—C16—C26	−36.8 (2)		