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(*E*)-2-Hydroxy-4-methoxy-3-(3-methylbut-2-enyl)-6-styrylbenzoic acid

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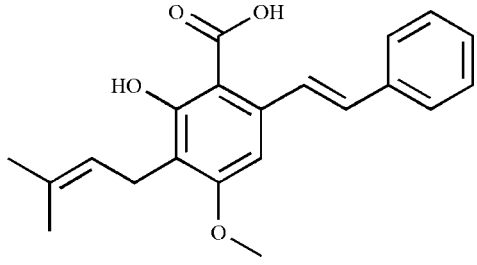
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.052; wR factor = 0.152; data-to-parameter ratio = 13.7.

The title compound, $C_{21}H_{22}O_4$, also known as cajanine, features an intramolecular O—H···O hydrogen bond between the adjacent carboxy and hydroxy groups. The benzene rings make an interplanar angle of 175.4 (2)°. In the crystal, molecules are linked by pairs of O—H···O hydrogen bonds, forming inversion dimers.

Related literature

Cajanine is an important component of the herb *Cajanus cajan* L., which is used in traditional Chinese medicine to treat osteonecrosis of the femoral head. For the total synthesis of cajanine, see: Ji *et al.* (2011). For the bioactivity of cajanine, see: Fu *et al.* (2009); Ji *et al.* (2011); Luo *et al.* (2008*a*,*b*); Zheng *et al.* (2007*a*,*b*); Inman & Hopp (2002); Ruan *et al.* (2009).



Experimental

Crystal data

$C_{21}H_{22}O_4$
M_r = 338.39
Triclinic, $P\overline{1}$
a = 6.9790 (3) Å
b = 9.9975 (8) Å
c = 13.8202 (11) Å
α = 77.899 (1)°
β = 78.956 (2)°
γ = 78.507 (2)°
V = 912.58 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 K
0.35 × 0.32 × 0.31 mm

Data collection

Bruker SMART APEX diffractometer
4547 measured reflections
3138 independent reflections
1735 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.152
S = 1.06
3138 reflections
229 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.85	2.667 (2)	176
O3—H3···O2	0.82	1.82	2.546 (2)	147

Symmetry code: (i) $-x+2, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5309).

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supporting information

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(*E*)-2-Hydroxy-4-methoxy-3-(3-methylbut-2-enyl)-6-styrylbenzoic acid

Xingyue Ji, Jie Jin, Guanghui Zheng and Zhuorong Li

S1. Comment

Cajanine, also known as longistylineA-2-carboxylicacid, is a stilbene derivative isolated from the herb Cajanus cajan *L*. The herb has been used in traditional Chinese medicine for many years to treat osteonecrosis of the femoralhead. Cajanine is a good drug candidate because of its wide range of pharmacological activities, which include antitumor (Ji *et al.* 2011), anti- HSV (Fu *et al.* 2009), anti-hyperlipidemic (Luo *et al.*, 2008*a*), anti-osteoporotic (Zheng *et al.*, 2007*a*,*b*), hypoglycemic (Inman & Hopp, 2002) and antioxidant (Luo *et al.*, 2008*b*) effects. It was also reported that cajanine can modulate Aβ_{25-35}-induced cognitive deficits, oxidative stress and cholinergic dysfunction in mice (Ruan *et al.*, 2009). We have accomplished its total synthesis previously (Ji *et al.* 2011), and the bioassay results showed that it showed some antiproliferative activity against human hepatoma cells.

The crystal structure of the title compound is reported here. In this crystal, the two benzene rings are not in the same plane, and the interplanar angle between them is 175.4 (2) °. A strong intramolecular O—H···O hydrogen bond is formed between the carboxyl group and a hydroxy group.

S2. Experimental

(*E*)-Methyl 2-hydroxy-4-methoxy-3-(3-methylbut-2-enyl)-6-styrylbenzoate (0.5 g, 1.42 mmol) was dissolved in EtOH/H_2O (15 ml/5 ml) and KOH (0.25 g, 4.26 mmol) was added. The mixture was heated under reflux for 3 h, and the reaction mixture was then added into ice water (50 ml) and the pH was adjusted to 2 with 10% HCl. The precipitate obtained was filtered and washed with water, dried in vacuum. The crude product was recrystallized from ethyl acetate / petroleum ether to give colorless crystals (0.38 g, 80%). m.p.168–170 °C.

^{1}H NMR(400 MHz,$CDCl_3$, 25 °C, TMS) δ: 11.58(s, 1H), 7.81(d, J = 16.0 Hz, 1H), 7.52(d, J = 7.2 Hz, 2H),7.38(t, J = 7.2 Hz,2*H*), 7.28(t, J = 7.2 Hz, 1H), 6.83(d, J = 16.0 Hz, 1H), 6.65(s, 1H), 5.22(t, J = 6.8 Hz, 1H), 3.95(s, 3H), 3.38(d, J = 6.8 Hz, 2H), 1.79(s, 3H), 1.68 (s, 3H), COOH was not observed. ^{13}C NMR(100 MHz, $CDCl_3$) δ: 174.95, 162.44, 162.25, 141.77, 137.28, 131.97, 130.86, 130.34, 128.74, 127.89, 126.79, 121.89, 116.77, 103.29, 102.97, 55.73, 25.82, 22.09, 17.80. HRMS(ESI) calcd for $C_{21}H_{22}O_4Na$ [*M*+Na]$^+$ 361.14158, found 361.14318.

S3. Refinement

Hydrogens were generated geometrically.

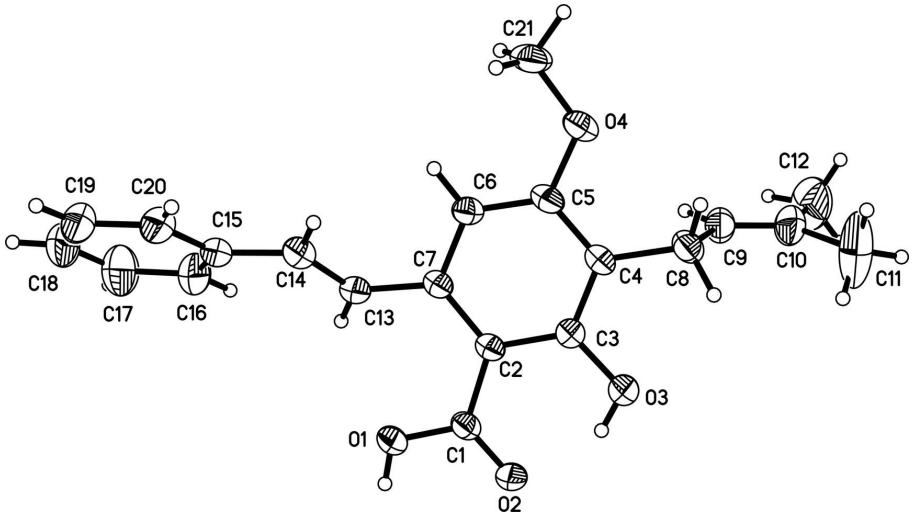

Figure 1

The title molecule with the atom-numbering scheme. Ddisplacement parameters are shown at the 30% probability level.

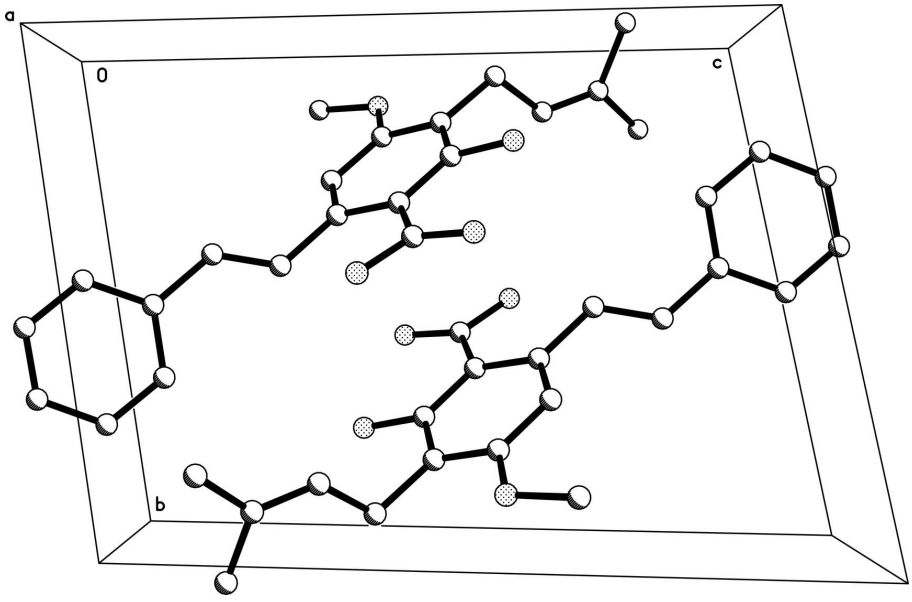

Figure 2

Packing of the title molecules viewed along the a direction.

(*E*)-2-Hydroxy-4-methoxy-3-(3-methylbut-2-enyl)-6-styrylbenzoic acid

Crystal data

$C_{21}H_{22}O_4$
$M_r = 338.39$
Triclinic, $P\overline{1}$
$a = 6.9790\ (3)$ Å
$b = 9.9975\ (8)$ Å
$c = 13.8202\ (11)$ Å
$\alpha = 77.899\ (1)°$
$\beta = 78.956\ (2)°$
$\gamma = 78.507\ (2)°$
$V = 912.58\ (11)$ Å^3
$Z = 2$
$F(000) = 360$
$D_x = 1.231$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1203 reflections
$\theta = 2.8–25.6°$

μ = 0.08 mm^{-1}
T = 298 K

Lump, colorless
0.35 × 0.32 × 0.31 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
4547 measured reflections
3138 independent reflections

1735 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.0°, θ_{min} = 3.0°
h = −8→8
k = −11→11
l = −16→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.152
S = 1.06
3138 reflections
229 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.057P)^2 + 0.0883P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.8842 (3)	0.47521 (18)	0.39744 (12)	0.0647 (5)
H1	0.9635	0.5150	0.4123	0.097*
O2	0.8460 (3)	0.39954 (17)	0.56073 (13)	0.0578 (5)
O3	0.6238 (3)	0.21943 (17)	0.64005 (12)	0.0622 (5)
H3	0.7100	0.2662	0.6362	0.093*
O4	0.1871 (3)	0.12244 (19)	0.45984 (13)	0.0699 (6)
C1	0.7933 (3)	0.4066 (2)	0.47912 (19)	0.0460 (6)
C2	0.6332 (3)	0.3384 (2)	0.46785 (17)	0.0425 (6)
C3	0.5566 (3)	0.2451 (2)	0.55136 (17)	0.0460 (6)
C4	0.4102 (3)	0.1710 (2)	0.54695 (18)	0.0474 (6)
C5	0.3353 (4)	0.1946 (3)	0.45837 (19)	0.0508 (7)
C6	0.4050 (4)	0.2864 (2)	0.37512 (18)	0.0500 (6)
H6	0.3517	0.2992	0.3165	0.060*
C7	0.5533 (3)	0.3596 (2)	0.37766 (17)	0.0442 (6)
C8	0.3312 (4)	0.0732 (3)	0.63820 (18)	0.0568 (7)

H8A	0.2964	−0.0038	0.6164	0.068*
H8B	0.4356	0.0358	0.6786	0.068*
C9	0.1559 (4)	0.1381 (3)	0.7015 (2)	0.0639 (8)
H9	0.0923	0.2237	0.6723	0.077*
C10	0.0802 (5)	0.0907 (3)	0.7923 (2)	0.0786 (9)
C11	0.1714 (8)	−0.0452 (5)	0.8471 (3)	0.170 (2)
H11A	0.1457	−0.1193	0.8198	0.255*
H11B	0.1155	−0.0549	0.9168	0.255*
H11C	0.3118	−0.0485	0.8400	0.255*
C12	−0.0985 (6)	0.1646 (4)	0.8487 (3)	0.1287 (15)
H12A	−0.1369	0.2547	0.8104	0.193*
H12B	−0.0693	0.1745	0.9117	0.193*
H12C	−0.2048	0.1124	0.8603	0.193*
C13	0.6113 (4)	0.4597 (3)	0.28730 (18)	0.0516 (7)
H13	0.6350	0.5444	0.2960	0.062*
C14	0.6320 (4)	0.4374 (3)	0.1946 (2)	0.0628 (8)
H14	0.6173	0.3498	0.1874	0.075*
C15	0.6759 (4)	0.5363 (4)	0.1019 (2)	0.0683 (8)
C16	0.6483 (5)	0.6766 (4)	0.1000 (2)	0.0940 (11)
H16	0.6044	0.7111	0.1593	0.113*
C17	0.6849 (7)	0.7665 (5)	0.0111 (3)	0.1376 (17)
H17	0.6664	0.8613	0.0107	0.165*
C18	0.7484 (8)	0.7173 (7)	−0.0768 (4)	0.139 (2)
H18	0.7703	0.7791	−0.1367	0.167*
C19	0.7796 (6)	0.5793 (7)	−0.0771 (3)	0.1203 (17)
H19	0.8273	0.5457	−0.1366	0.144*
C20	0.7398 (5)	0.4888 (4)	0.0121 (2)	0.0903 (11)
H20	0.7564	0.3943	0.0116	0.108*
C21	0.1162 (4)	0.1248 (3)	0.3689 (2)	0.0719 (8)
H21A	0.0509	0.2167	0.3455	0.108*
H21B	0.0245	0.0610	0.3810	0.108*
H21C	0.2257	0.0983	0.3191	0.108*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0679 (12)	0.0791 (13)	0.0572 (11)	−0.0449 (10)	−0.0144 (9)	0.0008 (10)
O2	0.0604 (12)	0.0644 (12)	0.0567 (11)	−0.0276 (9)	−0.0195 (9)	−0.0032 (9)
O3	0.0674 (12)	0.0704 (12)	0.0540 (11)	−0.0300 (10)	−0.0169 (9)	0.0021 (9)
O4	0.0663 (13)	0.0852 (14)	0.0689 (13)	−0.0438 (11)	−0.0076 (10)	−0.0106 (10)
C1	0.0412 (15)	0.0437 (15)	0.0537 (16)	−0.0126 (12)	−0.0063 (13)	−0.0060 (12)
C2	0.0386 (14)	0.0433 (14)	0.0484 (14)	−0.0123 (11)	−0.0041 (11)	−0.0114 (11)
C3	0.0459 (15)	0.0477 (15)	0.0452 (14)	−0.0110 (12)	−0.0071 (12)	−0.0068 (12)
C4	0.0431 (15)	0.0463 (15)	0.0539 (15)	−0.0160 (12)	−0.0011 (12)	−0.0089 (12)
C5	0.0436 (15)	0.0542 (16)	0.0600 (16)	−0.0195 (13)	−0.0015 (13)	−0.0171 (13)
C6	0.0474 (15)	0.0564 (16)	0.0513 (15)	−0.0165 (13)	−0.0098 (12)	−0.0119 (13)
C7	0.0400 (14)	0.0453 (14)	0.0491 (14)	−0.0129 (11)	−0.0039 (11)	−0.0103 (12)
C8	0.0527 (17)	0.0517 (16)	0.0648 (17)	−0.0180 (13)	−0.0067 (14)	−0.0014 (13)

C9	0.0547 (18)	0.0699 (19)	0.0581 (18)	−0.0097 (15)	−0.0068 (14)	0.0062 (15)
C10	0.085 (2)	0.092 (2)	0.0524 (18)	−0.0209 (19)	−0.0035 (17)	0.0007 (17)
C11	0.214 (5)	0.129 (4)	0.099 (3)	0.012 (4)	0.032 (3)	0.041 (3)
C12	0.112 (3)	0.169 (4)	0.081 (3)	−0.009 (3)	0.022 (2)	−0.016 (3)
C13	0.0487 (16)	0.0574 (16)	0.0534 (16)	−0.0189 (13)	−0.0129 (12)	−0.0063 (13)
C14	0.0596 (18)	0.075 (2)	0.0587 (18)	−0.0266 (15)	−0.0070 (14)	−0.0099 (15)
C15	0.0539 (18)	0.102 (3)	0.0540 (18)	−0.0332 (17)	−0.0130 (14)	−0.0010 (17)
C16	0.110 (3)	0.101 (3)	0.068 (2)	−0.039 (2)	−0.0156 (19)	0.015 (2)
C17	0.161 (4)	0.140 (4)	0.099 (3)	−0.062 (3)	−0.025 (3)	0.045 (3)
C18	0.124 (4)	0.208 (6)	0.077 (3)	−0.080 (4)	−0.030 (3)	0.055 (4)
C19	0.085 (3)	0.221 (5)	0.055 (2)	−0.051 (4)	−0.0123 (19)	0.001 (3)
C20	0.075 (2)	0.145 (3)	0.056 (2)	−0.038 (2)	−0.0091 (16)	−0.014 (2)
C21	0.0644 (19)	0.083 (2)	0.085 (2)	−0.0313 (16)	−0.0194 (16)	−0.0250 (17)

Geometric parameters (Å, º)

O1—C1	1.312 (3)	C11—H11A	0.9600
O1—H1	0.8200	C11—H11B	0.9600
O2—C1	1.236 (3)	C11—H11C	0.9600
O3—C3	1.352 (3)	C12—H12A	0.9600
O3—H3	0.8200	C12—H12B	0.9600
O4—C5	1.368 (3)	C12—H12C	0.9600
O4—C21	1.430 (3)	C13—C14	1.322 (3)
C1—C2	1.467 (3)	C13—H13	0.9300
C2—C3	1.414 (3)	C14—C15	1.467 (4)
C2—C7	1.420 (3)	C14—H14	0.9300
C3—C4	1.393 (3)	C15—C16	1.372 (4)
C4—C5	1.379 (3)	C15—C20	1.384 (4)
C4—C8	1.511 (3)	C16—C17	1.375 (4)
C5—C6	1.387 (3)	C16—H16	0.9300
C6—C7	1.391 (3)	C17—C18	1.367 (6)
C6—H6	0.9300	C17—H17	0.9300
C7—C13	1.472 (3)	C18—C19	1.354 (6)
C8—C9	1.482 (4)	C18—H18	0.9300
C8—H8A	0.9700	C19—C20	1.384 (5)
C8—H8B	0.9700	C19—H19	0.9300
C9—C10	1.294 (4)	C20—H20	0.9300
C9—H9	0.9300	C21—H21A	0.9600
C10—C12	1.487 (4)	C21—H21B	0.9600
C10—C11	1.494 (5)	C21—H21C	0.9600
C1—O1—H1	109.5	C10—C11—H11C	109.5
C3—O3—H3	109.5	H11A—C11—H11C	109.5
C5—O4—C21	119.8 (2)	H11B—C11—H11C	109.5
O2—C1—O1	120.0 (2)	C10—C12—H12A	109.5
O2—C1—C2	122.9 (2)	C10—C12—H12B	109.5
O1—C1—C2	117.1 (2)	H12A—C12—H12B	109.5
C3—C2—C7	118.5 (2)	C10—C12—H12C	109.5

C3—C2—C1	117.8 (2)	H12A—C12—H12C	109.5
C7—C2—C1	123.7 (2)	H12B—C12—H12C	109.5
O3—C3—C4	115.6 (2)	C14—C13—C7	124.5 (2)
O3—C3—C2	122.2 (2)	C14—C13—H13	117.8
C4—C3—C2	122.2 (2)	C7—C13—H13	117.8
C5—C4—C3	117.8 (2)	C13—C14—C15	126.9 (3)
C5—C4—C8	121.7 (2)	C13—C14—H14	116.6
C3—C4—C8	120.5 (2)	C15—C14—H14	116.6
O4—C5—C4	115.0 (2)	C16—C15—C20	118.1 (3)
O4—C5—C6	123.2 (2)	C16—C15—C14	122.2 (3)
C4—C5—C6	121.7 (2)	C20—C15—C14	119.6 (3)
C5—C6—C7	121.3 (2)	C15—C16—C17	120.5 (4)
C5—C6—H6	119.4	C15—C16—H16	119.7
C7—C6—H6	119.4	C17—C16—H16	119.7
C6—C7—C2	118.5 (2)	C18—C17—C16	120.4 (5)
C6—C7—C13	117.4 (2)	C18—C17—H17	119.8
C2—C7—C13	124.0 (2)	C16—C17—H17	119.8
C9—C8—C4	114.1 (2)	C19—C18—C17	120.4 (4)
C9—C8—H8A	108.7	C19—C18—H18	119.8
C4—C8—H8A	108.7	C17—C18—H18	119.8
C9—C8—H8B	108.7	C18—C19—C20	119.2 (4)
C4—C8—H8B	108.7	C18—C19—H19	120.4
H8A—C8—H8B	107.6	C20—C19—H19	120.4
C10—C9—C8	128.2 (3)	C19—C20—C15	121.3 (4)
C10—C9—H9	115.9	C19—C20—H20	119.4
C8—C9—H9	115.9	C15—C20—H20	119.4
C9—C10—C12	123.6 (3)	O4—C21—H21A	109.5
C9—C10—C11	120.6 (3)	O4—C21—H21B	109.5
C12—C10—C11	115.8 (3)	H21A—C21—H21B	109.5
C10—C11—H11A	109.5	O4—C21—H21C	109.5
C10—C11—H11B	109.5	H21A—C21—H21C	109.5
H11A—C11—H11B	109.5	H21B—C21—H21C	109.5

O2—C1—C2—C3	−9.3 (3)	C3—C2—C7—C6	−0.8 (3)
O1—C1—C2—C3	169.4 (2)	C1—C2—C7—C6	178.3 (2)
O2—C1—C2—C7	171.6 (2)	C3—C2—C7—C13	176.3 (2)
O1—C1—C2—C7	−9.7 (3)	C1—C2—C7—C13	−4.6 (4)
C7—C2—C3—O3	−179.7 (2)	C5—C4—C8—C9	−86.0 (3)
C1—C2—C3—O3	1.1 (3)	C3—C4—C8—C9	91.3 (3)
C7—C2—C3—C4	1.8 (3)	C4—C8—C9—C10	−165.1 (3)
C1—C2—C3—C4	−177.4 (2)	C8—C9—C10—C12	−179.4 (3)
O3—C3—C4—C5	179.4 (2)	C8—C9—C10—C11	0.7 (6)
C2—C3—C4—C5	−2.1 (3)	C6—C7—C13—C14	−41.1 (3)
O3—C3—C4—C8	1.9 (3)	C2—C7—C13—C14	141.8 (3)
C2—C3—C4—C8	−179.5 (2)	C7—C13—C14—C15	175.4 (2)
C21—O4—C5—C4	−171.9 (2)	C13—C14—C15—C16	−18.2 (5)
C21—O4—C5—C6	8.9 (4)	C13—C14—C15—C20	164.4 (3)
C3—C4—C5—O4	−177.8 (2)	C20—C15—C16—C17	−0.5 (5)

C8—C4—C5—O4	−0.4 (3)	C14—C15—C16—C17	−177.9 (3)
C3—C4—C5—C6	1.4 (4)	C15—C16—C17—C18	0.4 (6)
C8—C4—C5—C6	178.8 (2)	C16—C17—C18—C19	−1.3 (8)
O4—C5—C6—C7	178.7 (2)	C17—C18—C19—C20	2.3 (7)
C4—C5—C6—C7	−0.4 (4)	C18—C19—C20—C15	−2.4 (6)
C5—C6—C7—C2	0.1 (3)	C16—C15—C20—C19	1.5 (5)
C5—C6—C7—C13	−177.2 (2)	C14—C15—C20—C19	179.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.85	2.667 (2)	176
O3—H3···O2	0.82	1.82	2.546 (2)	147

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.