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# (*E*)-2,3-Bis(4-methoxyphenyl)acrylic acid

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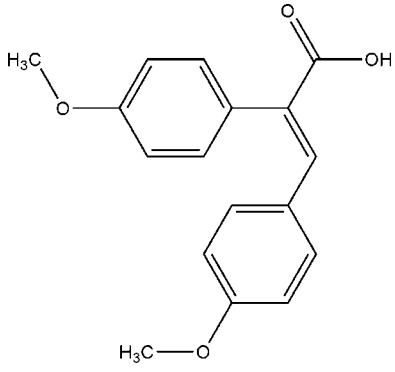
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.056; $wR$ factor = 0.151; data-to-parameter ratio = 14.9.

In the title molecule, $C_{17}H_{16}O_4$, the angle between the aromatic ring planes is 69.1 (6)°. The crystal structure is stabilized by intermolecular O—H···O hydrogen bonds; molecules related by a centre of symmetry are linked to form inversion dimers.

## Related literature

For the biological properties and synthesis of resveratrol (*trans*-3,4′,5-trihydroxystilbene) and its derivatives, see: Huang, Ruan *et al.* (2007); Huang *et al.* (2008); Jang *et al.* (1997); Ruan *et al.* (2006); Schulze *et al.* (2005); Shi *et al.* (2005). For related crystal structures, see: Huang, Li *et al.* (2007); Stomberg *et al.* (2001).




## Experimental

### Crystal data

$C_{17}H_{16}O_4$
$M_r$ = 284.30
Triclinic, $P\overline{1}$
$a$ = 5.8690 (12) Å
$b$ = 9.1480 (18) Å
$c$ = 13.992 (3) Å
$\alpha$ = 83.65 (3)°
$\beta$ = 85.43 (3)°
$\gamma$ = 80.92 (3)°
$V$ = 735.8 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 298 K
0.30 × 0.20 × 0.10 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.973, $T_{max}$ = 0.991
3196 measured reflections
2895 independent reflections
1779 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.151
$S$ = 1.08
2895 reflections
194 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3···O2$^{i}$ | 0.82 | 1.80 | 2.608 (2) | 169 |

Symmetry code: (i) $-x+3, -y+2, -z+1$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); 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: WN2320).

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# supporting information

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## (*E*)-2,3-Bis(4-methoxyphenyl)acrylic acid

**Banfeng Ruan, Ying Yang, Zhenwei Zhu, Pengcheng Lv and Hailiang Zhu**

### S1. Comment

Resveratrol (*trans*-3, 4′,5-trihydroxystilbene) and its derivatives have attracted much attention since it was first isolated in 1939, because of their physiological properties and potential therapeutic values (Schulze *et al.*, 2005; Jang *et al.*, 1997). In our laboratory, we have synthesized two series of resveratrol derivatives (Ruan *et al.*, 2006; Huang *et al.*, 2007). As part of an extensive structure-activity relationship (SAR) study on resveratrol derivatives, another series of analogues of resveratrol has been synthesized. One of them, namely the title compound, was obtained as single crystals and its crystal structure determined to establish its configuration.

The crystal structure demonstrated that it had the E configuration (Fig. 1). All bond lengths are within normal ranges and very similar to those in related crystal structures (Stomberg *et al.*, 2001). The torsion angles C5—C8—C10—C11 and C9—C8—C10—C11 are 5.9 (4)° and -176.6 (2)°, respectively. The angle between the aromatic ring planes is 69.1 (6)°. In the crystal structure, molecules related by a centre of symmetry are linked to form dimers *via* intermolecular O—H—O hydrogen bonds (Table 1 and Fig. 2).

### S2. Experimental

2-(4-Methoxyphenyl)acetic acid (1.66 g, 0.01 mol), 4-methoxybenzaldehyde (1.36 g, 0.01 mol) and acetic anhydride (15 ml) were added to a three-necked flask in an icewater bath with stirring. Triethylamine (5 ml) was added dropwise into this solution and the mixture was allowed to react at 100°C for 12 h. After cooling to room temperature, the mixture was slowly poured into 50 ml 10% NaOH solution, yielding a white precipitate. This was collected by vacuum filtration, washed with a large amount of water and dried in air. Colorless single crystals were obtained after a week upon evaporation of a solution of the reaction product in a mixture of ethyl acetate (10 ml) and petroleum ether (5 ml).

### S3. Refinement

All hydrogen atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å ($Csp^2$), 0.96 Å (methyl) and O—H = 0.82 Å. $U_{iso}(H) = 1.2U_{eq}(Csp^2)$, $1.5U_{eq}$(methyl C and hydroxyl O).

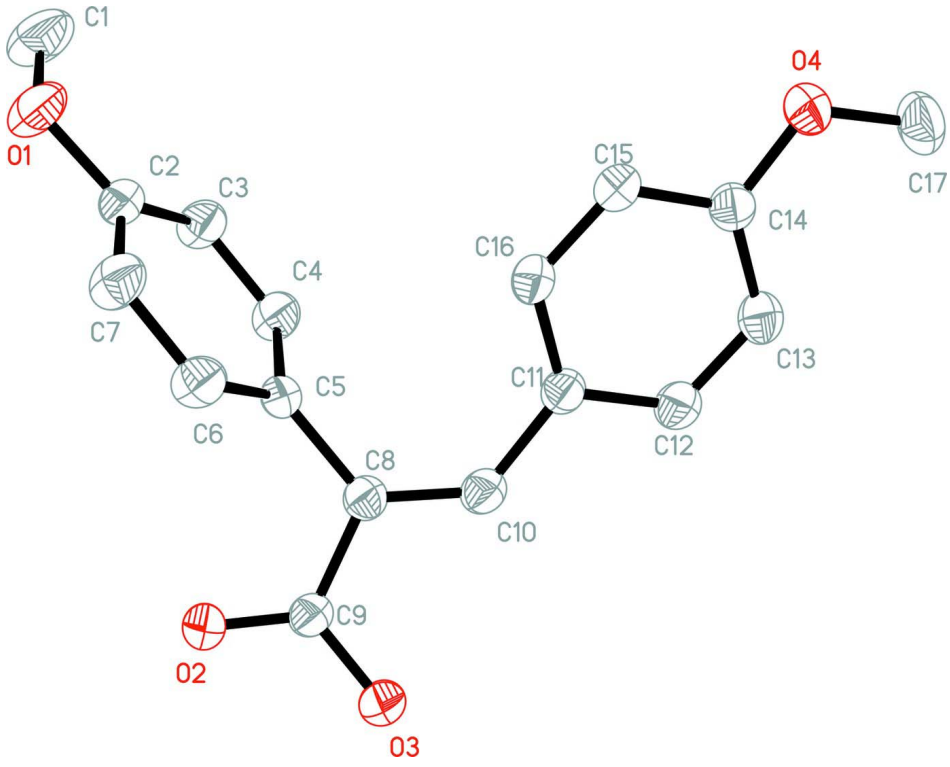


**Figure 1**

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. All H atoms have been omitted.

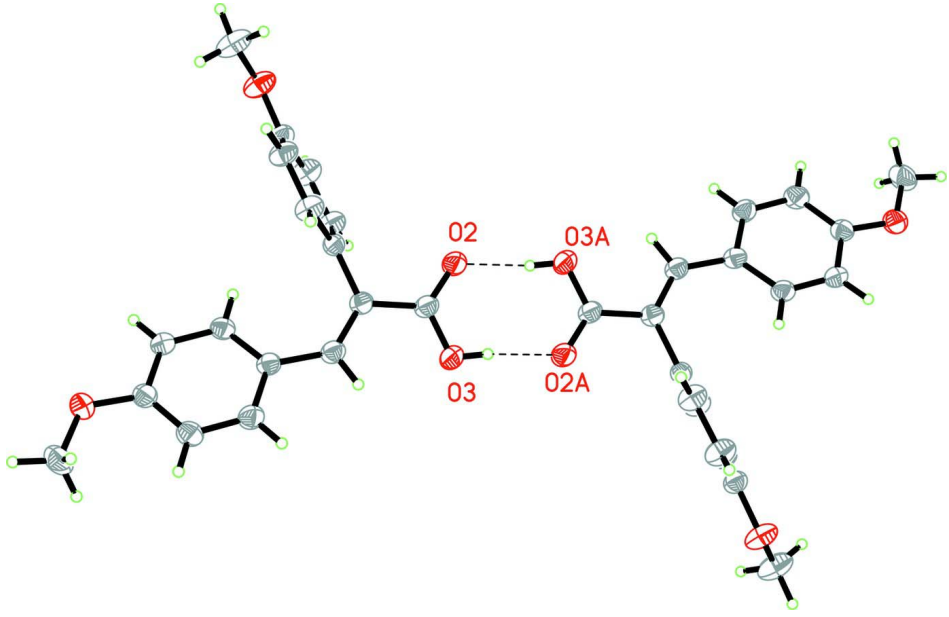


**Figure 2**

A view of the hydrogen-bonded dimer of the title compound. Dashed lines indicate hydrogen bonds. [Symmetry code: (A) -*x* + 3, -*y* + 2, -*z* + 1]

## (*E*)-2,3-Bis(4-methoxyphenyl)acrylic acid

*Crystal data*

$C_{17}H_{16}O_4$
$M_r = 284.30$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.8690\ (12)$ Å
$b = 9.1480\ (18)$ Å
$c = 13.992\ (3)$ Å
$\alpha = 83.65\ (3)°$
$\beta = 85.43\ (3)°$
$\gamma = 80.92\ (3)°$
$V = 735.8\ (3)$ Å$^3$
$Z = 2$
$F(000) = 300$
$D_x = 1.283$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1625 reflections
$\theta = 2.2–24.8°$
$\mu = 0.09$ mm$^{-1}$
$T = 298$ K
Block, colorless
0.30 × 0.20 × 0.10 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min} = 0.973$, $T_{max} = 0.991$
3196 measured reflections
2895 independent reflections
1779 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.5°$
$h = 0\rightarrow7$
$k = -11\rightarrow11$
$l = -17\rightarrow17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.151$
$S = 1.08$
2895 reflections
194 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
$w = 1/[\sigma^2(F_o^2) + (0.0675P)^2 + 0.024P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å$^{-3}$
$\Delta\rho_{min} = -0.17$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.044 (7)

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.7983 (6) | 1.3447 (4) | −0.0150 (2) | 0.0938 (11) |
| H1A | 0.6774 | 1.2848 | −0.0132 | 0.141* |

| | | | | |
|---|---|---|---|---|
| H1B | 0.8108 | 1.3993 | −0.0774 | 0.141* |
| H1C | 0.7629 | 1.4130 | 0.0333 | 0.141* |
| C2 | 1.0269 (4) | 1.1661 (3) | 0.08912 (15) | 0.0505 (6) |
| C3 | 0.8532 (4) | 1.1641 (3) | 0.16030 (17) | 0.0565 (6) |
| H3A | 0.7103 | 1.2225 | 0.1513 | 0.068* |
| C4 | 0.8905 (4) | 1.0754 (3) | 0.24524 (17) | 0.0548 (6) |
| H4 | 0.7705 | 1.0752 | 0.2929 | 0.066* |
| C5 | 1.0983 (4) | 0.9870 (2) | 0.26254 (15) | 0.0423 (5) |
| C6 | 1.2741 (4) | 0.9919 (3) | 0.19039 (16) | 0.0553 (6) |
| H6 | 1.4182 | 0.9357 | 0.2001 | 0.066* |
| C7 | 1.2382 (4) | 1.0786 (3) | 0.10484 (17) | 0.0621 (7) |
| H7 | 1.3573 | 1.0786 | 0.0568 | 0.074* |
| C8 | 1.1324 (4) | 0.8926 (2) | 0.35563 (15) | 0.0462 (6) |
| C9 | 1.2916 (4) | 0.9385 (3) | 0.41980 (16) | 0.0495 (6) |
| C10 | 1.0275 (4) | 0.7750 (2) | 0.38730 (16) | 0.0500 (6) |
| H10 | 1.0582 | 0.7349 | 0.4498 | 0.060* |
| C11 | 0.8736 (4) | 0.6996 (2) | 0.34031 (15) | 0.0466 (6) |
| C12 | 0.7562 (4) | 0.5977 (3) | 0.39652 (17) | 0.0563 (7) |
| H12 | 0.7770 | 0.5821 | 0.4623 | 0.068* |
| C13 | 0.6106 (4) | 0.5188 (3) | 0.35884 (17) | 0.0577 (7) |
| H13 | 0.5354 | 0.4505 | 0.3985 | 0.069* |
| C14 | 0.5767 (4) | 0.5414 (2) | 0.26176 (17) | 0.0495 (6) |
| C15 | 0.6987 (4) | 0.6386 (3) | 0.20313 (16) | 0.0550 (6) |
| H15 | 0.6826 | 0.6504 | 0.1370 | 0.066* |
| C16 | 0.8418 (4) | 0.7169 (2) | 0.24152 (16) | 0.0521 (6) |
| H16 | 0.9198 | 0.7831 | 0.2013 | 0.063* |
| C17 | 0.2995 (5) | 0.3745 (3) | 0.2726 (2) | 0.0746 (8) |
| H17A | 0.3998 | 0.2948 | 0.3053 | 0.112* |
| H17B | 0.2067 | 0.3345 | 0.2315 | 0.112* |
| H17C | 0.2009 | 0.4283 | 0.3192 | 0.112* |
| O1 | 1.0108 (3) | 1.2517 (2) | 0.00292 (12) | 0.0753 (6) |
| O2 | 1.3849 (3) | 1.04878 (19) | 0.39719 (11) | 0.0674 (6) |
| O3 | 1.3251 (3) | 0.85636 (19) | 0.50110 (11) | 0.0691 (6) |
| H3 | 1.4025 | 0.8958 | 0.5341 | 0.104* |
| O4 | 0.4348 (3) | 0.47241 (18) | 0.21611 (12) | 0.0641 (5) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.091 (2) | 0.104 (2) | 0.074 (2) | 0.007 (2) | −0.0214 (18) | 0.0273 (18) |
| C2 | 0.0525 (15) | 0.0561 (14) | 0.0426 (12) | −0.0126 (12) | −0.0038 (11) | 0.0029 (10) |
| C3 | 0.0391 (13) | 0.0660 (16) | 0.0582 (14) | 0.0010 (12) | −0.0025 (11) | 0.0085 (12) |
| C4 | 0.0350 (12) | 0.0696 (16) | 0.0543 (14) | −0.0040 (11) | 0.0048 (10) | 0.0067 (12) |
| C5 | 0.0397 (12) | 0.0455 (12) | 0.0429 (12) | −0.0120 (10) | −0.0034 (9) | −0.0004 (9) |
| C6 | 0.0366 (13) | 0.0690 (16) | 0.0543 (14) | 0.0024 (11) | 0.0015 (11) | 0.0018 (12) |
| C7 | 0.0468 (15) | 0.0817 (18) | 0.0506 (14) | −0.0023 (13) | 0.0095 (12) | 0.0054 (13) |
| C8 | 0.0419 (13) | 0.0483 (13) | 0.0475 (12) | −0.0076 (10) | −0.0032 (10) | 0.0010 (10) |
| C9 | 0.0472 (13) | 0.0552 (14) | 0.0451 (13) | −0.0108 (11) | −0.0061 (11) | 0.0061 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.0515 (14) | 0.0544 (14) | 0.0432 (12) | −0.0101 (11) | −0.0037 (11) | 0.0034 (10) |
| C11 | 0.0437 (13) | 0.0481 (13) | 0.0465 (13) | −0.0074 (10) | −0.0032 (10) | 0.0030 (10) |
| C12 | 0.0595 (16) | 0.0638 (16) | 0.0461 (13) | −0.0183 (13) | −0.0028 (11) | 0.0053 (11) |
| C13 | 0.0527 (15) | 0.0620 (15) | 0.0595 (15) | −0.0223 (12) | 0.0017 (12) | 0.0050 (12) |
| C14 | 0.0434 (13) | 0.0456 (13) | 0.0588 (14) | −0.0050 (11) | −0.0071 (11) | −0.0009 (11) |
| C15 | 0.0662 (16) | 0.0519 (14) | 0.0475 (13) | −0.0145 (12) | −0.0108 (12) | 0.0059 (11) |
| C16 | 0.0544 (14) | 0.0522 (14) | 0.0502 (14) | −0.0178 (12) | −0.0027 (11) | 0.0064 (11) |
| C17 | 0.0668 (18) | 0.0648 (17) | 0.097 (2) | −0.0284 (15) | −0.0050 (16) | −0.0028 (15) |
| O1 | 0.0737 (13) | 0.0920 (14) | 0.0513 (10) | −0.0045 (11) | −0.0040 (9) | 0.0201 (9) |
| O2 | 0.0759 (12) | 0.0728 (12) | 0.0594 (11) | −0.0376 (10) | −0.0217 (9) | 0.0176 (9) |
| O3 | 0.0865 (14) | 0.0735 (12) | 0.0535 (10) | −0.0355 (10) | −0.0255 (9) | 0.0150 (9) |
| O4 | 0.0639 (11) | 0.0610 (11) | 0.0720 (11) | −0.0240 (9) | −0.0171 (9) | 0.0030 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—O1 | 1.418 (3) | C9—O3 | 1.303 (2) |
| C1—H1A | 0.9600 | C10—C11 | 1.455 (3) |
| C1—H1B | 0.9600 | C10—H10 | 0.9300 |
| C1—H1C | 0.9600 | C11—C12 | 1.384 (3) |
| C2—O1 | 1.364 (3) | C11—C16 | 1.398 (3) |
| C2—C3 | 1.368 (3) | C12—C13 | 1.371 (3) |
| C2—C7 | 1.385 (3) | C12—H12 | 0.9300 |
| C3—C4 | 1.375 (3) | C13—C14 | 1.377 (3) |
| C3—H3A | 0.9300 | C13—H13 | 0.9300 |
| C4—C5 | 1.376 (3) | C14—O4 | 1.356 (3) |
| C4—H4 | 0.9300 | C14—C15 | 1.386 (3) |
| C5—C6 | 1.387 (3) | C15—C16 | 1.362 (3) |
| C5—C8 | 1.490 (3) | C15—H15 | 0.9300 |
| C6—C7 | 1.372 (3) | C16—H16 | 0.9300 |
| C6—H6 | 0.9300 | C17—O4 | 1.423 (3) |
| C7—H7 | 0.9300 | C17—H17A | 0.9600 |
| C8—C10 | 1.339 (3) | C17—H17B | 0.9600 |
| C8—C9 | 1.482 (3) | C17—H17C | 0.9600 |
| C9—O2 | 1.222 (3) | O3—H3 | 0.8200 |
| | | | |
| O1—C1—H1A | 109.5 | C8—C10—C11 | 130.8 (2) |
| O1—C1—H1B | 109.5 | C8—C10—H10 | 114.6 |
| H1A—C1—H1B | 109.5 | C11—C10—H10 | 114.6 |
| O1—C1—H1C | 109.5 | C12—C11—C16 | 116.9 (2) |
| H1A—C1—H1C | 109.5 | C12—C11—C10 | 117.9 (2) |
| H1B—C1—H1C | 109.5 | C16—C11—C10 | 125.1 (2) |
| O1—C2—C3 | 124.8 (2) | C13—C12—C11 | 122.4 (2) |
| O1—C2—C7 | 116.4 (2) | C13—C12—H12 | 118.8 |
| C3—C2—C7 | 118.8 (2) | C11—C12—H12 | 118.8 |
| C2—C3—C4 | 119.8 (2) | C12—C13—C14 | 119.5 (2) |
| C2—C3—H3A | 120.1 | C12—C13—H13 | 120.3 |
| C4—C3—H3A | 120.1 | C14—C13—H13 | 120.3 |
| C3—C4—C5 | 122.6 (2) | O4—C14—C13 | 125.2 (2) |

| | | | |
|---|---|---|---|
| C3—C4—H4 | 118.7 | O4—C14—C15 | 115.5 (2) |
| C5—C4—H4 | 118.7 | C13—C14—C15 | 119.3 (2) |
| C4—C5—C6 | 117.04 (19) | C16—C15—C14 | 120.6 (2) |
| C4—C5—C8 | 121.03 (19) | C16—C15—H15 | 119.7 |
| C6—C5—C8 | 121.9 (2) | C14—C15—H15 | 119.7 |
| C7—C6—C5 | 121.0 (2) | C15—C16—C11 | 121.2 (2) |
| C7—C6—H6 | 119.5 | C15—C16—H16 | 119.4 |
| C5—C6—H6 | 119.5 | C11—C16—H16 | 119.4 |
| C6—C7—C2 | 120.8 (2) | O4—C17—H17A | 109.5 |
| C6—C7—H7 | 119.6 | O4—C17—H17B | 109.5 |
| C2—C7—H7 | 119.6 | H17A—C17—H17B | 109.5 |
| C10—C8—C9 | 117.8 (2) | O4—C17—H17C | 109.5 |
| C10—C8—C5 | 126.2 (2) | H17A—C17—H17C | 109.5 |
| C9—C8—C5 | 115.95 (18) | H17B—C17—H17C | 109.5 |
| O2—C9—O3 | 122.1 (2) | C2—O1—C1 | 118.0 (2) |
| O2—C9—C8 | 121.2 (2) | C9—O3—H3 | 109.5 |
| O3—C9—C8 | 116.7 (2) | C14—O4—C17 | 118.3 (2) |
| | | | |
| O1—C2—C3—C4 | −178.7 (2) | C9—C8—C10—C11 | −176.6 (2) |
| C7—C2—C3—C4 | −0.3 (4) | C5—C8—C10—C11 | 5.9 (4) |
| C2—C3—C4—C5 | 0.1 (4) | C8—C10—C11—C12 | −168.2 (2) |
| C3—C4—C5—C6 | 0.9 (4) | C8—C10—C11—C16 | 14.8 (4) |
| C3—C4—C5—C8 | 179.8 (2) | C16—C11—C12—C13 | −1.5 (4) |
| C4—C5—C6—C7 | −1.7 (4) | C10—C11—C12—C13 | −178.8 (2) |
| C8—C5—C6—C7 | 179.4 (2) | C11—C12—C13—C14 | −0.5 (4) |
| C5—C6—C7—C2 | 1.5 (4) | C12—C13—C14—O4 | −178.9 (2) |
| O1—C2—C7—C6 | 178.1 (2) | C12—C13—C14—C15 | 2.9 (4) |
| C3—C2—C7—C6 | −0.4 (4) | O4—C14—C15—C16 | 178.3 (2) |
| C4—C5—C8—C10 | 66.9 (3) | C13—C14—C15—C16 | −3.3 (4) |
| C6—C5—C8—C10 | −114.2 (3) | C14—C15—C16—C11 | 1.3 (4) |
| C4—C5—C8—C9 | −110.7 (2) | C12—C11—C16—C15 | 1.1 (3) |
| C6—C5—C8—C9 | 68.2 (3) | C10—C11—C16—C15 | 178.2 (2) |
| C10—C8—C9—O2 | −176.7 (2) | C3—C2—O1—C1 | −0.5 (4) |
| C5—C8—C9—O2 | 1.1 (3) | C7—C2—O1—C1 | −178.9 (2) |
| C10—C8—C9—O3 | 2.9 (3) | C13—C14—O4—C17 | 3.6 (3) |
| C5—C8—C9—O3 | −179.4 (2) | C15—C14—O4—C17 | −178.2 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H3···O2$^{i}$ | 0.82 | 1.80 | 2.608 (2) | 169 |

Symmetry code: (i) −*x*+3, −*y*+2, −*z*+1.