

## 5-[2-(4-Acetoxyphenyl)ethenyl]-benzene-1,3-diol

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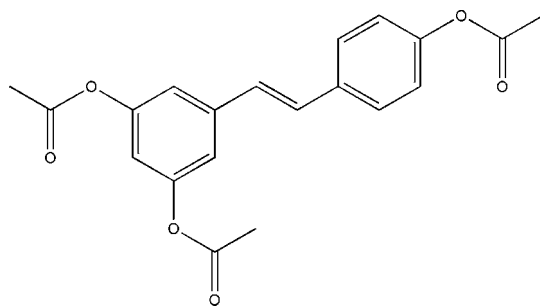
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å; R factor = 0.060; wR factor = 0.191; data-to-parameter ratio = 13.5.

The title compound,  $\text{C}_{20}\text{H}_{18}\text{O}_6$ , was prepared from resveratrol {systematic name: 5-[(*E*)-2-(4-hydroxyphenyl)ethenyl]benzene-1,3-diol}, which can be isolated from grapes, through triacetylation with using acetic anhydride in pyridine. The two benzene rings are approximately coplanar, making a dihedral angle of  $6.64$  ( $14$ )°, and the three acetoxy group are located on the same side of the plane. The skeleton of the compound resembles a table with three legs. In the crystal, molecules are linked *via* C—H...O interactions, forming inversion dimers. These dimers are further linked *via* C—H...O interactions, forming a three-dimensional structure.

## Related literature

For background to this class of compound, see: González-Barrio *et al.* (2006). For the preparation of the title compound, see: Sarpierto *et al.* (2007). For a study of its potential use in radioprotective drug development, see: Koide *et al.* (2011).



## Experimental

## Crystal data

$\text{C}_{20}\text{H}_{18}\text{O}_6$	$V = 3624.2$ ( $14$ ) Å <sup>3</sup>
$M_r = 354.34$	$Z = 8$
Monoclinic, $C2/c$	Cu $K\alpha$ radiation
$a = 31.520$ ( $6$ ) Å	$\mu = 0.80$ mm <sup>-1</sup>
$b = 6.1211$ ( $12$ ) Å	$T = 296$ K
$c = 20.110$ ( $4$ ) Å	$0.23 \times 0.10 \times 0.08$ mm
$\beta = 110.92$ ( $3$ )°	

## Data collection

Bruker APEXII CCD diffractometer	11742 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2009)	3181 independent reflections
$T_{\min} = 0.837$ , $T_{\max} = 0.939$	2532 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.020$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$	235 parameters
$wR(F^2) = 0.191$	H-atom parameters constrained
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.57$ e Å <sup>-3</sup>
3181 reflections	$\Delta\rho_{\text{min}} = -0.19$ e Å <sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C}20-H20C\cdots\text{O}1^i$	0.96	2.56	3.402 (4)	147
$\text{C}16-H16B\cdots\text{O}5^{ii}$	0.96	2.56	3.438 (4)	153
$\text{C}18-H18A\cdots\text{O}3^{iii}$	0.96	2.60	3.494 (4)	156
$\text{C}8-H8A\cdots\text{O}6^{iv}$	0.93	2.58	3.441 (4)	154

Symmetry codes: (i)  $-x, y - 1, -z + \frac{1}{2}$ ; (ii)  $-x, y, -z + \frac{1}{2}$ ; (iii)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (iv)  $-x, -y + 1, -z$ .

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); 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.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2305).

## References

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**supplementary materials**

*Acta Cryst.* (2011). E67, o3129 [ doi:10.1107/S1600536811044722 ]

## 5-[2-(4-Acetyloxyphenyl)ethenyl]benzene-1,3-diyl diacetate

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### Comment

The title molecule, 3,4',5-triacetoxy-*trans*-stilbene (Fig. 1), is the triacetylation product of resveratrol, which can be isolated from grapes (González-Barrio *et al.*, 2006). In the molecular structure of the title compound, two benzene rings were substantially coplanar with dihedral angle  $6.64 (14)^\circ$ . Three acetoxy group located in the same side of the plane. As a result, the whole structure looks like an interesting long table with three legs.

In the crystal, molecules of title compound packed with formation an infinite *Z* form (Fig. 2). Molecules are linked by non-classical C–H $\cdots$ O hydrogen bonds, which played an important role for the stability of the crystal structure (Table 1).

Koide's study (Koide *et al.*, 2011) showed that the title compound effectively protected the live cells after  $\gamma$ -irradiation and it may be a leading candidate for radioprotective drug development.

### Experimental

The title compound was prepared according to the procedure (Sarpierito *et al.*, 2007) through triacetylation by using acetic anhydride in pyridine (1:1, v/v). Crystals appropriate for X-ray diffraction data collection were obtained from methanol solution, yielding colourless block-like crystals after a week at room temperature.

### Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C–H distances of  $0.93 \text{ \AA}$  ( $0.96 \text{ \AA}$  for methyl group) and  $U_{\text{iso}}(\text{H}) = 1.2(1.5 \text{ for } \text{CH}_3)U_{\text{eq}}(\text{C})$ .

### Figures

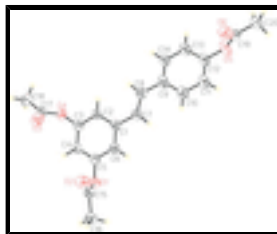


Fig. 1. The title molecule structure with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as a small spheres of arbitrary radius.

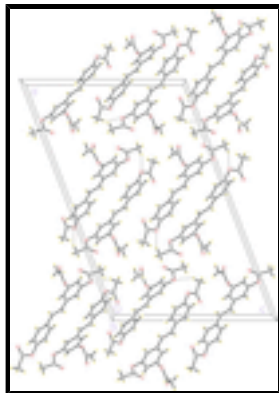


Fig. 2. The packing diagram of the title compound, viewed down the *b* axis.

5-[2-(4-Acetyloxyphenyl)ethenyl]benzene-1,3-diyl diacetate

*Crystal data*

$C_{20}H_{18}O_6$

$M_r = 354.34$

Monoclinic,  $C2/c$

Hall symbol:  $-C\ 2yc$

$a = 31.520\ (6)\ \text{\AA}$

$b = 6.1211\ (12)\ \text{\AA}$

$c = 20.110\ (4)\ \text{\AA}$

$\beta = 110.92\ (3)^\circ$

$V = 3624.2\ (14)\ \text{\AA}^3$

$Z = 8$

$F(000) = 1488$

$D_x = 1.299\ \text{Mg m}^{-3}$

Cu  $K\alpha$  radiation,  $\lambda = 1.54178\ \text{\AA}$

Cell parameters from 3228 reflections

$\theta = 4.7\text{--}67.0^\circ$

$\mu = 0.80\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Block, colourless

$0.23 \times 0.10 \times 0.08\ \text{mm}$

*Data collection*

Bruker APEXII CCD  
diffractometer

Radiation source: fine-focus sealed tube  
graphite

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2009)

$T_{\min} = 0.837$ ,  $T_{\max} = 0.939$

11742 measured reflections

3181 independent reflections

2532 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$

$\theta_{\max} = 67.0^\circ$ ,  $\theta_{\min} = 4.7^\circ$

$h = -37 \rightarrow 36$

$k = -7 \rightarrow 7$

$l = -19 \rightarrow 24$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.060$

$wR(F^2) = 0.191$

$S = 1.05$

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

$w = 1/[\sigma^2(F_o^2) + (0.1023P)^2 + 2.2789P]$

3181 reflections  
235 parameters  
0 restraints

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.57 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$$

### Special details

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.16481 (6)	0.7332 (3)	0.46756 (9)	0.0754 (5)
O2	0.21472 (8)	0.5358 (4)	0.43718 (12)	0.0992 (7)
O3	0.21702 (7)	1.1732 (4)	0.29763 (12)	0.0906 (6)
O4	0.14826 (6)	1.2873 (3)	0.29000 (10)	0.0714 (5)
O5	-0.11728 (7)	0.1955 (4)	-0.02189 (12)	0.1001 (7)
O6	-0.07902 (11)	0.0003 (4)	-0.07410 (13)	0.1110 (8)
C1	0.08924 (7)	0.7665 (4)	0.28105 (13)	0.0645 (6)
C2	0.10294 (7)	0.9669 (4)	0.26198 (12)	0.0646 (6)
H2A	0.0887	1.0215	0.2162	0.077*
C3	0.13752 (7)	1.0835 (4)	0.31104 (12)	0.0600 (5)
C4	0.15881 (7)	1.0105 (4)	0.37985 (12)	0.0620 (6)
H4A	0.1815	1.0918	0.4130	0.074*
C5	0.14503 (8)	0.8119 (4)	0.39738 (12)	0.0617 (6)
C6	0.11048 (8)	0.6919 (4)	0.34968 (13)	0.0642 (6)
H6A	0.1015	0.5605	0.3638	0.077*
C7	0.05373 (8)	0.6257 (5)	0.23138 (15)	0.0767 (7)
H7A	0.0469	0.4975	0.2502	0.092*
C8	0.03135 (9)	0.6616 (5)	0.16494 (15)	0.0761 (7)
H8A	0.0389	0.7872	0.1456	0.091*
C9	-0.00525 (8)	0.5237 (5)	0.11593 (16)	0.0741 (7)
C10	-0.01673 (9)	0.3156 (5)	0.13435 (16)	0.0803 (8)
H10A	0.0004	0.2548	0.1781	0.096*
C11	-0.05336 (9)	0.2001 (5)	0.08785 (16)	0.0792 (7)
H11A	-0.0613	0.0633	0.1000	0.095*
C12	-0.07737 (9)	0.2943 (5)	0.02379 (16)	0.0772 (7)
C13	-0.06570 (10)	0.4942 (5)	0.00422 (17)	0.0835 (8)
H13A	-0.0823	0.5524	-0.0402	0.100*
C14	-0.02968 (10)	0.6077 (5)	0.05012 (16)	0.0808 (7)

## supplementary materials

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H14A	-0.0217	0.7424	0.0366	0.097*
C15	0.19909 (8)	0.5858 (4)	0.48039 (14)	0.0699 (6)
C16	0.21382 (11)	0.5035 (6)	0.55443 (17)	0.0948 (9)
H16A	0.2381	0.4006	0.5623	0.142*
H16B	0.1887	0.4330	0.5621	0.142*
H16C	0.2242	0.6235	0.5870	0.142*
C17	0.18971 (9)	1.3158 (4)	0.28572 (12)	0.0668 (6)
C18	0.19501 (12)	1.5425 (5)	0.26272 (19)	0.0925 (9)
H18A	0.2247	1.5590	0.2602	0.139*
H18B	0.1914	1.6449	0.2965	0.139*
H18C	0.1724	1.5698	0.2167	0.139*
C19	-0.11458 (13)	0.0548 (5)	-0.07061 (14)	0.0847 (8)
C20	-0.16046 (14)	-0.0225 (7)	-0.11694 (17)	0.1184 (14)
H20A	-0.1575	-0.1227	-0.1518	0.178*
H20B	-0.1785	0.1002	-0.1406	0.178*
H20C	-0.1749	-0.0949	-0.0883	0.178*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0720 (10)	0.0922 (12)	0.0612 (10)	0.0095 (9)	0.0228 (8)	0.0065 (8)
O2	0.0966 (14)	0.1150 (17)	0.0855 (14)	0.0354 (13)	0.0319 (12)	0.0047 (12)
O3	0.0806 (12)	0.1032 (15)	0.1010 (15)	0.0186 (11)	0.0483 (11)	0.0178 (11)
O4	0.0629 (9)	0.0650 (10)	0.0877 (12)	0.0039 (7)	0.0287 (8)	0.0061 (8)
O5	0.0743 (12)	0.1182 (17)	0.0978 (15)	-0.0211 (11)	0.0186 (11)	-0.0451 (13)
O6	0.141 (2)	0.1095 (18)	0.0868 (15)	-0.0075 (16)	0.0461 (15)	-0.0264 (12)
C1	0.0513 (11)	0.0761 (15)	0.0679 (14)	-0.0055 (10)	0.0235 (10)	-0.0116 (11)
C2	0.0519 (11)	0.0831 (16)	0.0554 (12)	0.0072 (11)	0.0150 (10)	-0.0011 (11)
C3	0.0544 (11)	0.0611 (12)	0.0664 (13)	0.0046 (10)	0.0239 (10)	-0.0005 (10)
C4	0.0534 (11)	0.0670 (14)	0.0632 (13)	-0.0008 (10)	0.0178 (10)	-0.0098 (10)
C5	0.0565 (12)	0.0715 (14)	0.0577 (12)	0.0044 (10)	0.0212 (10)	-0.0025 (10)
C6	0.0607 (13)	0.0670 (14)	0.0685 (14)	-0.0035 (10)	0.0275 (11)	-0.0031 (11)
C7	0.0627 (14)	0.0930 (18)	0.0749 (16)	-0.0060 (13)	0.0252 (12)	-0.0037 (14)
C8	0.0691 (15)	0.0825 (17)	0.0778 (17)	-0.0064 (13)	0.0277 (13)	-0.0042 (13)
C9	0.0584 (13)	0.0822 (17)	0.0881 (18)	-0.0114 (12)	0.0338 (13)	-0.0290 (14)
C10	0.0642 (14)	0.097 (2)	0.0773 (16)	0.0033 (13)	0.0220 (12)	-0.0157 (14)
C11	0.0681 (15)	0.0801 (17)	0.0874 (19)	-0.0074 (12)	0.0255 (14)	-0.0200 (14)
C12	0.0637 (14)	0.0838 (18)	0.0844 (18)	-0.0133 (13)	0.0266 (13)	-0.0318 (14)
C13	0.0751 (16)	0.096 (2)	0.0774 (17)	-0.0051 (14)	0.0248 (14)	-0.0176 (14)
C14	0.0764 (16)	0.0869 (18)	0.0805 (18)	-0.0104 (14)	0.0299 (14)	-0.0170 (14)
C15	0.0592 (13)	0.0694 (14)	0.0734 (15)	-0.0003 (11)	0.0143 (11)	0.0024 (12)
C16	0.0807 (18)	0.110 (2)	0.085 (2)	0.0081 (17)	0.0194 (15)	0.0267 (17)
C17	0.0672 (14)	0.0792 (16)	0.0565 (12)	0.0017 (12)	0.0253 (11)	-0.0013 (11)
C18	0.104 (2)	0.088 (2)	0.102 (2)	-0.0070 (17)	0.0569 (19)	0.0091 (16)
C19	0.114 (2)	0.0813 (18)	0.0563 (14)	-0.0215 (17)	0.0277 (15)	-0.0038 (13)
C20	0.147 (3)	0.118 (3)	0.0649 (17)	-0.054 (2)	0.0076 (19)	-0.0127 (17)

*Geometric parameters (Å, °)*

O1—C15	1.360 (3)	C9—C14	1.372 (4)
O1—C5	1.409 (3)	C9—C10	1.409 (4)
O2—C15	1.182 (3)	C10—C11	1.392 (4)
O3—C17	1.188 (3)	C10—H10A	0.9300
O4—C17	1.351 (3)	C11—C12	1.367 (4)
O4—C3	1.397 (3)	C11—H11A	0.9300
O5—C19	1.330 (4)	C12—C13	1.375 (4)
O5—C12	1.403 (3)	C13—C14	1.369 (4)
O6—C19	1.195 (4)	C13—H13A	0.9300
C1—C6	1.379 (3)	C14—H14A	0.9300
C1—C2	1.399 (4)	C15—C16	1.481 (4)
C1—C7	1.481 (4)	C16—H16A	0.9600
C2—C3	1.380 (3)	C16—H16B	0.9600
C2—H2A	0.9300	C16—H16C	0.9600
C3—C4	1.379 (3)	C17—C18	1.491 (4)
C4—C5	1.378 (3)	C18—H18A	0.9600
C4—H4A	0.9300	C18—H18B	0.9600
C5—C6	1.378 (3)	C18—H18C	0.9600
C6—H6A	0.9300	C19—C20	1.490 (5)
C7—C8	1.288 (4)	C20—H20A	0.9600
C7—H7A	0.9300	C20—H20B	0.9600
C8—C9	1.484 (4)	C20—H20C	0.9600
C8—H8A	0.9300		
C15—O1—C5	117.03 (19)	C11—C12—C13	122.0 (3)
C17—O4—C3	118.62 (19)	C11—C12—O5	120.0 (3)
C19—O5—C12	118.9 (2)	C13—C12—O5	117.7 (3)
C6—C1—C2	118.5 (2)	C14—C13—C12	120.0 (3)
C6—C1—C7	117.5 (2)	C14—C13—H13A	120.0
C2—C1—C7	123.9 (2)	C12—C13—H13A	120.0
C3—C2—C1	120.0 (2)	C13—C14—C9	120.3 (3)
C3—C2—H2A	120.0	C13—C14—H14A	119.8
C1—C2—H2A	120.0	C9—C14—H14A	119.8
C4—C3—C2	121.8 (2)	O2—C15—O1	123.0 (2)
C4—C3—O4	120.6 (2)	O2—C15—C16	126.0 (3)
C2—C3—O4	117.4 (2)	O1—C15—C16	111.0 (2)
C5—C4—C3	117.2 (2)	C15—C16—H16A	109.5
C5—C4—H4A	121.4	C15—C16—H16B	109.5
C3—C4—H4A	121.4	H16A—C16—H16B	109.5
C4—C5—C6	122.3 (2)	C15—C16—H16C	109.5
C4—C5—O1	119.4 (2)	H16A—C16—H16C	109.5
C6—C5—O1	118.2 (2)	H16B—C16—H16C	109.5
C5—C6—C1	120.0 (2)	O3—C17—O4	122.7 (2)
C5—C6—H6A	120.0	O3—C17—C18	126.3 (3)
C1—C6—H6A	120.0	O4—C17—C18	111.0 (2)
C8—C7—C1	127.1 (3)	C17—C18—H18A	109.5
C8—C7—H7A	116.5	C17—C18—H18B	109.5

## supplementary materials

C1—C7—H7A	116.5	H18A—C18—H18B	109.5
C7—C8—C9	126.9 (3)	C17—C18—H18C	109.5
C7—C8—H8A	116.6	H18A—C18—H18C	109.5
C9—C8—H8A	116.6	H18B—C18—H18C	109.5
C14—C9—C10	118.9 (2)	O6—C19—O5	122.2 (3)
C14—C9—C8	117.6 (3)	O6—C19—C20	126.5 (3)
C10—C9—C8	123.4 (3)	O5—C19—C20	111.3 (3)
C11—C10—C9	120.8 (3)	C19—C20—H20A	109.5
C11—C10—H10A	119.6	C19—C20—H20B	109.5
C9—C10—H10A	119.6	H20A—C20—H20B	109.5
C12—C11—C10	117.8 (3)	C19—C20—H20C	109.5
C12—C11—H11A	121.1	H20A—C20—H20C	109.5
C10—C11—H11A	121.1	H20B—C20—H20C	109.5
C6—C1—C2—C3	1.1 (3)	C7—C8—C9—C10	-8.3 (4)
C7—C1—C2—C3	-177.6 (2)	C14—C9—C10—C11	-2.5 (4)
C1—C2—C3—C4	-1.4 (3)	C8—C9—C10—C11	175.7 (2)
C1—C2—C3—O4	-177.03 (19)	C9—C10—C11—C12	0.6 (4)
C17—O4—C3—C4	68.8 (3)	C10—C11—C12—C13	1.4 (4)
C17—O4—C3—C2	-115.5 (2)	C10—C11—C12—O5	-173.5 (2)
C2—C3—C4—C5	1.8 (3)	C19—O5—C12—C11	-91.5 (3)
O4—C3—C4—C5	177.33 (19)	C19—O5—C12—C13	93.4 (3)
C3—C4—C5—C6	-2.1 (3)	C11—C12—C13—C14	-1.6 (4)
C3—C4—C5—O1	-178.2 (2)	O5—C12—C13—C14	173.4 (3)
C15—O1—C5—C4	-98.1 (3)	C12—C13—C14—C9	-0.4 (4)
C15—O1—C5—C6	85.7 (3)	C10—C9—C14—C13	2.4 (4)
C4—C5—C6—C1	1.9 (3)	C8—C9—C14—C13	-175.9 (2)
O1—C5—C6—C1	178.0 (2)	C5—O1—C15—O2	5.8 (4)
C2—C1—C6—C5	-1.3 (3)	C5—O1—C15—C16	-175.1 (2)
C7—C1—C6—C5	177.4 (2)	C3—O4—C17—O3	1.7 (4)
C6—C1—C7—C8	-177.1 (3)	C3—O4—C17—C18	-179.9 (2)
C2—C1—C7—C8	1.5 (4)	C12—O5—C19—O6	4.4 (5)
C1—C7—C8—C9	-177.9 (2)	C12—O5—C19—C20	-176.5 (3)
C7—C8—C9—C14	170.0 (3)		

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C20—H20C $\cdots$ O1 <sup>i</sup>	0.96	2.56	3.402 (4)	147.
C16—H16B $\cdots$ O5 <sup>ii</sup>	0.96	2.56	3.438 (4)	153.
C18—H18A $\cdots$ O3 <sup>iii</sup>	0.96	2.60	3.494 (4)	156.
C8—H8A $\cdots$ O6 <sup>iv</sup>	0.93	2.58	3.441 (4)	154.
C16—H16A $\cdots$ O3 <sup>v</sup>	0.96	2.70	3.185 (4)	112.

Symmetry codes: (i)  $-x, y-1, -z+1/2$ ; (ii)  $-x, y, -z+1/2$ ; (iii)  $-x+1/2, y+1/2, -z+1/2$ ; (iv)  $-x, -y+1, -z$ ; (v)  $-x+1/2, -y+3/2, -z+1$ .



Fig. 1

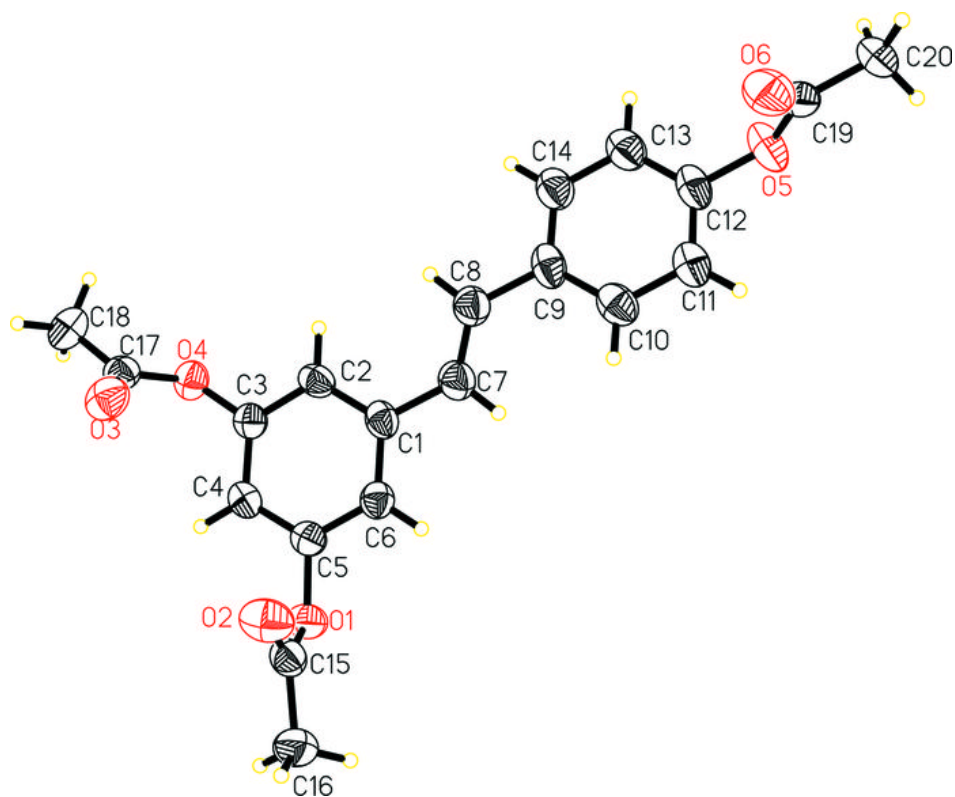


Fig. 2

