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2,6-Dibromo-4-formylphenyl 3-phenylprop-2-enoate

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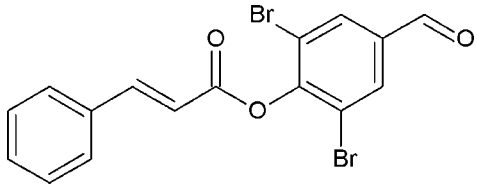
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.041; wR factor = 0.107; data-to-parameter ratio = 19.8.

Molecules of the title compound, $C_{16}H_{10}Br_2O_3$, adopt an E conformation about the C=C double bond. The dihedral angle between the two aromatic rings is 78.0 (7)°. In the crystal, molecules are linked through weak C—H···O hydrogen bonds.

Related literature

For the biological activity of cinnamoyl derivatives, see: De *et al.* (2011); Obioran *et al.* (1986); Cremlyn *et al.* (1984).



Experimental

Crystal data

$C_{16}H_{10}Br_2O_3$
M_r = 410.06
Triclinic, $P\overline{1}$
a = 8.0846 (3) Å
b = 9.0149 (4) Å
c = 11.8995 (5) Å
α = 77.429 (2)°
β = 73.918 (2)°
γ = 70.236 (2)°
V = 776.83 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 5.22 mm^{-1}
T = 293 K
0.25 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker 2004)
T_{min} = 0.979, T_{max} = 0.983
15811 measured reflections
3764 independent reflections
2282 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.107
S = 0.98
3764 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1^{i}	0.93	2.48	3.221 (6)	136

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT6828).

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supporting information

Acta Cryst. (2012). E**68**, o2873 [https://doi.org/10.1107/S1600536812037427]

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S1. Comment

Cinnamoyl derivatives exhibit a variety of pharmacological properties, e.g anticancer, antitumor and antimicrobial activities (De *et al.*, 2011; Obioran *et al.*, 1986; Cremlyn *et al.*, 1984). In view of their importance, the crystal structure determination of the title compound was carried out and the results are presented herein. The molecular structure of the title compound is shown in Fig. 1. In the molecule, the configuration about the C═C double bond is *E*. The dihedral angle between the two aromatic rings is 78.0 (7)°. In the crystal packing, molecules are linked through weak C—H···O hydrogen bonds (Fig. 2).

S2. Experimental

To a solution of 3,5-dibromo benzaldehyde (0.03 mol) in chloroform (100 ml) cinnamoyl chloride (0.03 mol) was added followed by addition of triethyl amine (0.03 mol). Then the reaction was stirred at room temperature for 3 h. The reaction mixture was quenched with water and the chloroform layer was separated. The combined chloroform layers were washed with 5% NaOH solution followed by water wash and dried with sodium sulfate. Then the mixture was concentrated under reduced pressure. The obtained solid was crystallized in a mixture of methanol:chloroform.

S3. Refinement

H atoms were refined with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C)] using a riding model with C—H = 0.93 Å.

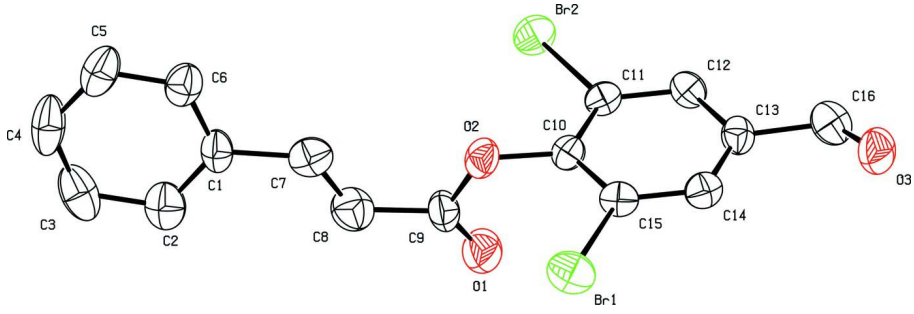

Figure 1

The molecular structure of the title compound showing 30% probability displacement ellipsoids. H atoms are omitted for clarity.

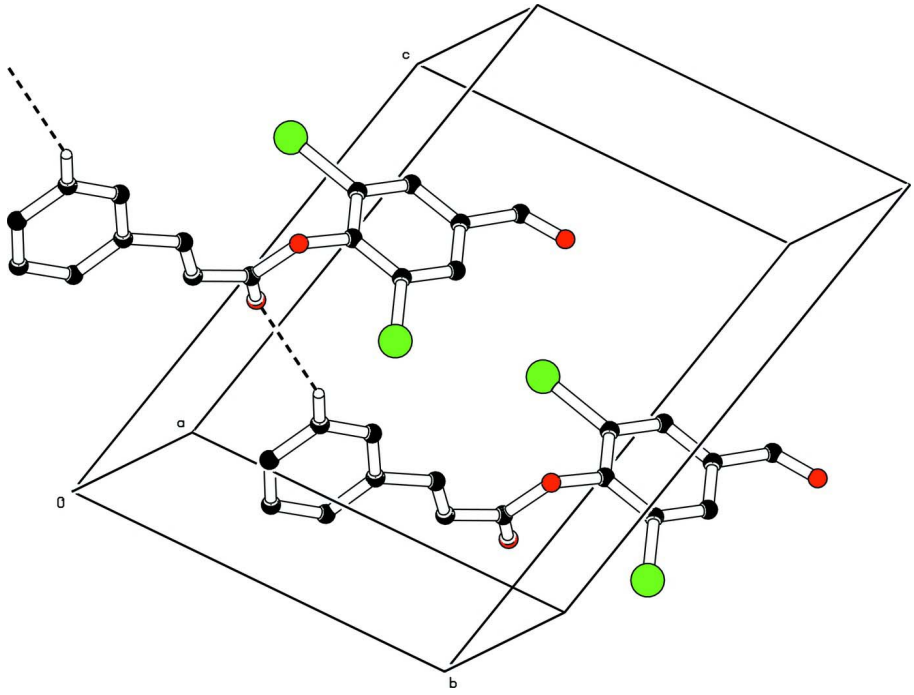

Figure 2

Crystal packing diagram. H atoms not involved in intermolecular hydrogen bonding (dashed lines) have been omitted for clarity.

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Crystal data

$C_{16}H_{10}Br_2O_3$
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$\alpha = 77.429$ (2)°
$\beta = 73.918$ (2)°
$\gamma = 70.236$ (2)°
$V = 776.83$ (6) Å^3
$Z = 2$
$F(000) = 400$
$D_x = 1.753$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8834 reflections
$\theta = 2.1$–$31.2°$
$\mu = 5.22$ mm^{-1}
$T = 293$ K
Block, colourless
0.25 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker 2004)
$T_{min} = 0.979$, $T_{max} = 0.983$
15811 measured reflections
3764 independent reflections
2282 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 28.2°$, $\theta_{min} = 2.4°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.107$
$S = 0.98$
3764 reflections
190 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
$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2 + 0.7467P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.63$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.5056 (3)	0.8407 (3)	0.3049 (2)	0.0643 (7)
Br2	0.28505 (7)	0.69030 (5)	0.52006 (4)	0.07858 (18)
Br1	0.54158 (7)	1.17400 (6)	0.21211 (4)	0.08435 (18)
C10	0.3929 (4)	0.9517 (4)	0.3796 (3)	0.0499 (8)
C15	0.3931 (5)	1.1088 (4)	0.3529 (3)	0.0555 (9)
C12	0.1796 (5)	1.0109 (4)	0.5601 (3)	0.0562 (9)
H12	0.1060	0.9786	0.6297	0.067*
C1	0.8079 (5)	0.4509 (4)	0.1110 (4)	0.0612 (10)
C16	0.0729 (6)	1.2807 (6)	0.6205 (4)	0.0745 (12)
H16	−0.0078	1.2465	0.6849	0.089*
C13	0.1840 (5)	1.1664 (4)	0.5332 (3)	0.0559 (9)
C5	1.0667 (7)	0.2245 (5)	0.1043 (5)	0.0881 (14)
H5	1.1658	0.1610	0.1351	0.106*
O3	0.0815 (5)	1.4077 (4)	0.6125 (3)	0.0920 (10)
C11	0.2853 (5)	0.9037 (4)	0.4828 (3)	0.0517 (8)
C2	0.7771 (6)	0.4158 (6)	0.0153 (4)	0.0796 (13)
H2	0.6803	0.4821	−0.0168	0.096*
C9	0.4246 (7)	0.8097 (5)	0.2269 (4)	0.0657 (11)
C7	0.6899 (6)	0.5893 (5)	0.1768 (4)	0.0704 (11)
H7	0.7306	0.6079	0.2368	0.085*
C14	0.2892 (5)	1.2157 (4)	0.4296 (3)	0.0573 (9)
H14	0.2901	1.3212	0.4114	0.069*
C8	0.5420 (7)	0.6811 (6)	0.1574 (4)	0.0830 (13)
H8	0.5037	0.6671	0.0946	0.100*
C6	0.9537 (6)	0.3553 (5)	0.1536 (4)	0.0721 (11)

H6	0.9770	0.3801	0.2184	0.087*
O1	0.2767 (5)	0.8782 (4)	0.2205 (3)	0.0886 (9)
C4	1.0338 (8)	0.1871 (6)	0.0099 (6)	0.0954 (18)
H4	1.1101	0.0970	−0.0237	0.114*
C3	0.8902 (8)	0.2802 (7)	−0.0361 (5)	0.0943 (17)
H3	0.8673	0.2543	−0.1006	0.113*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0470 (14)	0.0607 (15)	0.0710 (17)	−0.0052 (12)	−0.0006 (13)	−0.0138 (13)
Br2	0.1027 (4)	0.0525 (2)	0.0777 (3)	−0.0311 (2)	−0.0149 (2)	0.00322 (19)
Br1	0.0860 (3)	0.0953 (3)	0.0707 (3)	−0.0500 (3)	−0.0005 (2)	0.0062 (2)
C10	0.0397 (19)	0.0526 (19)	0.056 (2)	−0.0126 (15)	−0.0095 (16)	−0.0082 (17)
C15	0.050 (2)	0.063 (2)	0.056 (2)	−0.0249 (17)	−0.0117 (17)	−0.0009 (18)
C12	0.053 (2)	0.066 (2)	0.051 (2)	−0.0247 (18)	−0.0061 (17)	−0.0090 (18)
C1	0.064 (3)	0.052 (2)	0.062 (2)	−0.0278 (19)	0.0140 (19)	−0.0159 (18)
C16	0.072 (3)	0.090 (3)	0.074 (3)	−0.031 (2)	−0.016 (2)	−0.025 (2)
C13	0.052 (2)	0.059 (2)	0.063 (2)	−0.0162 (17)	−0.0154 (18)	−0.0196 (18)
C5	0.077 (3)	0.055 (2)	0.121 (4)	−0.017 (2)	−0.003 (3)	−0.016 (3)
O3	0.110 (3)	0.076 (2)	0.098 (2)	−0.0113 (19)	−0.037 (2)	−0.0376 (19)
C11	0.051 (2)	0.0473 (18)	0.060 (2)	−0.0200 (16)	−0.0151 (17)	−0.0012 (16)
C2	0.067 (3)	0.084 (3)	0.086 (3)	−0.033 (2)	0.005 (2)	−0.018 (3)
C9	0.079 (3)	0.057 (2)	0.060 (2)	−0.020 (2)	−0.002 (2)	−0.0219 (19)
C7	0.064 (3)	0.073 (3)	0.073 (3)	−0.034 (2)	−0.007 (2)	0.006 (2)
C14	0.061 (2)	0.052 (2)	0.067 (2)	−0.0254 (18)	−0.0200 (19)	−0.0054 (18)
C8	0.085 (3)	0.089 (3)	0.084 (3)	−0.029 (3)	−0.025 (3)	−0.017 (3)
C6	0.071 (3)	0.058 (2)	0.080 (3)	−0.022 (2)	−0.001 (2)	−0.009 (2)
O1	0.090 (2)	0.087 (2)	0.092 (2)	−0.0086 (19)	−0.0341 (19)	−0.0304 (18)
C4	0.083 (4)	0.067 (3)	0.131 (5)	−0.037 (3)	0.029 (3)	−0.047 (3)
C3	0.102 (4)	0.118 (4)	0.085 (3)	−0.069 (4)	0.015 (3)	−0.045 (3)

Geometric parameters (Å, º)

O2—C9	1.393 (5)	C13—C14	1.370 (5)
O2—C10	1.394 (4)	C5—C4	1.355 (8)
Br2—C11	1.878 (3)	C5—C6	1.358 (6)
Br1—C15	1.878 (4)	C5—H5	0.9300
C10—C11	1.373 (5)	C2—C3	1.401 (7)
C10—C15	1.383 (5)	C2—H2	0.9300
C15—C14	1.371 (5)	C9—O1	1.161 (5)
C12—C13	1.379 (5)	C9—C8	1.473 (6)
C12—C11	1.379 (5)	C7—C8	1.252 (6)
C12—H12	0.9300	C7—H7	0.9300
C1—C2	1.352 (6)	C14—H14	0.9300
C1—C6	1.357 (6)	C8—H8	0.9300
C1—C7	1.512 (6)	C6—H6	0.9300
C16—O3	1.152 (5)	C4—C3	1.358 (8)

C16—C13	1.507 (6)	C4—H4	0.9300
C16—H16	0.9300	C3—H3	0.9300
C9—O2—C10	115.2 (3)	C1—C2—C3	120.4 (5)
C11—C10—C15	119.6 (3)	C1—C2—H2	119.8
C11—C10—O2	119.8 (3)	C3—C2—H2	119.8
C15—C10—O2	120.6 (3)	O1—C9—O2	122.1 (3)
C14—C15—C10	120.5 (3)	O1—C9—C8	124.1 (4)
C14—C15—Br1	120.0 (3)	O2—C9—C8	113.8 (4)
C10—C15—Br1	119.5 (3)	C8—C7—C1	125.6 (5)
C13—C12—C11	119.5 (3)	C8—C7—H7	117.2
C13—C12—H12	120.3	C1—C7—H7	117.2
C11—C12—H12	120.3	C15—C14—C13	119.6 (3)
C2—C1—C6	118.6 (4)	C15—C14—H14	120.2
C2—C1—C7	124.8 (4)	C13—C14—H14	120.2
C6—C1—C7	116.5 (4)	C7—C8—C9	124.6 (5)
O3—C16—C13	124.2 (5)	C7—C8—H8	117.7
O3—C16—H16	117.9	C9—C8—H8	117.7
C13—C16—H16	117.9	C1—C6—C5	122.0 (5)
C14—C13—C12	120.6 (3)	C1—C6—H6	119.0
C14—C13—C16	120.5 (4)	C5—C6—H6	119.0
C12—C13—C16	118.8 (4)	C3—C4—C5	120.5 (5)
C4—C5—C6	119.5 (5)	C3—C4—H4	119.8
C4—C5—H5	120.3	C5—C4—H4	119.8
C6—C5—H5	120.3	C4—C3—C2	119.0 (5)
C10—C11—C12	120.3 (3)	C4—C3—H3	120.5
C10—C11—Br2	119.8 (3)	C2—C3—H3	120.5
C12—C11—Br2	119.9 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	0.93	2.48	3.221 (6)	136
C7—H7···O2	0.93	2.39	2.764 (3)	104

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