

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Ethyl 2-(4-chlorophenyl)-3-(3,5-dimethoxyphenoxy)acrylate

Wu Chen, Yong-Ming Cui, Fei Pan, Dong-Sheng Xia and Qing-Fu Zeng*

Engineering Research Center for Clean Production of Textile Printing, Ministry of Education, Wuhan University of Science & Engineering, Wuhan 430073, People's Republic of China

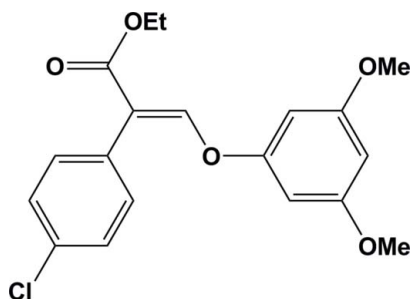
Correspondence e-mail: qingfu_zeng@163.com

Received 31 October 2008; accepted 21 November 2008

 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.058; wR factor = 0.147; data-to-parameter ratio = 14.3.

 The title compound, $\text{C}_{19}\text{H}_{19}\text{ClO}_5$, displays a dihedral angle of $74.7(3)^\circ$ between the mean planes of the 4-chlorophenyl and phenol rings.

Related literature

 For phenylacetate and styrene derivatives, see: Fang *et al.* (2007); Huang *et al.* (2007); Li *et al.* (2007).


Experimental

Crystal data

 $\text{C}_{19}\text{H}_{19}\text{ClO}_5$
 $M_r = 362.80$

 Triclinic, $P\bar{1}$
 $a = 9.601(2)$ Å
 $b = 9.607(3)$ Å
 $c = 10.368(2)$ Å
 $\alpha = 77.84(2)^\circ$
 $\beta = 75.42(3)^\circ$
 $\gamma = 87.40(3)^\circ$
 $V = 904.7(4)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.24$ mm⁻¹
 $T = 298(2)$ K
 $0.30 \times 0.20 \times 0.10$ mm

Data collection

 Bruker SMART 1000 CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\min} = 0.932$, $T_{\max} = 0.977$

 6132 measured reflections
 3280 independent reflections
 2153 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.147$
 $S = 1.03$
 3280 reflections

 230 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.48$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.40$ e Å⁻³

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

This work was supported by the National Science & Technology Program of China (No. 2006BAC02A11), the Key Technologies R & D Program of the Education Commission of Hubei Province of China (No. Z20081701) and the Technologies R & D Program of Hubei Province of China (No. 2007AA301B62).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2078).

References

- Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Bruker (2007). *SMART* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Fang, R.-Q., Li, H.-Q., Shi, L., Xiao, Z.-P. & Zhu, H.-L. (2007). *Acta Cryst.* **E63**, o3975.
 Huang, X.-F., Ruan, B.-F., Wang, X.-T., Xu, C., Ge, H.-M. & Zhu, H.-L. (2007). *Eur. J. Med. Chem.* **42**, 263–267.
 Li, H.-Q., Xu, C., Li, H.-S., Xiao, Z.-P., Shi, L. & Zhu, H.-L. (2007). *Chem. Med. Chem.* **2**, 1361–1369.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supporting information

Acta Cryst. (2008). E64, o2471 [doi:10.1107/S1600536808039263]

Ethyl 2-(4-chlorophenyl)-3-(3,5-dimethoxyphenoxy)acrylate**Wu Chen, Yong-Ming Cui, Fei Pan, Dong-Sheng Xia and Qing-Fu Zeng****S1. Comment**

Phenylacetate and styrene derivatives are important for their extensive biological activities. Recently a large number of such compounds have been synthesized, and found to have good biological activities (Fang *et al.*, 2007; Huang *et al.*, 2007; Li *et al.*, 2007). Here report on the crystal structure of the new acrylate compound, (I).

The molecular structure of compound (I) is illustrated in Fig. 1. All the bond lengths and angles are within normal values. The dihedral angle between the mean plane of the 4-chlorophenyl ring (C1—C6) and the mean plane through the phenol ring (C7—C12) is 74.7 (3)°. The [O5/C13—C15/O1/O2] mean plane forms dihedral angles of 23.6 (3)° and 59.6 (3)° with the mean planes of rings (C1—C6) and (C7—C12), respectively.

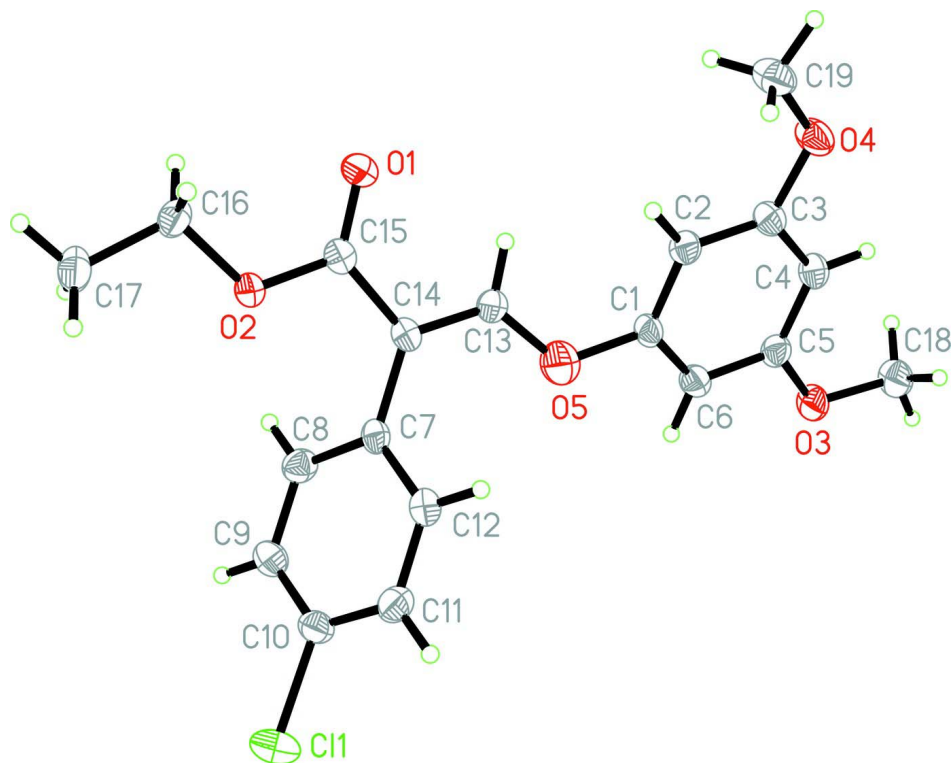
In the crystal structure the molecules stack head-to-head along the *c* direction.

S2. Experimental

Ethyl 3-bromo-2-(4-chlorophenyl)acrylate (0.1 mmol) and 3,5-dimethoxyphenol (0.1 mmol) were reacted in chloroform for 12 h, giving a clear colorless solution. Crystals of compound (I) were formed by gradual evaporation of the solution.

S3. Refinement

All the H-atoms were placed in calculated positions and treated as riding atoms: C—H = 0.93–0.97 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and $1.5U_{\text{eq}}(\text{methyl C})$.

**Figure 1**

The molecular structure of compound (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level.

Ethyl 2-(4-chlorophenyl)-3-(3,5-dimethoxyphenoxy)acrylate

Crystal data

$C_{19}H_{19}ClO_5$

$M_r = 362.80$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 9.601\ (2)\ \text{\AA}$

$b = 9.607\ (3)\ \text{\AA}$

$c = 10.368\ (2)\ \text{\AA}$

$\alpha = 77.84\ (2)^\circ$

$\beta = 75.42\ (3)^\circ$

$\gamma = 87.40\ (3)^\circ$

$V = 904.7\ (4)\ \text{\AA}^3$

$Z = 2$

$F(000) = 382$

$D_x = 1.335\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1273 reflections

$\theta = 2.4\text{--}25.3^\circ$

$\mu = 0.24\ \text{mm}^{-1}$

$T = 298\ \text{K}$

Block, colorless

$0.30 \times 0.20 \times 0.10\ \text{mm}$

Data collection

Bruker SMART 1000 CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2001)

$T_{\min} = 0.932$, $T_{\max} = 0.977$

6132 measured reflections

3280 independent reflections

2153 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.028$

$\theta_{\max} = 25.3^\circ$, $\theta_{\min} = 2.1^\circ$

$h = -11 \rightarrow 11$

$k = -11 \rightarrow 11$

$l = -12 \rightarrow 12$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.058$ $wR(F^2) = 0.147$ $S = 1.03$

3280 reflections

230 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0584P)^2 + 0.3443P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.48 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.40 \text{ e } \text{\AA}^{-3}$ Extinction correction: *SHELXTL* (Sheldrick,
2008), $F_c^* = kF_c[1 + 0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.015 (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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.9387 (3)	0.1311 (3)	0.7046 (3)	0.0377 (7)
C2	1.0552 (3)	0.1122 (3)	0.5995 (3)	0.0393 (7)
H2	1.0797	0.1812	0.5197	0.047*
C3	1.1345 (3)	-0.0115 (3)	0.6159 (3)	0.0411 (7)
C4	1.0993 (3)	-0.1153 (3)	0.7352 (3)	0.0433 (8)
H4	1.1517	-0.1990	0.7447	0.052*
C5	0.9853 (3)	-0.0911 (3)	0.8389 (3)	0.0399 (7)
C6	0.9046 (3)	0.0313 (3)	0.8241 (3)	0.0424 (7)
H6	0.8276	0.0461	0.8947	0.051*
C7	0.6961 (3)	0.5299 (3)	0.6619 (3)	0.0341 (7)
C8	0.5498 (3)	0.5569 (3)	0.6821 (3)	0.0429 (7)
H8	0.5004	0.5304	0.6245	0.051*
C9	0.4755 (3)	0.6225 (3)	0.7858 (3)	0.0476 (8)
H9	0.3773	0.6391	0.7982	0.057*
C10	0.5490 (3)	0.6624 (3)	0.8697 (3)	0.0442 (8)
C11	0.6936 (3)	0.6343 (3)	0.8557 (3)	0.0472 (8)
H11	0.7414	0.6591	0.9154	0.057*
C12	0.7665 (3)	0.5688 (3)	0.7519 (3)	0.0416 (7)
H12	0.8642	0.5503	0.7417	0.050*
C13	0.8483 (3)	0.3402 (3)	0.5672 (3)	0.0400 (7)
H13	0.8987	0.3089	0.4896	0.048*
C14	0.7768 (3)	0.4626 (3)	0.5486 (3)	0.0352 (7)
C15	0.7837 (3)	0.5296 (3)	0.4060 (3)	0.0378 (7)

C16	0.7084 (4)	0.7295 (3)	0.2597 (3)	0.0469 (8)
H16A	0.6915	0.6667	0.2031	0.056*
H16B	0.8017	0.7750	0.2182	0.056*
C17	0.5928 (4)	0.8392 (4)	0.2728 (4)	0.0638 (10)
H17A	0.5009	0.7929	0.3116	0.096*
H17B	0.5941	0.8959	0.1844	0.096*
H17C	0.6095	0.8993	0.3307	0.096*
C18	1.0305 (4)	-0.3072 (3)	0.9843 (3)	0.0595 (10)
H18A	1.0336	-0.3627	0.9167	0.089*
H18B	0.9906	-0.3639	1.0731	0.089*
H18C	1.1262	-0.2773	0.9788	0.089*
C19	1.2980 (4)	0.0648 (3)	0.3998 (3)	0.0580 (9)
H19A	1.2229	0.0832	0.3525	0.087*
H19B	1.3822	0.0325	0.3418	0.087*
H19C	1.3206	0.1506	0.4242	0.087*
Cl1	0.45938 (11)	0.75361 (11)	0.99503 (10)	0.0720 (4)
O5	0.8538 (3)	0.2570 (3)	0.6900 (3)	0.0694 (7)
O1	0.8506 (2)	0.4862 (2)	0.3068 (2)	0.0560 (6)
O2	0.7048 (2)	0.6494 (2)	0.39530 (19)	0.0412 (5)
O3	0.9429 (2)	-0.1850 (2)	0.9607 (2)	0.0501 (6)
O4	1.2510 (2)	-0.0425 (2)	0.5203 (2)	0.0545 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0428 (17)	0.0281 (15)	0.0451 (17)	0.0087 (13)	-0.0152 (14)	-0.0104 (13)
C2	0.0505 (19)	0.0275 (15)	0.0389 (16)	0.0037 (14)	-0.0133 (14)	-0.0030 (13)
C3	0.0410 (17)	0.0355 (16)	0.0457 (18)	0.0035 (14)	-0.0090 (14)	-0.0092 (14)
C4	0.0502 (19)	0.0317 (16)	0.0469 (18)	0.0087 (14)	-0.0154 (15)	-0.0037 (14)
C5	0.0468 (18)	0.0340 (16)	0.0392 (17)	0.0037 (14)	-0.0143 (14)	-0.0047 (13)
C6	0.0441 (18)	0.0400 (17)	0.0417 (17)	0.0064 (14)	-0.0088 (14)	-0.0085 (14)
C7	0.0346 (16)	0.0272 (14)	0.0382 (16)	0.0018 (12)	-0.0096 (13)	-0.0011 (12)
C8	0.0400 (18)	0.0495 (19)	0.0417 (17)	-0.0017 (14)	-0.0125 (14)	-0.0117 (14)
C9	0.0367 (17)	0.056 (2)	0.0488 (19)	0.0084 (15)	-0.0066 (15)	-0.0145 (16)
C10	0.051 (2)	0.0403 (17)	0.0370 (17)	0.0070 (15)	-0.0037 (15)	-0.0091 (14)
C11	0.053 (2)	0.0493 (19)	0.0432 (18)	0.0025 (16)	-0.0194 (15)	-0.0101 (15)
C12	0.0383 (17)	0.0409 (17)	0.0461 (17)	0.0061 (14)	-0.0136 (14)	-0.0073 (14)
C13	0.0464 (18)	0.0365 (17)	0.0361 (16)	0.0070 (14)	-0.0114 (14)	-0.0048 (13)
C14	0.0323 (16)	0.0321 (15)	0.0404 (16)	0.0037 (13)	-0.0078 (13)	-0.0078 (13)
C15	0.0351 (16)	0.0352 (16)	0.0441 (17)	0.0025 (13)	-0.0106 (14)	-0.0097 (13)
C16	0.059 (2)	0.0425 (18)	0.0396 (17)	0.0061 (16)	-0.0195 (16)	-0.0024 (14)
C17	0.082 (3)	0.053 (2)	0.066 (2)	0.0239 (19)	-0.038 (2)	-0.0124 (18)
C18	0.074 (2)	0.0423 (19)	0.053 (2)	0.0162 (18)	-0.0132 (18)	0.0046 (16)
C19	0.063 (2)	0.046 (2)	0.051 (2)	0.0065 (17)	0.0064 (17)	-0.0061 (16)
Cl1	0.0792 (7)	0.0803 (7)	0.0582 (6)	0.0120 (5)	-0.0040 (5)	-0.0363 (5)
O5	0.0825 (19)	0.0557 (15)	0.0689 (17)	0.0162 (14)	-0.0212 (14)	-0.0105 (13)
O1	0.0676 (16)	0.0554 (14)	0.0401 (12)	0.0240 (12)	-0.0068 (11)	-0.0121 (11)
O2	0.0476 (12)	0.0376 (11)	0.0373 (11)	0.0130 (10)	-0.0115 (9)	-0.0068 (9)

O3	0.0569 (14)	0.0403 (12)	0.0454 (12)	0.0099 (11)	-0.0100 (11)	0.0031 (10)
O4	0.0587 (15)	0.0414 (13)	0.0512 (13)	0.0129 (11)	0.0011 (11)	-0.0028 (11)

Geometric parameters (Å, °)

C1—C6	1.373 (4)	C12—H12	0.9300
C1—C2	1.387 (4)	C13—C14	1.338 (4)
C1—O5	1.430 (3)	C13—O5	1.366 (4)
C2—C3	1.385 (4)	C13—H13	0.9300
C2—H2	0.9300	C14—C15	1.469 (4)
C3—O4	1.363 (3)	C15—O1	1.212 (3)
C3—C4	1.392 (4)	C15—O2	1.349 (3)
C4—C5	1.378 (4)	C16—O2	1.446 (3)
C4—H4	0.9300	C16—C17	1.496 (4)
C5—O3	1.367 (3)	C16—H16A	0.9700
C5—C6	1.381 (4)	C16—H16B	0.9700
C6—H6	0.9300	C17—H17A	0.9600
C7—C8	1.388 (4)	C17—H17B	0.9600
C7—C12	1.398 (4)	C17—H17C	0.9600
C7—C14	1.487 (4)	C18—O3	1.427 (4)
C8—C9	1.385 (4)	C18—H18A	0.9600
C8—H8	0.9300	C18—H18B	0.9600
C9—C10	1.370 (4)	C18—H18C	0.9600
C9—H9	0.9300	C19—O4	1.429 (4)
C10—C11	1.379 (4)	C19—H19A	0.9600
C10—C11	1.745 (3)	C19—H19B	0.9600
C11—C12	1.382 (4)	C19—H19C	0.9600
C11—H11	0.9300		
C6—C1—C2	120.9 (3)	C14—C13—H13	117.1
C6—C1—O5	119.2 (3)	O5—C13—H13	117.1
C2—C1—O5	119.9 (3)	C13—C14—C15	115.3 (3)
C3—C2—C1	118.7 (3)	C13—C14—C7	123.7 (3)
C3—C2—H2	120.7	C15—C14—C7	121.0 (2)
C1—C2—H2	120.7	O1—C15—O2	122.0 (3)
O4—C3—C2	124.2 (3)	O1—C15—C14	126.0 (3)
O4—C3—C4	114.6 (3)	O2—C15—C14	112.0 (2)
C2—C3—C4	121.2 (3)	O2—C16—C17	107.5 (3)
C5—C4—C3	118.5 (3)	O2—C16—H16A	110.2
C5—C4—H4	120.7	C17—C16—H16A	110.2
C3—C4—H4	120.7	O2—C16—H16B	110.2
O3—C5—C4	123.3 (3)	C17—C16—H16B	110.2
O3—C5—C6	115.7 (3)	H16A—C16—H16B	108.5
C4—C5—C6	121.0 (3)	C16—C17—H17A	109.5
C1—C6—C5	119.7 (3)	C16—C17—H17B	109.5
C1—C6—H6	120.2	H17A—C17—H17B	109.5
C5—C6—H6	120.2	C16—C17—H17C	109.5
C8—C7—C12	117.6 (3)	H17A—C17—H17C	109.5

C8—C7—C14	121.8 (3)	H17B—C17—H17C	109.5
C12—C7—C14	120.6 (3)	O3—C18—H18A	109.5
C9—C8—C7	121.7 (3)	O3—C18—H18B	109.5
C9—C8—H8	119.1	H18A—C18—H18B	109.5
C7—C8—H8	119.1	O3—C18—H18C	109.5
C10—C9—C8	118.9 (3)	H18A—C18—H18C	109.5
C10—C9—H9	120.5	H18B—C18—H18C	109.5
C8—C9—H9	120.5	O4—C19—H19A	109.5
C9—C10—C11	121.4 (3)	O4—C19—H19B	109.5
C9—C10—C11	119.6 (2)	H19A—C19—H19B	109.5
C11—C10—C11	119.1 (3)	O4—C19—H19C	109.5
C10—C11—C12	119.1 (3)	H19A—C19—H19C	109.5
C10—C11—H11	120.4	H19B—C19—H19C	109.5
C12—C11—H11	120.4	C13—O5—C1	123.7 (2)
C11—C12—C7	121.2 (3)	C15—O2—C16	117.4 (2)
C11—C12—H12	119.4	C5—O3—C18	117.4 (2)
C7—C12—H12	119.4	C3—O4—C19	116.9 (2)
C14—C13—O5	125.8 (3)		
