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3-(4-Bromophenyl)-2-ethylacrylic acid

Niaz Muhammad,[a] Zia-ur-Rehman,[a] Saqib Ali[a] and Auke Meetsma[b]*

[a]Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, and [b]Crystal Structure Center, Chemical Physics, Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, NL-9747 AG Groningen, The Netherlands

Correspondence e-mail: a.meetsma@rug.nl

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Key indicators

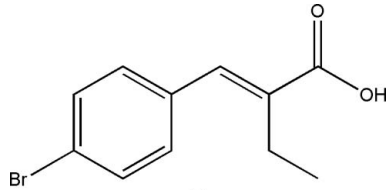
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.026
wR factor = 0.067
Data-to-parameter ratio = 18.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The configuration in the solid state structure of the title compound, $C_{11}H_{11}BrO_2$, about the C=C double bond is *E*. In the crystal structure, symmetry-related molecules are linked by O—H···O hydrogen bonds, forming centrosymmetric carboxylic acid dimers.

Comment

Cinnamic acid derivatives are used in the shikimic acid metabolic pathways of higher plants (Forgó *et al.*, 2005). These compounds are also widely used as starting materials for the synthesis of antimalarial drugs. The most active compounds in this group are halo-substituted (Nodiff *et al.*, 1971).



(I)

The molecular structure of the title compound, (I), is shown in Fig. 1 and selected bond distances and angles are given in Table 1. The length of the C7=C8 bond [1.348 (2) Å] shows its double-bond character. The configuration about the C=C double bond is *E*. The bond lengths within the phenyl ring range from 1.382 (2) to 1.408 (2) Å, typical of aromatic character (Allen *et al.*, 1987). The Br—C3 bond distance is normal. In the crystal structure of (I), centrosymmetric dimers are formed *via* O—H···O hydrogen bonds involving the carboxylic acid groups (Fig. 2 and Table 2). The dimers are

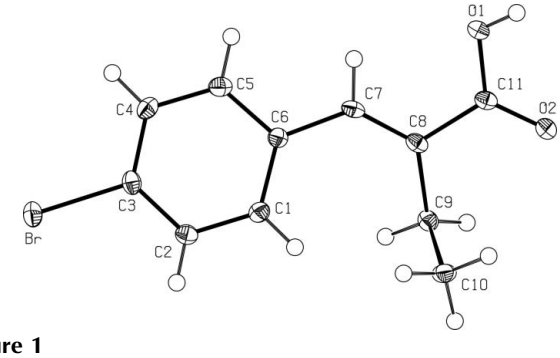


Figure 1
The molecular structure of the title compound, showing the atom numbering scheme. Displacement ellipsoids for non-H atoms are represented at the 50% probability level. The H atoms are drawn with an arbitrary radius.

further linked by C—H···O bonds, forming a sheet-like structure.

Experimental

Compound (I) was synthesized according to a previously reported method (Gensler *et al.*, 1958). A mixture of 4-bromobenzaldehyde (1.85 g 10 mmol), ethylmalonic acid (2.64 g 20 mmol) and piperidine (1.98 ml 20 mmol) in a pyridine (12.5 ml) solution was heated on a steam-bath for 24 h. The reaction mixture was cooled and added to a mixture of 25 ml of concentrated HCl and 50 g of ice. The precipitate formed in the acidified mixture was filtered off and washed with ice-cold water. The product was recrystallized from an alcohol–water mixture (4:1). The yield was 65%.

Crystal data

$C_{11}H_{11}BrO_2$
$M_r = 255.11$
Monoclinic, $P2_1/c$
$a = 11.9803$ (9) Å
$b = 5.0008$ (4) Å
$c = 16.986$ (1) Å
$\beta = 101.880$ (1)°
$V = 995.85$ (12) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 4.10$ mm^{-1}
$T = 100$ (1) K
0.49 × 0.39 × 0.21 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min} = 0.164$, $T_{max} = 0.423$
8570 measured reflections
2461 independent reflections
2168 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.067$
$S = 1.03$
2461 reflections
132 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.73$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br—C3	1.9034 (16)	O2—C11	1.227 (2)
O1—C11	1.330 (2)		
Br—C3—C2	118.83 (12)	O2—C11—C8	121.63 (15)
Br—C3—C4	119.78 (12)	O1—C11—O2	122.22 (15)
O1—C11—C8	116.16 (14)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H11···O2^{i}	0.79 (4)	1.89 (3)	2.6716 (18)	172 (3)
C4—H4···O2^{ii}	0.95	2.52	3.457 (2)	167
C7—H7···O1	0.95	2.28	2.722 (2)	107

Symmetry codes: (i) $-x+1, -y+3, -z+1$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

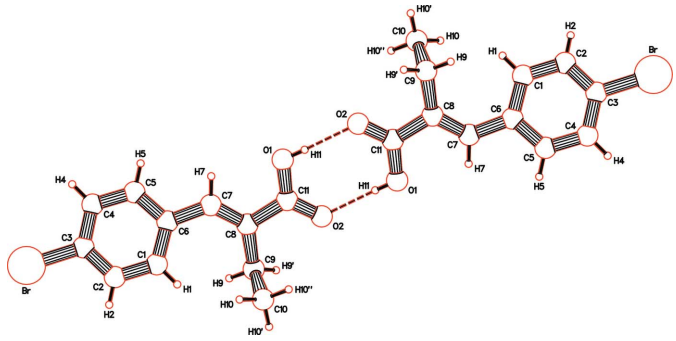


Figure 2
Perspective drawing of the dimer formed by O—H···O hydrogen bonds, shown as dashed lines.

All H atoms except H11 were included in the riding model approximation, with C—H = 0.95–0.98 and $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.5$ for methyl and $x = 1.2$ for other H atoms. Atom H11 was located in a difference Fourier map and refined freely with an isotropic displacement parameter.

Data collection: *SMART* (Bruker, 2006); cell refinement: *SAINT-Plus* (Bruker, 2006); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2006); program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLUTO* (Meetsma, 2007) and *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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References

Allen, F. H., Kennard, O., Waston, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Beurskens, P. T., Beurskens, G., de Gelder, R., García-Granda, S., Gould, R. O., Israël, R. & Smits, J. M. M. (1999). *The DIRDIF99 Program System.* Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.
Bruker, (2006). *SMART*, *SAINT-Plus* and *XPREP*. Bruker AXS Inc., Madison, Wisconsin, USA.
Forgó, P., Felföldi, K. & Pálinkó, I. (2005). *J. Mol. Struct.* **744–747**, 273–276.
Gensler, W. J. & Berman, E. (1958). *J. Am. Chem. Soc.* **80**, 4949–4954.
Meetsma, A. (2007). Extended version of the program *PLUTO*. University of Groningen, The Netherlands. (Unpublished.)
Nodiff, E. A., Tanabe, K., Seyfried, C., Matsuura, S., Kondo, Y., Chen, E. H. & Tyagi, M. P. (1971). *J. Med. Chem.* **14**, 921–925.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2001). *SADABS*. Version 2.03. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.