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3-(4-Hydroxy-3-methoxy-2-nitrophenyl)acrylic acid

Chun-Nian Xia, Wei-Xiao Hu* and Wei Zhou

College of Pharmaceutical Science, Zhejiang University of Technology, Hangzhou 310032, People's Republic of China

Correspondence e-mail: huyang@mail.hz.zj.cn

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Key indicators

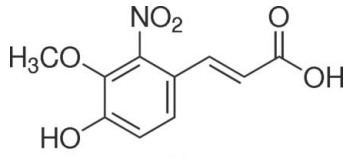
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.095
wR factor = 0.243
Data-to-parameter ratio = 12.2

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

The title compound, $C_{10}H_9NO_6$, has an *E* configuration, with the carboxyl group and the benzene ring located on opposite sides of the C=C bond. Intermolecular O—H···O hydrogen bonding helps to stabilize the crystal structure.

Comment

Caffeic acid and its derivatives have antiatherosclerotic and neuroprotective properties (Son & Lewis, 2002). Also these compounds can inhibit the peroxynitrite-dependent tyrosine nitration (Pannala *et al.*, 1998). As part of our ongoing research on caffeic acid derivatives (Xia & Hu, 2005), we present here the structure of the title compound, (I).



(I)

The molecular structure of (I) is illustrated in Fig. 1. The molecule has an *E* configuration, with the carboxyl group and the benzene ring located on opposite sides of the C7=C8 bond. The nitro group is twisted by 60.66 (18)° with respect to the benzene ring. Intermolecular O—H···O hydrogen bonding occurs in the crystal structure (Table 1).

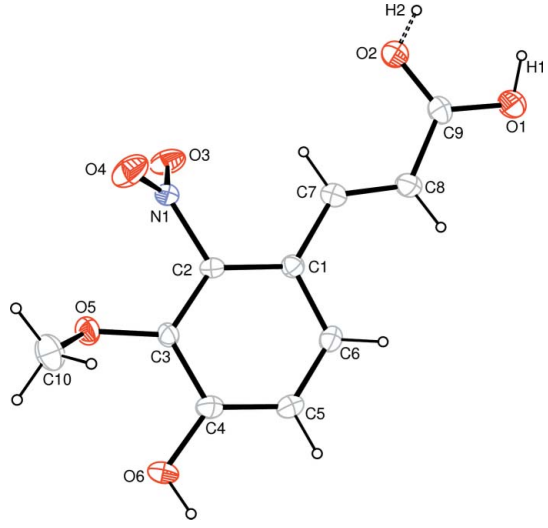


Figure 1
The structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). The dashed line indicates one of the disordered components.

Experimental

Compound (I) was synthesized according to the method reported by Grenier *et al.* (2000). Single crystals were obtained by slow evaporation of a methanol/water solution (1:1).

Crystal data

$C_{10}H_9NO_6$
$M_r = 239.18$
Monoclinic, $P2_1/c$
$a = 3.8710\ (14)$ Å
$b = 8.049\ (5)$ Å
$c = 34.342\ (5)$ Å
$\beta = 90.03\ (2)^\circ$
$V = 1070.0\ (8)$ Å^3
$Z = 4$
$D_x = 1.485$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.13$ mm^{-1}
$T = 298\ (2)$ K
Prism, light yellow
$0.15 \times 0.10 \times 0.05$ mm

Data collection

Bruker SMART1000 CCD diffractometer
φ and ω scans
Absorption correction: none
4259 measured reflections
1885 independent reflections
1477 reflections with $I > 2\sigma(I)$
$R_{int} = 0.127$
$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.095$
$wR(F^2) = 0.243$
$S = 1.10$
1885 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0647P)^2 + 3.1253P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.89	1.80	2.670 (6)	164
O2—H2···O1^{i}	0.92	1.76	2.670 (6)	171
O6—H6A···O3^{ii}	0.84	2.01	2.847 (5)	171

Symmetry codes: (i) $-x+2, -y+2, -z$; (ii) $x, y-1, z$.

The carboxyl group is disordered over two sites; in a difference Fourier map two peaks were found at positions near to both O1 and O2. They were set as H1 and H2 with each having 0.5 occupancy. The hydroxy H was also located in a difference Fourier map. H atoms bonded to O atoms were refined as riding in their as-found relative positions, with $U_{iso}(H) = 1.5U_{eq}(O)$. Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and the torsion angle was refined to fit the electron density, with $U_{iso}(H) = 1.5U_{eq}(C)$. Other H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined in riding mode, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1999); software used to prepare material for publication: *SHELXL97*.

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