organic papers

2-Cyano-3-(4-hydroxyphenyl)propenoic acid

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The title compound, $C_{10}H_7NO_3$, has the cyano, carboxylic acid
and phenol groups in a *trans* configuration with respect to the
C=C double bond. Intramolecular O—H···N and eight-
membered O—H···O hydrogen-bonding interactions form an
infinite two-dimensional layer structure.

Comment

2-Cyano-3-(4-hydroxyphenyl)propenoic acid (or α-cyano-4-
hydroxycinnamic acid), (I), is a very useful intermediate for
organic synthesis, especially for preparing some esters (Kim *et
al.*, 1988; Cho *et al.*, 1991; Takagi *et al.*, 1992). It can also be
used as the lactate transport inhibitor, increasing the magni-
tude of the acidification and resulting in a significantly faster
reduction in tone in response to hypoxia (Otter & Austin,
1999; Coss *et al.*, 2003). More importantly, (I) is a typical
matrix material for research into matrix-assisted laser deso-
rption/ionization time-of-flight mass spectra (MALDI–
TOFMS), because it has a conjugated π-system which can
absorb the energy of the laser and help to ionize the sample.
Although several of its derivatives have been structurally
elucidated (Voznyi *et al.*, 1992; He *et al.*, 1993; Shi *et al.*, 1993,
2002; Nesterov *et al.*, 2001), its crystal structure has not been
described. In this communication, we report the crystal
structure of (I).

(I)
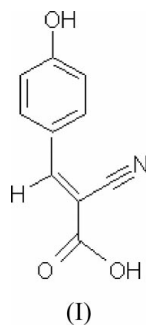
The atom-numbering scheme of the title compound is
shown in Fig. 1, while selected bond distances and angles are
given in Table 1. The geometries of the phenol ring and
carboxylic acid group are in the normal ranges. The phenol
and carboxylic acid groups adopt a *trans* orientation with
respect to the C=C double bond (C2=C3), with angles of
C1—C2—C3 = 120.6 (2)° and C2—C3—C5 = 132.9 (2)°. The
linear cyano group [N1—C4—C2 = 176.6 (2)°] and one H
atom occupy the other two positions [C3—C2—C4 =
125.2 (2)° and C2—C3—H3*A* = 114°]. All atoms in (I) are
almost coplanar, with a mean deviation of 0.0377 (1) Å.

Hydrogen-bonding interactions are the most remarkable
structural feature of (I). In its crystal packing, O—H···N and
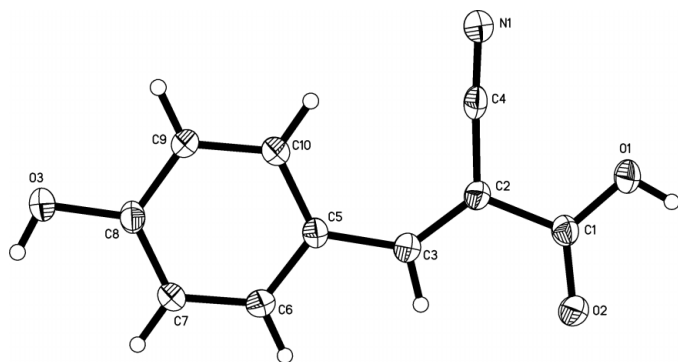
Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering scheme.

O—H···O hydrogen-bonding interactions are observed (Table 2). The former stems from the cyano N atom and a neighboring phenol H atom, whilst the latter comes from two vicinal carboxylic acid groups, forming an eight-membered O—H···O hydrogen-bonding ring. With the assistance of these crosslinked supramolecular contacts, an infinite two-dimensional layer structure is formed (Fig. 2). All layers in the crystal structure are parallel with a short separation of 3.08 (2) Å *via* van der Waals packing interactions; there are no π–π stacking interactions between the aromatic rings.

Experimental

The title compound was purchased from Aldrich. Yellow crystals suitable for X-ray analysis were grown from a solution in ethanol and a small amount of water (5:1). The UV–vis spectrum of the title compound gives a maximum absorbance at 337.5 nm in ethanol corresponding to the conjugated π–π^* transition.

Crystal data

$C_{10}H_7NO_3$	$D_x = 1.448$ Mg m^{-3}
$M_r = 189.17$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2966
$a = 5.839$ (2) Å	reflections
$b = 9.498$ (3) Å	$\theta = 3.4$–$27.5°$
$c = 15.663$ (5) Å	$\mu = 0.11$ mm^{-1}
$\beta = 92.76$ (2)°	$T = 296$ (2) K
$V = 867.6$ (5) Å^3	Block, yellow
$Z = 4$	$0.30 \times 0.30 \times 0.20$ mm

Data collection

Rigaku Mercury CCD area-detector diffractometer	1513 independent reflections
	1415 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.067$
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)	$\theta_{max} = 25.0°$
	$h = -6 \rightarrow 6$
$T_{min} = 0.969$, $T_{max} = 0.977$	$k = -10 \rightarrow 11$
7176 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0104P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.058$	$+ 1.0945P]$
$wR(F^2) = 0.115$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{max} < 0.001$
1513 reflections	$\Delta\rho_{max} = 0.18$ e Å^{-3}
129 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
H-atom parameters constrained	
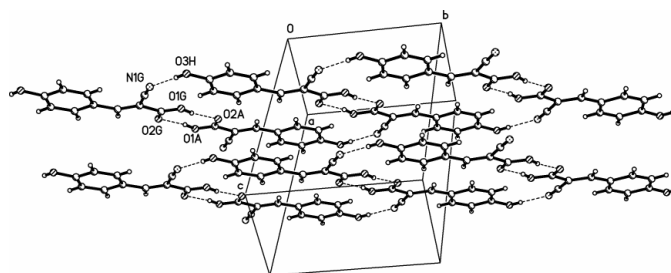
Figure 2
A perspective view of the infinite hydrogen-bond-sustained one-dimensional chain of dimers of (I). For clarity, labels are given only once for the hydrogen-bond contacts. Hydrogen bonds are shown as dashed lines.

Table 1
Selected geometric parameters (Å, °).

C1—O2	1.262 (3)	C2—C4	1.431 (3)
C1—O1	1.267 (3)	C3—C5	1.435 (3)
C1—C2	1.477 (3)	C4—N1	1.147 (3)
C2—C3	1.346 (3)	C8—O3	1.354 (3)
O2—C1—O1	124.3 (2)	C4—C2—C1	114.17 (19)
O2—C1—C2	119.0 (2)	C2—C3—C5	132.9 (2)
O1—C1—C2	116.7 (2)	N1—C4—C2	176.6 (2)
C3—C2—C4	125.2 (2)	O3—C8—C7	123.2 (2)
C3—C2—C1	120.6 (2)	O3—C8—C9	116.8 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1B···O2^i	0.82	1.79	2.600 (2)	168
O3—H3···N1^{ii}	0.82	2.03	2.853 (3)	178

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

All H atoms were positioned geometrically (C—H = 0.93 Å and O—H = 0.82 Å) and refined as riding, with U_{iso}(H) = $1.2U_{eq}$(C) or $1.5U_{eq}$(O).

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *TEXSAN* (Molecular Structure Corporation & Rigaku, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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