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

Michael Karas,[a] Isabelle Fournier[a] and Michael Bolte[b]*

[a]Institut für Pharmazeutische Chemie, Instrumentelle Analytische Chemie, J. W. Goethe-Universität Frankfurt, Marie-Curie-Str. 9-11, 60439 Frankfurt/Main, Germany, and [b]Institut für Organische Chemie, J. W. Goethe-Universität Frankfurt, Marie-Curie-Str. 11, 60439 Frankfurt/Main, Germany

Correspondence e-mail: bolte@chemie.uni-frankfurt.de

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.001 Å
Disorder in main residue
R factor = 0.032
wR factor = 0.093
Data-to-parameter ratio = 14.2

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

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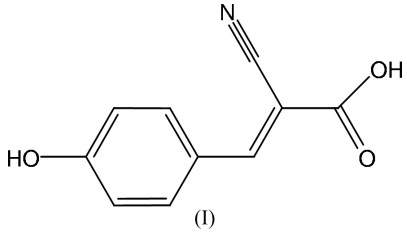
The title compound, $C_{10}H_7NO_3$, has an almost planar molecule, forming hydrogen-bonded dimers *via* the carboxyl groups. These dimers are further connected by hydrogen bonds between the hydroxy groups of the benzene rings and the cyano N atoms into ribbons, which are arranged in layers. The H atom of the carboxyl group is disordered over two sites.

Comment

The title compound (Fig. 1) has an almost planar molecule (the r.m.s. deviation for all non-H atoms is 0.053 Å). Two molecules form centrosymmetric hydrogen-bonded dimers *via* the carboxyl groups. These dimers are further connected into ribbons (Fig. 2) *via* hydrogen bonds between the hydroxy groups on the benzene rings and the cyano N atoms. These ribbons are arranged into layers perpendicular to [103] so that a two-dimensional structure is formed (Fig. 3). The interplanar distance is 3.12 Å.



(I)

Experimental

The title compound was prepared according to the procedure described by Karchgaudhuri *et al.* (2002).

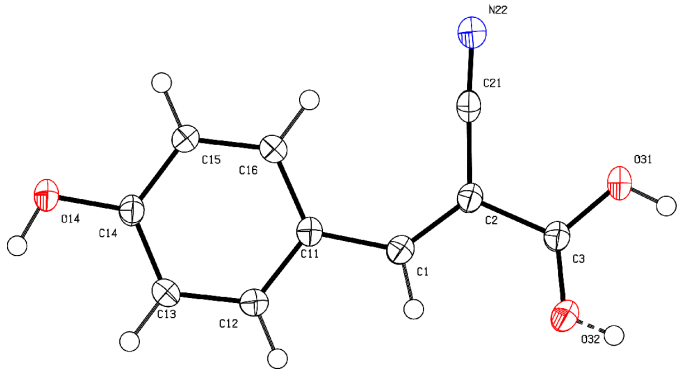


Figure 1
Perspective view of the title compound, with the atom numbering; displacement ellipsoids are shown at the 50% probability level. The bond of the disordered H atom with the minor site occupation factor is drawn with a broken line.

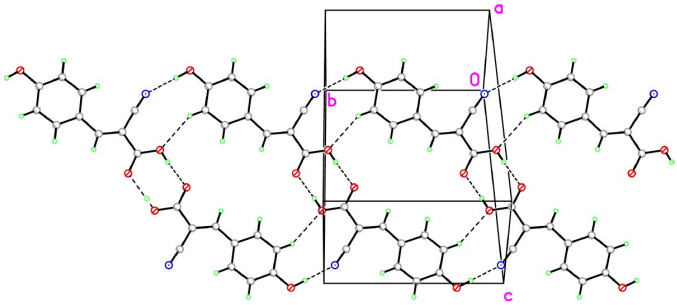


Figure 2
Packing diagram. View along [103]; only the major occupied site of the disordered hydroxy H atom is shown. Hydrogen bonding is indicated by broken lines.

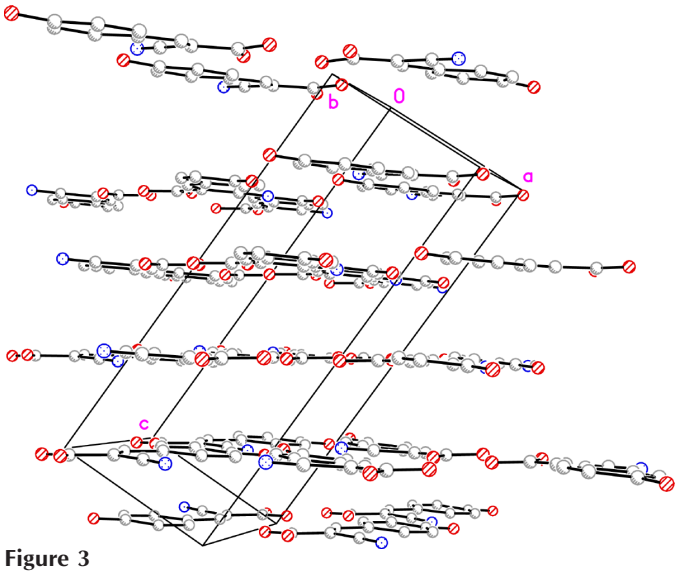


Figure 3
Packing diagram. View approximately on to the *ac* plane. H atoms have been omitted.

Crystal data

$C_{10}H_7NO_3$
M_r = 189.17
Monoclinic, $P2_1/c$
a = 5.8182 (5) Å
b = 9.5061 (7) Å
c = 15.461 (1) Å
β = 93.890 (6)°
V = 853.15 (11) Å^3
Z = 4
D_x = 1.473 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 508 reflections
θ = 3.4–20.9°
μ = 0.11 mm^{-1}
T = 173 (2) K
Block, yellow
0.52 × 0.48 × 0.32 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: none
12 012 measured reflections
1986 independent reflections
1798 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 28.7°
$h = -7 \rightarrow 7$
$k = -12 \rightarrow 11$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.093
S = 1.05
1986 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 0.1987P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected bond lengths (Å).

C1—C2	1.3551 (14)	C21—N22	1.1503 (14)
C2—C21	1.4309 (13)	C3—O32	1.2510 (12)
C2—C3	1.4831 (12)	C3—O31	1.2842 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
O14—H14···N22^{i}	0.910 (17)	1.934 (17)	2.8435 (12)	177.2 (15)
O31—H31···O32^{ii}	0.81 (3)	1.79 (3)	2.5967 (10)	176 (2)
O32—H32···O31^{ii}	0.83 (6)	1.77 (6)	2.5967 (10)	173 (4)

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

All H atoms were found in a difference map. Those bonded to C atoms were refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C)] using a riding model with $C_{aromatic}$—H = 0.95 Å, H atoms bonded to O atoms were refined freely. The H atom of the carboxyl group is disordered over two sites. The ratio of the site occupation factors of the disordered H atoms refined to 0.63 (5)/0.37 (5).

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *XP* in *SHELXTL* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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