Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-[(4-Formylphenyl)(hydroxy)methyl]-acrylonitrile

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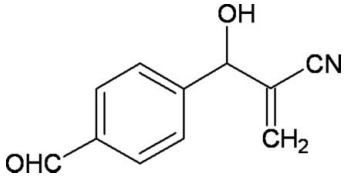
Received 5 July 2011; accepted 22 July 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.137; data-to-parameter ratio = 21.7.

In the title compound, $C_{11}H_9NO_2$, the mean planes formed by the phenyl and acryl group are almost orthogonal to each other, with a dihedral angle of 88.61 (7)°. The carbonitrile side chain is almost linear, the C—C—N angle being 179.54 (16)°. In the crystal, molecules are linked by intermolecular O—H···O interactions into infinite chains running parallel to the b axis.

Related literature

For uses of acrylonitrile derivatives, see: Ohsumi *et al.* (1998). For related structures, see: Cobo *et al.* (2005); Nizam Mohideen *et al.* (2007).



Experimental

Crystal data

$C_{11}H_9NO_2$
M_r = 187.19
Monoclinic, $P2_1/n$
a = 7.6089 (5) Å
b = 6.0895 (3) Å
c = 20.5135 (14) Å
β = 93.615 (2)°
V = 948.59 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
12108 measured reflections
2778 independent reflections
2109 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.137
S = 1.04
2778 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.82	1.99	2.8107 (15)	175

Symmetry code: (i) $x+1, y-1, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

CMS and KS thank Dr Babu Varghese, SAIF, IIT, Chennai, India, for the X-ray intensity data collection and Dr V. Murugan, Head of the Department of Physics, for providing facilities in the department to carry out this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2428).

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supporting information

Acta Cryst. (2011). E**67**, o2176 [doi:10.1107/S160053681102976X]

2-[(4-Formylphenyl)(hydroxy)methyl]acrylonitrile

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S1. Comment

Acrylonitrile derivatives have been shown to possess antitubercular and antitumour activities (Ohsumi *et al.*, 1998).

In the title compound (Fig. 1), the mean planes formed by the phenyl ring C2—C7 and acryl group (N1/C8—C11) are almost orthogonal to each other with a dihedral angle 88.61 (7)°. The bond length C9—C11 [1.4338 (18) Å] is significantly shorter than the expected value for a C—C single bond because of conjugation effects (Nizam Mohideen *et al.*, 2007). The mean plane of C2—C1—O1 is slightly twisted out of the mean plane of phenyl ring C2—C7 with a dihedral angle 2.62 (9)°. The carbonitrile side chain (C9—C11—N1) is almost linear, with the angle around central carbon atom being 179.54 (16)°. The title compound exhibits structural similarities with closely related structures (Cobo *et al.*2005, Nizam Mohideen *et al.*2007).

In the title compound, the crystal packing is stabilized by O2—H2···O1 intermolecular interactions which link the molecules into infinite chains running parallel to the *b*-axis (Tab. 1 & Fig. 2).

S2. Experimental

To a reaction mixture of terephthalaldehyde (1 mmol) and acrylonitrile (2 mmol) was added a catalytic quantity of 1,4-diazabicyclo[2.2.2]octane (10–15 mol %). The reaction mixture was left standing at room temperature in a stoppered sample flask. The progress of the reaction was monitored by Thin Layer Chromatography (TLC) over a period of several days. After 6 days the TLC revealed the presence of a product. The reaction mixture was dissolved in ethyl acetate and washed with aqueous HCl solution (0.25 *M*) and water followed by brine solution. The organic layer was separated and dried over sodium sulfate, filtering and evaporation of the organic solvent under reduced pressure. The product was seperated by flash column chromatography using hexane and ethyl acetate (4:1) as an eluent to give colorless solid. The product was dissolved in chloroform and heated for two minutes. The resulting solution was subjected to crystallization by slow evaporation of the solvent resulting in single crystals suitable for XRD studies.

S3. Refinement

The hydrogen atoms were placed in calculated positions with C—H = 0.93 to 0.98 Å and O—H = 0.82 Å and refined in the riding model with isotropic displacement parameters: U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O).

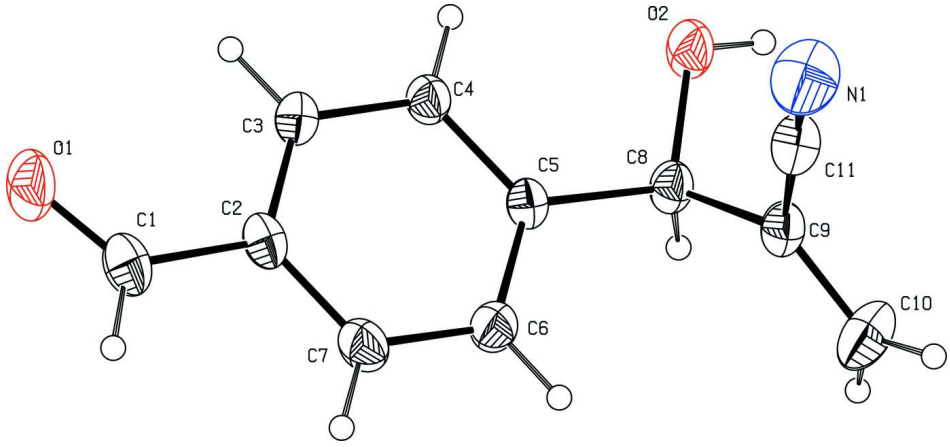

Figure 1

The molecular structure of the title compound showing 30% probability displacement ellipsoids.

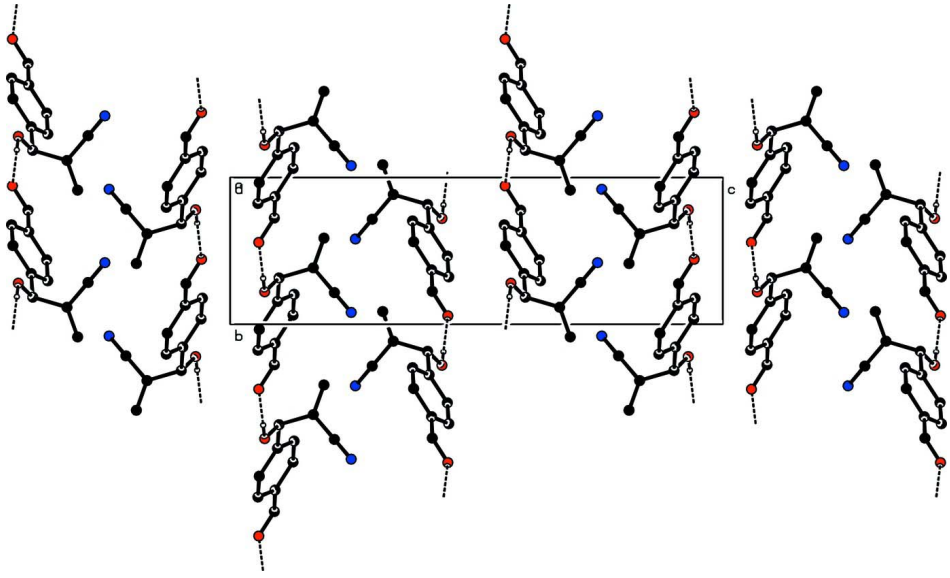

Figure 2

A view of the unit cell of the title compound viewed down *a*-axis; O—H···O intermolecular interactions are indicated by dashed lines.

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Crystal data

$C_{11}H_9NO_2$
$M_r = 187.19$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.6089\ (5)$ Å
$b = 6.0895\ (3)$ Å
$c = 20.5135\ (14)$ Å
$\beta = 93.615\ (2)°$
$V = 948.59\ (10)$ Å^3
$Z = 4$

$F(000) = 392$
$D_x = 1.311$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2778 reflections
$\theta = 2.0–30.1°$
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
12108 measured reflections
2778 independent reflections
2109 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 30.1°$, $\theta_{min} = 2.0°$
$h = -10 \rightarrow 10$
$k = -8 \rightarrow 5$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.137$
$S = 1.04$
2778 reflections
128 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.068P)^2 + 0.1498P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.29788 (17)	1.2762 (2)	0.08969 (7)	0.0530 (3)
H1	0.2060	1.2372	0.1152	0.064*
C2	0.45120 (15)	1.1299 (2)	0.09117 (6)	0.0402 (3)
C3	0.59636 (15)	1.17738 (19)	0.05636 (6)	0.0403 (3)
H3	0.5982	1.3042	0.0312	0.048*
C4	0.73929 (15)	1.03554 (19)	0.05910 (6)	0.0377 (3)
H4	0.8374	1.0683	0.0361	0.045*
C5	0.73630 (14)	0.84482 (18)	0.09612 (5)	0.0341 (2)
C6	0.58917 (16)	0.7961 (2)	0.12973 (6)	0.0440 (3)
H6	0.5855	0.6670	0.1538	0.053*
C7	0.44760 (16)	0.9386 (2)	0.12758 (6)	0.0473 (3)
H7	0.3496	0.9059	0.1507	0.057*
C8	0.88910 (15)	0.68441 (19)	0.09921 (6)	0.0386 (3)
H8	0.8530	0.5530	0.0742	0.046*
C9	0.94025 (16)	0.6160 (2)	0.16879 (6)	0.0416 (3)
C10	0.9246 (2)	0.4136 (2)	0.19036 (8)	0.0658 (4)
H10A	0.9592	0.3799	0.2335	0.079*

H10B	0.8788	0.3045	0.1625	0.079*
C11	1.01071 (18)	0.7847 (2)	0.21163 (7)	0.0499 (3)
N1	1.0657 (2)	0.9196 (3)	0.24571 (8)	0.0783 (4)
O1	0.28115 (14)	1.44271 (18)	0.05813 (6)	0.0647 (3)
O2	1.03273 (12)	0.77961 (17)	0.07008 (5)	0.0550 (3)
H2	1.1103	0.6874	0.0670	0.083*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0386 (6)	0.0578 (8)	0.0626 (8)	0.0154 (6)	0.0044 (6)	−0.0036 (6)
C2	0.0328 (5)	0.0454 (6)	0.0420 (6)	0.0090 (4)	−0.0012 (4)	−0.0055 (5)
C3	0.0394 (6)	0.0378 (6)	0.0434 (6)	0.0073 (4)	−0.0005 (5)	0.0030 (5)
C4	0.0336 (5)	0.0409 (6)	0.0390 (6)	0.0055 (4)	0.0047 (4)	0.0040 (4)
C5	0.0326 (5)	0.0371 (5)	0.0326 (5)	0.0067 (4)	0.0007 (4)	−0.0005 (4)
C6	0.0402 (6)	0.0457 (6)	0.0466 (7)	0.0051 (5)	0.0073 (5)	0.0104 (5)
C7	0.0337 (6)	0.0579 (7)	0.0512 (7)	0.0058 (5)	0.0099 (5)	0.0057 (6)
C8	0.0390 (6)	0.0381 (5)	0.0389 (6)	0.0101 (4)	0.0055 (4)	0.0029 (4)
C9	0.0417 (6)	0.0405 (6)	0.0426 (6)	0.0102 (5)	0.0018 (5)	0.0033 (5)
C10	0.0954 (12)	0.0465 (8)	0.0535 (8)	0.0048 (8)	−0.0100 (8)	0.0109 (6)
C11	0.0546 (7)	0.0469 (7)	0.0476 (7)	0.0105 (6)	−0.0009 (6)	0.0022 (5)
N1	0.0984 (12)	0.0638 (8)	0.0706 (9)	0.0003 (8)	−0.0120 (8)	−0.0121 (7)
O1	0.0556 (6)	0.0605 (6)	0.0781 (7)	0.0279 (5)	0.0057 (5)	0.0043 (5)
O2	0.0419 (5)	0.0599 (6)	0.0653 (6)	0.0204 (4)	0.0195 (4)	0.0194 (5)

Geometric parameters (Å, º)

C1—O1	1.2055 (18)	C6—H6	0.9300
C1—C2	1.4664 (16)	C7—H7	0.9300
C1—H1	0.9300	C8—O2	1.4036 (15)
C2—C3	1.3829 (17)	C8—C9	1.5139 (16)
C2—C7	1.3853 (18)	C8—H8	0.9800
C3—C4	1.3871 (15)	C9—C10	1.3173 (18)
C3—H3	0.9300	C9—C11	1.4338 (18)
C4—C5	1.3887 (15)	C10—H10A	0.9300
C4—H4	0.9300	C10—H10B	0.9300
C5—C6	1.3835 (16)	C11—N1	1.1410 (19)
C5—C8	1.5168 (14)	O2—H2	0.8200
C6—C7	1.3818 (17)		
O1—C1—C2	125.37 (14)	C6—C7—C2	120.24 (11)
O1—C1—H1	117.3	C6—C7—H7	119.9
C2—C1—H1	117.3	C2—C7—H7	119.9
C3—C2—C7	119.84 (10)	O2—C8—C9	110.75 (10)
C3—C2—C1	121.51 (12)	O2—C8—C5	109.36 (9)
C7—C2—C1	118.64 (12)	C9—C8—C5	111.56 (9)
C2—C3—C4	119.92 (11)	O2—C8—H8	108.4
C2—C3—H3	120.0	C9—C8—H8	108.4

C4—C3—H3	120.0	C5—C8—H8	108.4
C3—C4—C5	120.20 (11)	C10—C9—C11	120.17 (13)
C3—C4—H4	119.9	C10—C9—C8	123.43 (12)
C5—C4—H4	119.9	C11—C9—C8	116.39 (11)
C6—C5—C4	119.58 (10)	C9—C10—H10A	120.0
C6—C5—C8	118.90 (10)	C9—C10—H10B	120.0
C4—C5—C8	121.50 (10)	H10A—C10—H10B	120.0
C7—C6—C5	120.20 (11)	N1—C11—C9	179.54 (16)
C7—C6—H6	119.9	C8—O2—H2	109.5
C5—C6—H6	119.9		

O1—C1—C2—C3	1.9 (2)	C3—C2—C7—C6	0.60 (19)
O1—C1—C2—C7	−177.02 (14)	C1—C2—C7—C6	179.52 (12)
C7—C2—C3—C4	−1.32 (18)	C6—C5—C8—O2	−171.48 (11)
C1—C2—C3—C4	179.80 (11)	C4—C5—C8—O2	10.23 (15)
C2—C3—C4—C5	0.69 (18)	C6—C5—C8—C9	−48.61 (15)
C3—C4—C5—C6	0.66 (17)	C4—C5—C8—C9	133.09 (11)
C3—C4—C5—C8	178.94 (10)	O2—C8—C9—C10	−122.89 (15)
C4—C5—C6—C7	−1.38 (19)	C5—C8—C9—C10	115.05 (15)
C8—C5—C6—C7	−179.71 (11)	O2—C8—C9—C11	56.40 (14)
C5—C6—C7—C2	0.8 (2)	C5—C8—C9—C11	−65.67 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.82	1.99	2.8107 (15)	175

Symmetry code: (i) *x*+1, *y*−1, *z*.