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(*E*)-2-Bromomethyl-3-(*o*-tolyl)acrylonitrile

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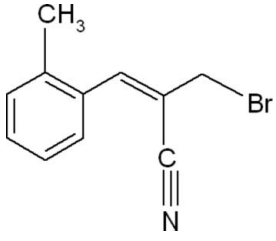
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.035; wR factor = 0.085; data-to-parameter ratio = 16.5.

The title compound $C_{11}H_{10}BrN$, has an *E* conformation at the C=C bond of the acrylonitrile unit. The vinyl group makes a dihedral angle of 44.53 (12)° with the benzene ring. In the crystal, weak C—H···π interactions involving the benzene ring are observed.

Related literature

For the biological activity of cyanoacrylates, see: Zhang *et al.* (2009); Obniska *et al.* (2005); For related structures, see: Ye *et al.* (2009); Suresh *et al.* (2012).



Experimental

Crystal data

$C_{11}H_{10}BrN$
M_r = 236.11
Monoclinic, $P2_1/n$
a = 7.5473 (8) Å
b = 11.7362 (10) Å
c = 11.5228 (11) Å
β = 96.436 (3)°
V = 1014.22 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.00 mm^{-1}
T = 295 K
0.20 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.435, T_{max} = 0.535
8718 measured reflections
1960 independent reflections
1261 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.085
S = 1.00
1960 reflections
119 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C6 ring

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···*Cg*1^{i}	0.93	2.97	3.654 (7)	131
C11—H11*B*···*Cg*1^{ii}	0.96	2.86	3.699 (1)	146

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

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

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2587).

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supplementary materials

Acta Cryst. (2013). E**69**, o1367 [doi:10.1107/S1600536813021041]

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J. Kanchanadevi, G. Anbalagan, R. Selvakumar, M. Bakthadoss, B. Gunasekaran and V. Manivannan

Comment

Cyanoacrylates and its derivatives have been widely used as agrochemicals (Zhang *et al.*, 2009) and are an important intermediate in drug synthesis (Obniska *et al.*, 2005).

The geometric parameters of the title molecule (Fig. 1) agree well with reported similar structure (Ye *et al.*, 2009; Suresh *et al.*, 2012). The vinyl group makes a dihedral angle of 44.53 (12) ° with the benzene ring. The acrylonitrile (C7–C8) and cyano (C9–N1) groups deviate from the mean plane of the benzene (C1–C6) ring.

The crystal packing is controlled by weak C—H···π [C7—H7···*Cg*1(1 - *x*, -*y*, 1 - *z*) distance of 3.654 (7) Å, C11—H11B···*Cg*1(2 - *x*, -*y*, 1 - *z*) distance of 3.699 (1) Å, (*Cg*1 is the centroid of the ring defined by the atoms C1—C6)] interactions.

Experimental

To a stirred solution of 2-[hydroxy(*o*-tolyl)methyl]acrylonitrile (1 equivalent) in dichloromethane (DCM) was added a 48% hydrobromic acid (2 equivalent) solution and then a concentrated sulfuric acid solution (catalytic amount) at 273 K. After stirring overnight at room temperature, the mixture was diluted with DCM and water. The aqueous phase was extracted twice with DCM. The combined organic phase was washed twice with water an then dried with sodiumsulfate. Removal of the solvent led to the crude product which was purified through a pad of silica gel (100–200 mesh) using ethylacetate and hexanes (1:9) as solvents. The pure title compound was obtained as a colorless solid (yield 90%; m.p. 383-387 K).

Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic C—H, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for CH_2 and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for CH_3.

Computing details

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

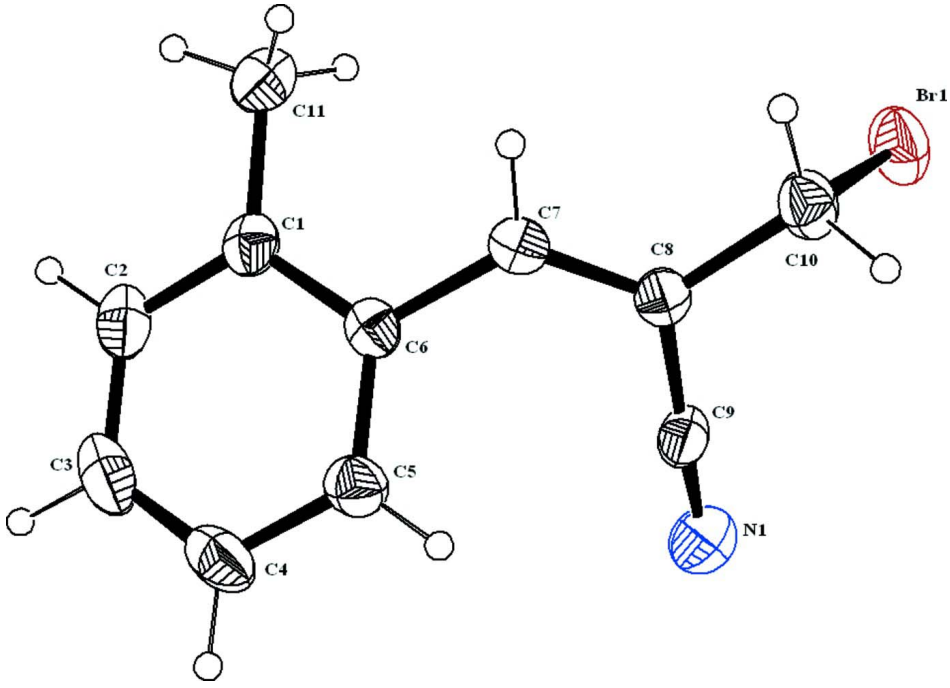

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

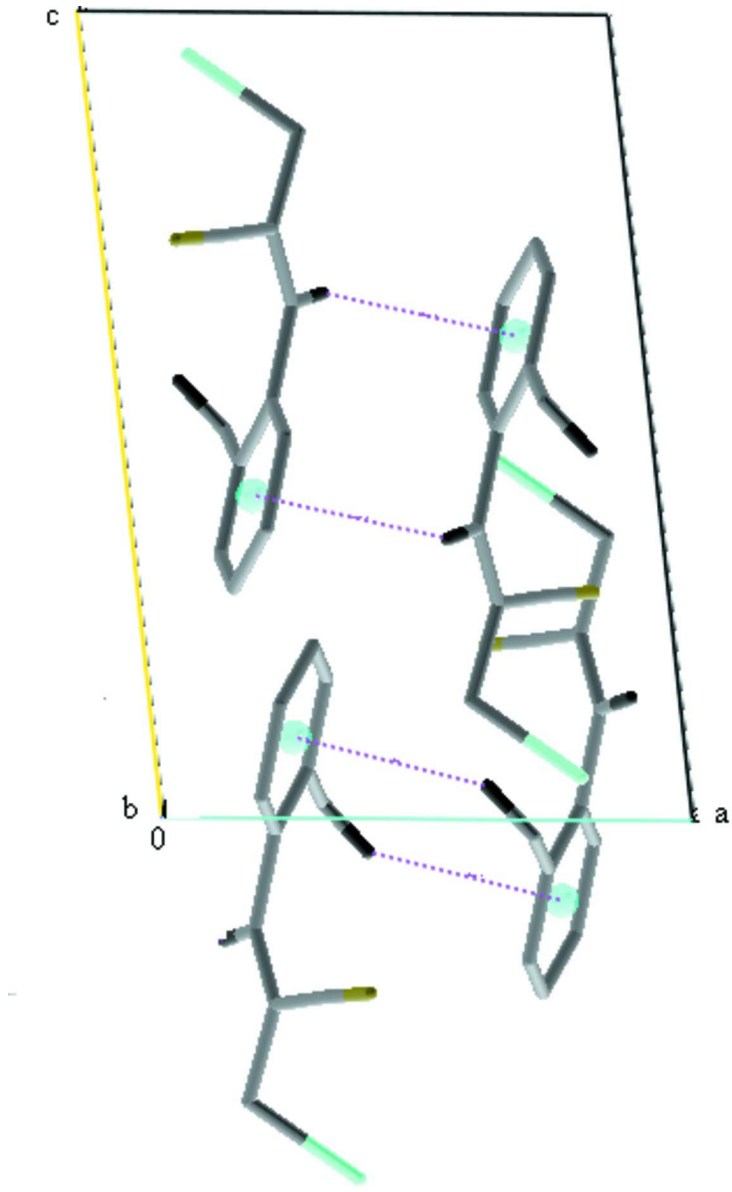

Figure 2

The packing diagram showing C-H···π interactions as dashed lines.

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Crystal data

$C_{11}H_{10}BrN$
$M_r = 236.11$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.5473\ (8)$ Å
$b = 11.7362\ (10)$ Å
$c = 11.5228\ (11)$ Å
$\beta = 96.436\ (3)°$
$V = 1014.22\ (17)$ Å^3
$Z = 4$

$F(000) = 472$
$D_x = 1.546$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1980 reflections
$\theta = 2.5–25.8°$
$\mu = 4.00$ mm^{-1}
$T = 295$ K
Block, colourless
0.20 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.435, T_{max} = 0.535
8718 measured reflections
1960 independent reflections
1261 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 25.9°, θ_{min} = 2.5°
h = −9→9
k = −14→13
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.085
S = 1.00
1960 reflections
119 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
$w = 1/[\sigma^2(F_o^2) + (0.036P)^2 + 0.5483P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.7824 (4)	−0.0112 (3)	0.5604 (3)	0.0451 (8)
C2	0.8374 (5)	0.0182 (4)	0.6742 (3)	0.0587 (10)
H2	0.8886	−0.0372	0.7252	0.070*
C3	0.8186 (5)	0.1269 (4)	0.7146 (3)	0.0702 (12)
H3	0.8563	0.1443	0.7922	0.084*
C4	0.7448 (5)	0.2096 (4)	0.6414 (3)	0.0634 (11)
H4	0.7307	0.2831	0.6691	0.076*
C5	0.6911 (5)	0.1840 (3)	0.5260 (3)	0.0508 (9)
H5	0.6417	0.2406	0.4759	0.061*
C6	0.7101 (4)	0.0752 (3)	0.4843 (3)	0.0398 (8)
C7	0.6525 (4)	0.0464 (3)	0.3617 (3)	0.0411 (7)
H7	0.5936	−0.0227	0.3480	0.049*
C8	0.6760 (4)	0.1091 (3)	0.2682 (2)	0.0410 (8)
C9	0.7740 (5)	0.2128 (3)	0.2782 (3)	0.0496 (9)
C10	0.6063 (5)	0.0732 (3)	0.1480 (3)	0.0530 (9)
H10A	0.5312	0.1331	0.1112	0.064*
H10B	0.5336	0.0055	0.1521	0.064*
C11	0.8037 (5)	−0.1309 (3)	0.5196 (3)	0.0582 (9)
H11A	0.8550	−0.1767	0.5838	0.087*
H11B	0.8807	−0.1316	0.4587	0.087*
H11C	0.6892	−0.1611	0.4903	0.087*
N1	0.8572 (5)	0.2944 (3)	0.2831 (3)	0.0750 (10)
Br1	0.79897 (5)	0.04122 (4)	0.05323 (3)	0.07015 (19)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0373 (19)	0.053 (2)	0.0457 (18)	−0.0111 (16)	0.0080 (14)	0.0050 (16)
C2	0.057 (2)	0.076 (3)	0.0429 (19)	−0.011 (2)	0.0049 (17)	0.0097 (18)
C3	0.071 (3)	0.101 (4)	0.039 (2)	−0.023 (3)	0.0111 (19)	−0.011 (2)
C4	0.069 (3)	0.069 (3)	0.057 (2)	−0.013 (2)	0.026 (2)	−0.022 (2)
C5	0.053 (2)	0.050 (2)	0.052 (2)	−0.0022 (17)	0.0165 (16)	−0.0044 (16)
C6	0.0321 (17)	0.049 (2)	0.0398 (16)	−0.0060 (14)	0.0106 (14)	−0.0021 (14)
C7	0.0353 (17)	0.043 (2)	0.0452 (17)	0.0012 (15)	0.0058 (14)	−0.0036 (15)
C8	0.0381 (18)	0.043 (2)	0.0412 (17)	0.0057 (16)	0.0041 (14)	0.0000 (15)
C9	0.062 (2)	0.048 (2)	0.0392 (18)	0.005 (2)	0.0082 (16)	0.0103 (16)
C10	0.051 (2)	0.062 (2)	0.0444 (18)	0.0072 (17)	−0.0035 (15)	−0.0007 (15)
C11	0.055 (2)	0.053 (2)	0.065 (2)	−0.0032 (18)	0.0013 (18)	0.0105 (18)
N1	0.099 (3)	0.059 (2)	0.068 (2)	−0.011 (2)	0.0173 (18)	0.0085 (17)
Br1	0.0798 (3)	0.0886 (4)	0.0435 (2)	0.0105 (2)	0.01345 (18)	−0.00341 (19)

Geometric parameters (Å, º)

C1—C2	1.374 (4)	C7—C8	1.334 (4)
C1—C6	1.409 (4)	C7—H7	0.9300
C1—C11	1.495 (5)	C8—C9	1.422 (5)
C2—C3	1.371 (6)	C8—C10	1.486 (4)
C2—H2	0.9300	C9—N1	1.143 (4)
C3—C4	1.364 (6)	C10—Br1	1.950 (3)
C3—H3	0.9300	C10—H10A	0.9700
C4—C5	1.379 (5)	C10—H10B	0.9700
C4—H4	0.9300	C11—H11A	0.9600
C5—C6	1.378 (4)	C11—H11B	0.9600
C5—H5	0.9300	C11—H11C	0.9600
C6—C7	1.470 (4)		
C2—C1—C6	117.9 (3)	C8—C7—H7	116.6
C2—C1—C11	120.2 (3)	C6—C7—H7	116.6
C6—C1—C11	121.8 (3)	C7—C8—C9	121.4 (3)
C3—C2—C1	121.7 (4)	C7—C8—C10	122.1 (3)
C3—C2—H2	119.2	C9—C8—C10	116.4 (3)
C1—C2—H2	119.2	N1—C9—C8	177.2 (4)
C4—C3—C2	120.2 (3)	C8—C10—Br1	111.6 (2)
C4—C3—H3	119.9	C8—C10—H10A	109.3
C2—C3—H3	119.9	Br1—C10—H10A	109.3
C3—C4—C5	119.8 (4)	C8—C10—H10B	109.3
C3—C4—H4	120.1	Br1—C10—H10B	109.3
C5—C4—H4	120.1	H10A—C10—H10B	108.0
C6—C5—C4	120.5 (3)	C1—C11—H11A	109.5
C6—C5—H5	119.8	C1—C11—H11B	109.5
C4—C5—H5	119.8	H11A—C11—H11B	109.5
C5—C6—C1	119.9 (3)	C1—C11—H11C	109.5
C5—C6—C7	121.1 (3)	H11A—C11—H11C	109.5
C1—C6—C7	119.0 (3)	H11B—C11—H11C	109.5

C8—C7—C6	126.7 (3)		
C6—C1—C2—C3	1.8 (5)	C2—C1—C6—C7	179.2 (3)
C11—C1—C2—C3	−179.6 (3)	C11—C1—C6—C7	0.6 (4)
C1—C2—C3—C4	−0.4 (5)	C5—C6—C7—C8	41.9 (5)
C2—C3—C4—C5	−0.9 (5)	C1—C6—C7—C8	−139.4 (3)
C3—C4—C5—C6	0.5 (5)	C6—C7—C8—C9	3.9 (5)
C4—C5—C6—C1	1.0 (5)	C6—C7—C8—C10	−177.8 (3)
C4—C5—C6—C7	179.6 (3)	C7—C8—C10—Br1	−114.5 (3)
C2—C1—C6—C5	−2.1 (4)	C9—C8—C10—Br1	63.9 (3)
C11—C1—C6—C5	179.3 (3)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1–C6 ring

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···*Cg*1^{i}	0.93	2.97	3.654 (7)	131
C11—H11*B*···*Cg*1^{ii}	0.96	2.86	3.699 (1)	146

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