Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(3-Methoxyphenyl)butanedinitrile

Wan-Xin Du, Yin Ye and Xian-Wen Wei*

College of Chemistry and Materials Science, Anhui Key Laboratory of Functional Molecular Solids, Anhui Normal University, Wuhu 241000, People's Republic of China
Correspondence e-mail: xwwei@mail.ahnu.edu.cn

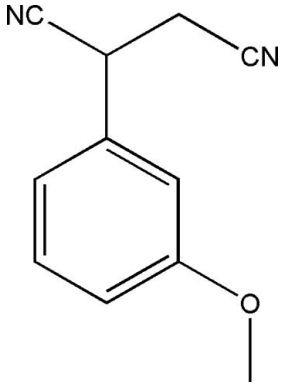
Received 8 April 2009; accepted 23 April 2009

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.128; data-to-parameter ratio = 17.3.

In the title compound, $C_{11}H_{10}N_2O$, the dicyanoethylene portion has an *anti* conformation. The crystal structure features non-classical C—H···N and C—H···O interactions.

Related literature

For the synthesis, see: Johnson *et al.* (1962). The title compound is an intermediate in the synthesis of drugs (Obniska *et al.*, 2005).



Experimental

Crystal data

$C_{11}H_{10}N_2O$
M_r = 186.21
Monoclinic, $P2_1/c$
a = 5.5263 (8) Å
b = 16.105 (2) Å
c = 11.0332 (16) Å
β = 97.179 (2)°
V = 974.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 K
0.4 × 0.2 × 0.1 mm

Data collection

Bruker SMART area-detector diffractometer
Absorption correction: none
8042 measured reflections
2210 independent reflections
1963 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.128
S = 1.04
2210 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···N1^{i}	0.98	2.61	3.4864 (17)	150
C10—H10A···O1^{ii}	0.97	2.38	3.2470 (15)	149
C10—H10B···N2^{iii}	0.97	2.60	3.4823 (18)	151

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x-1, y, z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Science and Technology Fund of Anhui Province for Outstanding Youth (No. 08040106906), the National Natural Science Foundation (No. 20671002) of China, the State Education Ministry (EYTP, SRF for ROCS, SRFDP 20070370001) and the Education Department (No. 2006KJ006TD) of Anhui Province.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2569).

References

Bruker (2000). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Johnson, F., Panella, J. P. & Carlson, A. A. (1962). *J. Org. Chem.* **28**, 2241–2243.
Obniska, J., Jurczyk, S., Zejc, A., Kamiński, K., Tatarczyńska, E. & Stachowicz, K. (2005). *Pharmacol. Rep.* **57**, 170–175.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2009). E**65**, o1165 [doi:10.1107/S1600536809015232]

2-(3-Methoxyphenyl)butanedinitrile

Wan-Xin Du, Yin Ye and Xian-Wen Wei

S1. Comment

The title compound is an important intermediate in drugs synthesis (Obniska *et al.*, 2005). In this paper, we report the structure of the title compound (I). In (I), the succinonitrite moiety adopts an anti conformation. Six atoms of succinonitrite moiety, (N1/C9/C8/N2/C11/C10), almost lie on one plane, the maximum deviations from the mean plane of the succinonitrite being 0.0275 (8) Å. This mean plane is almost perpendicular to the phenyl mean plane with a dihedral angle of 87.55 (6) Å. The crystal packing is stabilized by two intermolecular non-classic C—H···N hydrogen bonds and one intermolecular non-classic C—H···O hydrogen bond.

S2. Experimental

The compound (I) was obtained by reaction of (*Z*)-ethyl-2-cyano-3-(4-methoxyphenyl)acrylate and NaCN in ethanol-water mixture according to the reported method (Johnson *et al.*, 1962). Single crystals suitable for X-ray diffraction were obtained by evaporation of an ethanol solution at room temperature.

S3. Refinement

All non-hydrogen atoms were refined anisotropically. H atoms bonded to C atoms were introduced at calculated positions and refined using a riding model with C—H distances of 0.93–0.97 Å. In all cases, the H-atom U_{iso}(H) is 1.2 times U_{eq} of the parent atom.

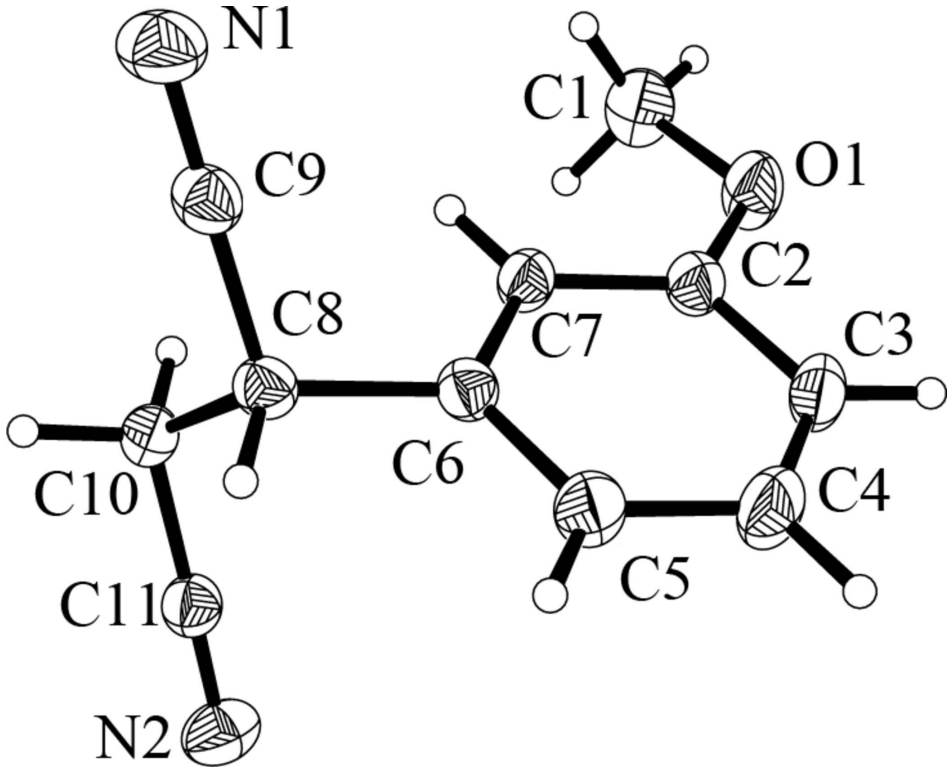


Figure 1

The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

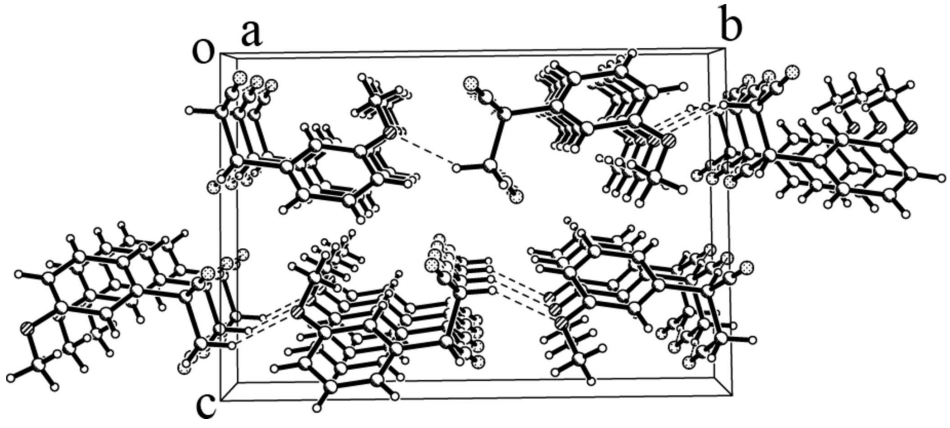


Figure 2

A packing diagram of (I) viewed down the *a* axis. Dotted lines show the C—H···N and C—H···O hydrogen bonds.

2-(3-Methoxyphenyl)butanedinitrile

Crystal data

$C_{11}H_{10}N_2O$
M_r = 186.21
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 5.5263 (8) Å
b = 16.105 (2) Å
c = 11.0332 (16) Å
β = 97.179 (2)°
V = 974.3 (2) Å^3
Z = 4

$F(000) = 392$
$D_x = 1.270$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5752 reflections
$\theta = 2.3$–$27.4°$
$\mu = 0.08$ mm^{-1}
$T = 298$ K
Block, colorless
0.4 × 0.2 × 0.1 mm

Data collection

Bruker SMART area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
8042 measured reflections
2210 independent reflections
1963 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -7 \rightarrow 7$
$k = -20 \rightarrow 20$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.128$
$S = 1.04$
2210 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
$w = 1/[\sigma^2(F_o^2) + (0.0729P)^2 + 0.1612P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ 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}
C6	0.6739 (2)	0.85144 (7)	0.67253 (10)	0.0379 (3)
C7	0.5211 (2)	0.80066 (7)	0.73097 (11)	0.0406 (3)
H7	0.4177	0.8237	0.7822	0.049*
C5	0.8292 (3)	0.81733 (9)	0.59747 (12)	0.0518 (3)
H5	0.9321	0.8512	0.5588	0.062*
C2	0.5237 (2)	0.71565 (7)	0.71258 (11)	0.0439 (3)
C3	0.6789 (3)	0.68150 (8)	0.63618 (14)	0.0551 (4)
H3	0.6799	0.6245	0.6231	0.066*
C4	0.8306 (3)	0.73211 (9)	0.58018 (15)	0.0622 (4)
H4	0.9358	0.7090	0.5299	0.075*
C8	0.6709 (2)	0.94492 (7)	0.69077 (10)	0.0384 (3)
H8	0.7891	0.9698	0.6423	0.046*

C10	0.7385 (2)	0.97151 (7)	0.82538 (11)	0.0414 (3)
H10A	0.7311	1.0315	0.8311	0.050*
H10B	0.6209	0.9485	0.8744	0.050*
C9	0.4279 (2)	0.97888 (7)	0.64751 (11)	0.0435 (3)
O1	0.37911 (19)	0.66090 (5)	0.76429 (10)	0.0605 (3)
C1	0.2421 (3)	0.69035 (10)	0.85616 (15)	0.0638 (4)
H1A	0.3505	0.7141	0.9218	0.096*
H1B	0.1545	0.6450	0.8867	0.096*
H1C	0.1286	0.7318	0.8221	0.096*
N1	0.2393 (2)	1.00418 (8)	0.61421 (12)	0.0604 (3)
C11	0.9826 (2)	0.94328 (7)	0.87350 (10)	0.0415 (3)
N2	1.1722 (2)	0.92210 (8)	0.91331 (11)	0.0581 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C6	0.0380 (6)	0.0381 (6)	0.0376 (5)	−0.0021 (4)	0.0054 (4)	−0.0030 (4)
C7	0.0415 (6)	0.0363 (6)	0.0462 (6)	−0.0003 (4)	0.0139 (5)	−0.0042 (4)
C5	0.0540 (8)	0.0522 (7)	0.0537 (7)	−0.0070 (6)	0.0239 (6)	−0.0074 (5)
C2	0.0443 (6)	0.0368 (6)	0.0518 (6)	−0.0028 (5)	0.0112 (5)	−0.0029 (5)
C3	0.0617 (8)	0.0384 (6)	0.0679 (8)	0.0001 (5)	0.0188 (6)	−0.0143 (6)
C4	0.0668 (9)	0.0565 (8)	0.0696 (9)	−0.0002 (7)	0.0339 (7)	−0.0175 (7)
C8	0.0364 (6)	0.0373 (6)	0.0417 (6)	−0.0028 (4)	0.0053 (4)	0.0024 (4)
C10	0.0399 (6)	0.0366 (5)	0.0467 (6)	0.0036 (4)	0.0019 (5)	−0.0048 (4)
C9	0.0436 (7)	0.0397 (6)	0.0460 (6)	−0.0049 (5)	0.0007 (5)	0.0055 (5)
O1	0.0694 (7)	0.0352 (5)	0.0829 (7)	−0.0077 (4)	0.0339 (5)	−0.0025 (4)
C1	0.0727 (10)	0.0539 (8)	0.0708 (9)	−0.0093 (7)	0.0331 (8)	0.0033 (7)
N1	0.0479 (7)	0.0619 (7)	0.0679 (8)	0.0001 (5)	−0.0065 (5)	0.0126 (6)
C11	0.0429 (6)	0.0402 (6)	0.0413 (6)	0.0009 (5)	0.0050 (5)	−0.0025 (4)
N2	0.0469 (6)	0.0739 (8)	0.0525 (6)	0.0129 (5)	0.0023 (5)	−0.0037 (5)

Geometric parameters (Å, º)

C6—C5	1.3791 (16)	C8—C9	1.4730 (16)
C6—C7	1.3903 (15)	C8—C10	1.5460 (16)
C6—C8	1.5193 (15)	C8—H8	0.9800
C7—C2	1.3843 (16)	C10—C11	1.4593 (16)
C7—H7	0.9300	C10—H10A	0.9700
C5—C4	1.386 (2)	C10—H10B	0.9700
C5—H5	0.9300	C9—N1	1.1365 (16)
C2—O1	1.3623 (15)	O1—C1	1.4205 (17)
C2—C3	1.3890 (17)	C1—H1A	0.9600
C3—C4	1.371 (2)	C1—H1B	0.9600
C3—H3	0.9300	C1—H1C	0.9600
C4—H4	0.9300	C11—N2	1.1368 (16)
C5—C6—C7	120.25 (11)	C6—C8—C10	113.36 (9)
C5—C6—C8	119.48 (10)	C9—C8—H8	108.3

C7—C6—C8	120.28 (9)	C6—C8—H8	108.3
C2—C7—C6	119.71 (10)	C10—C8—H8	108.3
C2—C7—H7	120.1	C11—C10—C8	111.38 (9)
C6—C7—H7	120.1	C11—C10—H10A	109.4
C6—C5—C4	119.46 (12)	C8—C10—H10A	109.4
C6—C5—H5	120.3	C11—C10—H10B	109.4
C4—C5—H5	120.3	C8—C10—H10B	109.4
O1—C2—C7	124.16 (11)	H10A—C10—H10B	108.0
O1—C2—C3	115.90 (11)	N1—C9—C8	179.20 (13)
C7—C2—C3	119.94 (11)	C2—O1—C1	118.40 (10)
C4—C3—C2	119.79 (11)	O1—C1—H1A	109.5
C4—C3—H3	120.1	O1—C1—H1B	109.5
C2—C3—H3	120.1	H1A—C1—H1B	109.5
C3—C4—C5	120.84 (12)	O1—C1—H1C	109.5
C3—C4—H4	119.6	H1A—C1—H1C	109.5
C5—C4—H4	119.6	H1B—C1—H1C	109.5
C9—C8—C6	110.45 (9)	N2—C11—C10	178.53 (13)
C9—C8—C10	108.02 (9)		

C5—C6—C7—C2	−0.64 (18)	C6—C5—C4—C3	0.3 (2)
C8—C6—C7—C2	179.32 (11)	C5—C6—C8—C9	118.72 (12)
C7—C6—C5—C4	0.4 (2)	C7—C6—C8—C9	−61.25 (14)
C8—C6—C5—C4	−179.55 (13)	C5—C6—C8—C10	−119.90 (12)
C6—C7—C2—O1	−179.11 (11)	C7—C6—C8—C10	60.14 (14)
C6—C7—C2—C3	0.13 (19)	C9—C8—C10—C11	−177.45 (10)
O1—C2—C3—C4	179.91 (14)	C6—C8—C10—C11	59.81 (13)
C7—C2—C3—C4	0.6 (2)	C7—C2—O1—C1	−9.4 (2)
C2—C3—C4—C5	−0.8 (2)	C3—C2—O1—C1	171.30 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···N1^{i}	0.98	2.61	3.4864 (17)	150
C10—H10*A*···O1^{ii}	0.97	2.38	3.2470 (15)	149
C10—H10*B*···N2^{iii}	0.97	2.60	3.4823 (18)	151

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+1, *y*+1/2, −*z*+3/2; (iii) *x*−1, *y*, *z*.