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2-(4-Nitrobenzylidene)malononitrile

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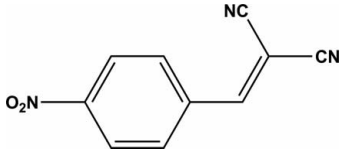
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.091; data-to-parameter ratio = 11.2.

In the title compound, $C_{10}H_5N_3O_2$, the benzylidenemalononitrile unit is nearly planar, with a maximum deviation of 0.129 (2) Å for a terminal N atom; the nitro group is approximately coplanar with the benzene ring [dihedral angle = 8.8 (3)°]. An intramolecular C—H···N hydrogen bond stabilizes the molecular conformation.

Related literature

For the preparation of the title compound, see: Baheti *et al.* (2011). For the spectroscopy and applications of benzylidenemalononitrile derivatives, see: Cao *et al.* (2010); Ding & Zhao (2010); Elinson *et al.* (2010); Herbivo *et al.* (2010); Shigemitsu *et al.* (2011); Ye *et al.* (2010). For related structures, see: El Brahmi *et al.* (2011); Karthikeyan *et al.* (2011); Mehdi *et al.* (2010); Ouzidan *et al.* (2011); Raza *et al.* (2010).



Experimental

Crystal data

$C_{10}H_5N_3O_2$
M_r = 199.17
Orthorhombic, $Pna2_1$
a = 19.5557 (9) Å
b = 3.8732 (2) Å
c = 11.9823 (5) Å
V = 907.58 (7) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.89 mm^{-1}
T = 297 K
0.76 × 0.60 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.674, T_{max} = 1.000
3111 measured reflections
1517 independent reflections
1420 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.091
S = 1.06
1517 reflections
136 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack (1983), 582 Friedel pairs
Flack parameter: −0.2 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···N3	0.93	2.58	3.431 (3)	152

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5449).

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supplementary materials

Acta Cryst. (2012). E**68**, o957 [doi:10.1107/S1600536812008896]

2-(4-Nitrobenzylidene)malononitrile

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Comment

Organic compounds bearing benzylidenemalononitrile moieties have attracted considerable attention due to their potential applications in the design of molecular devices (Cao *et al.*, 2010; Herbivo *et al.*, 2010; Shigemitsu *et al.*, 2011). In addition, the title compound and its derivatives have been used as potential precursors to prepare 5,7-diazaspiro-[2,5]octane (Elinson *et al.*, 2010), 2-amino-4*H*-chromene-3-carbonitrile (Ding *et al.*, 2010) and 4*H*-pyran derivatives (Ye *et al.*, 2010).

The molecular structure of the title compound is shown in Figure 1. The nitro group is close to being coplanar with the benzene ring (dihedral angle = 8.8 (3)°), which is consistent with previous studies (El Brahmi *et al.*, 2011; Mehdi *et al.*, 2010; Ouzidan *et al.*, 2011; Raza *et al.*, 2010). In addition, the benzylidenemalononitrile moiety is nearly planar with a maximum deviation of 0.129 (2))Å for atom N2 (Karthikeyan *et al.*, 2011). An intramolecular C—H···N hydrogen bond stabilizes the molecular conformation.

Experimental

The title compound was synthesized by the Knoevenagel condensation of malononitrile with 4-nitrobenzaldehyde (Baheti *et al.*, 2011). Colorless crystals suitable for the crystallographic studies reported here were isolated over a period of four weeks by slow evaporation from a chloroform solution.

Refinement

H atoms were positioned geometrically (C—H = 0.93 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Computing details

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

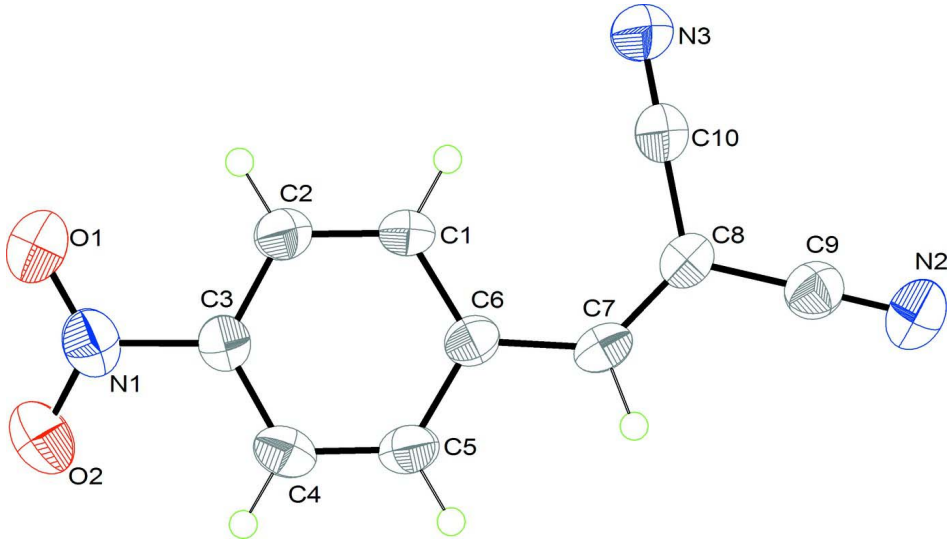

Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids.

2-(4-Nitrobenzylidene)propanedinitrile

Crystal data

$C_{10}H_5N_3O_2$
$M_r = 199.17$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 19.5557$ (9) Å
$b = 3.8732$ (2) Å
$c = 11.9823$ (5) Å
$V = 907.58$ (7) Å^3
$Z = 4$
$F(000) = 408$
$D_x = 1.458$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 2320 reflections
$\theta = 3.7$–$71.5°$
$\mu = 0.89$ mm^{-1}
$T = 297$ K
Parallelepiped, colorless
0.76 × 0.60 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.674$, $T_{max} = 1.000$
3111 measured reflections
1517 independent reflections
1420 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 71.7°$, $\theta_{min} = 4.5°$
$h = -24\rightarrow15$
$k = -4\rightarrow3$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.091$
$S = 1.06$
1517 reflections
136 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0621P)^2 + 0.0168P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

Absolute structure: Flack (1983), 582 Friedel pairs

Flack parameter: −0.2 (2)

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}
O1	0.19540 (9)	1.1888 (6)	−0.10487 (14)	0.0798 (6)
O2	0.17348 (9)	1.4626 (5)	0.04698 (17)	0.0790 (6)
N1	0.21000 (8)	1.2840 (4)	−0.01057 (15)	0.0530 (4)
N2	0.61988 (11)	0.5187 (6)	0.25478 (17)	0.0672 (5)
N3	0.53572 (10)	0.5513 (7)	−0.07973 (17)	0.0743 (6)
C1	0.38494 (10)	0.9176 (5)	0.00650 (14)	0.0445 (4)
H1A	0.4165	0.8120	−0.0404	0.053*
C2	0.32231 (10)	1.0153 (5)	−0.03437 (15)	0.0449 (4)
H2A	0.3110	0.9738	−0.1086	0.054*
C3	0.27635 (9)	1.1752 (5)	0.03563 (14)	0.0405 (4)
C4	0.29078 (10)	1.2411 (5)	0.14638 (16)	0.0471 (5)
H4A	0.2591	1.3505	0.1922	0.056*
C5	0.35351 (10)	1.1396 (5)	0.18681 (15)	0.0447 (4)
H5A	0.3641	1.1811	0.2613	0.054*
C6	0.40158 (9)	0.9766 (4)	0.11918 (14)	0.0387 (4)
C7	0.46578 (10)	0.8685 (5)	0.17120 (14)	0.0415 (4)
H7A	0.4690	0.9154	0.2471	0.050*
C8	0.52069 (10)	0.7129 (4)	0.12720 (15)	0.0408 (4)
C9	0.57642 (11)	0.6105 (5)	0.19838 (16)	0.0478 (5)
C10	0.52915 (9)	0.6242 (6)	0.01095 (17)	0.0489 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0629 (11)	0.1147 (15)	0.0617 (10)	0.0171 (10)	−0.0179 (8)	−0.0051 (10)
O2	0.0585 (9)	0.0933 (14)	0.0852 (13)	0.0283 (9)	0.0017 (9)	−0.0088 (10)
N1	0.0435 (9)	0.0578 (10)	0.0577 (12)	0.0029 (7)	0.0036 (8)	0.0085 (9)
N2	0.0659 (12)	0.0835 (14)	0.0521 (10)	0.0141 (11)	−0.0141 (10)	0.0016 (9)
N3	0.0567 (11)	0.1197 (18)	0.0464 (10)	0.0190 (11)	−0.0019 (9)	−0.0203 (11)
C1	0.0467 (9)	0.0544 (11)	0.0324 (8)	0.0064 (8)	0.0011 (7)	−0.0025 (8)
C2	0.0470 (9)	0.0543 (11)	0.0334 (8)	0.0003 (8)	−0.0011 (8)	−0.0006 (8)
C3	0.0391 (8)	0.0424 (9)	0.0399 (10)	−0.0019 (7)	0.0009 (7)	0.0045 (7)
C4	0.0480 (10)	0.0506 (11)	0.0426 (10)	0.0023 (9)	0.0106 (8)	−0.0029 (9)
C5	0.0501 (10)	0.0529 (11)	0.0312 (8)	−0.0032 (8)	0.0027 (8)	−0.0009 (8)
C6	0.0447 (9)	0.0394 (9)	0.0321 (8)	−0.0029 (7)	0.0016 (7)	0.0030 (7)

C7	0.0515 (10)	0.0439 (11)	0.0290 (7)	−0.0038 (8)	−0.0023 (7)	0.0013 (7)
C8	0.0447 (9)	0.0407 (9)	0.0370 (9)	−0.0041 (8)	−0.0039 (7)	0.0024 (8)
C9	0.0502 (10)	0.0520 (11)	0.0413 (10)	0.0009 (9)	−0.0029 (9)	0.0011 (9)
C10	0.0401 (9)	0.0618 (12)	0.0449 (10)	0.0041 (8)	−0.0009 (8)	−0.0037 (9)

Geometric parameters (Å, º)

O1—N1	1.222 (2)	C3—C4	1.381 (3)
O2—N1	1.210 (2)	C4—C5	1.376 (3)
N1—C3	1.472 (2)	C4—H4A	0.9300
N2—C9	1.143 (3)	C5—C6	1.393 (3)
N3—C10	1.130 (3)	C5—H5A	0.9300
C1—C2	1.372 (3)	C6—C7	1.463 (3)
C1—C6	1.407 (2)	C7—C8	1.339 (3)
C1—H1A	0.9300	C7—H7A	0.9300
C2—C3	1.377 (3)	C8—C10	1.444 (3)
C2—H2A	0.9300	C8—C9	1.440 (3)
O2—N1—O1	124.15 (19)	C4—C5—C6	121.76 (17)
O2—N1—C3	118.00 (17)	C4—C5—H5A	119.1
O1—N1—C3	117.85 (17)	C6—C5—H5A	119.1
C2—C1—C6	120.27 (17)	C5—C6—C1	118.41 (17)
C2—C1—H1A	119.9	C5—C6—C7	117.46 (17)
C6—C1—H1A	119.9	C1—C6—C7	124.11 (16)
C3—C2—C1	119.29 (17)	C8—C7—C6	130.47 (17)
C3—C2—H2A	120.4	C8—C7—H7A	114.8
C1—C2—H2A	120.4	C6—C7—H7A	114.8
C2—C3—C4	122.37 (17)	C7—C8—C10	125.34 (17)
C2—C3—N1	118.37 (15)	C7—C8—C9	119.85 (17)
C4—C3—N1	119.25 (16)	C10—C8—C9	114.78 (16)
C5—C4—C3	117.89 (18)	N2—C9—C8	177.8 (2)
C5—C4—H4A	121.1	N3—C10—C8	179.3 (3)
C3—C4—H4A	121.1		
C6—C1—C2—C3	0.8 (3)	C3—C4—C5—C6	0.2 (3)
C1—C2—C3—C4	−0.2 (3)	C4—C5—C6—C1	0.4 (3)
C1—C2—C3—N1	178.79 (16)	C4—C5—C6—C7	−177.94 (17)
O2—N1—C3—C2	−170.72 (19)	C2—C1—C6—C5	−0.9 (3)
O1—N1—C3—C2	9.0 (3)	C2—C1—C6—C7	177.29 (17)
O2—N1—C3—C4	8.3 (3)	C5—C6—C7—C8	−179.0 (2)
O1—N1—C3—C4	−172.0 (2)	C1—C6—C7—C8	2.8 (3)
C2—C3—C4—C5	−0.3 (3)	C6—C7—C8—C10	2.3 (3)
N1—C3—C4—C5	−179.30 (17)	C6—C7—C8—C9	−175.70 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···N3	0.93	2.58	3.431 (3)	152