Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Methyl-3-nitrobenzonitrile

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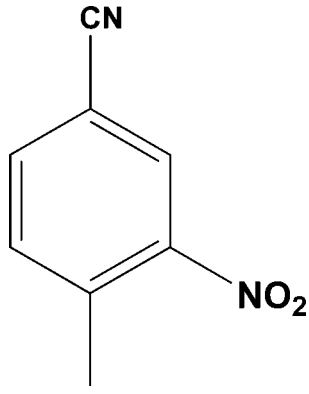
Received 29 July 2008; accepted 26 August 2008

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.068; wR factor = 0.208; data-to-parameter ratio = 16.1.

In the title compound, $C_8H_6N_2O_2$, the nitro group is rotated by 23.2 (3)° out of the plane of the benzene ring. The crystal structure is stabilized by van der Waals interactions.

Related literature

For the chemistry of nitrile derivatives, see: Xiong *et al.* (2002); Jin *et al.* (1994); Brewis *et al.* (2003); Dunica *et al.* (1991). For related literature, see: Fu & Zhao (2007); Liang & Wang, (2008).



Experimental

Crystal data

$C_8H_6N_2O_2$
M_r = 162.15
Monoclinic, $P2_1/c$
a = 3.9088 (8) Å
b = 13.576 (3) Å
c = 14.819 (4) Å
β = 99.13 (3)°
V = 776.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.35 × 0.30 × 0.1 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.965, T_{max} = 0.990
7589 measured reflections
1761 independent reflections
1336 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.208
S = 1.10
1753 reflections
109 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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 a start-up grant from Southeast University to Professor Ren-Gen Xiong.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WK2090).

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supporting information

Acta Cryst. (2008). E**64**, o1898 [doi:10.1107/S1600536808027414]

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S1. Comment

Nitrile derivatives have found a wide range of applications in industry and coordination chemistry as ligands. For example, phthalonitriles have been used as starting materials for phthalocyanines (Jin *et al.*, 1994), which are important components for dyes, pigments, gas sensors, optical limiters and liquid crystals, and which are also used in medicine, as singlet oxygen photosensitisers for photodynamic therapy (Brewis *et al.*, 2003). Also, nitrile compounds are the precursors of tetrazole complexes (Dunica *et al.*(1991); Xiong *et al.*(2002)). Recently, a series of benzonitrile compounds have been reported (Fu & Zhao, 2007; Liang & Wang, 2008). As an extension of these studies on structural characterization, we report here the crystal structure of the title compound, *p*-methyl-*m*-nitrobenzonitrile.

The crystal data show that in the title compound (Fig. 1), the benzene ring and the nitro group are not coplanar, they are twisted with respect to each other by torsion angles of O1—N1—C1—C6 (-23.2 (4)°) and O2—N1—C1—C2 (-25.6 (3)°); the nitrile group C8≡N2 bond length of 1.144 (3) Å is within the normal range. The crystal structure is stabilized only by van der Waals interactions.

S2. Experimental

The purchased *p*-methyl-*m*-nitrobenzonitrile (3 mmol, 486.44 mg) was dissolved in chloroform (20 ml) and evaporated in air, affording colorless block crystals of this compound suitable for X-ray analysis.

S3. Refinement

All H atoms bonded to C atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic), C—H = 0.96 Å (methyl), with U_{iso}(H) = 1.2U_{eq}(aromatic C) and U_{iso}(H) = 1.5U_{eq}(methyl C).

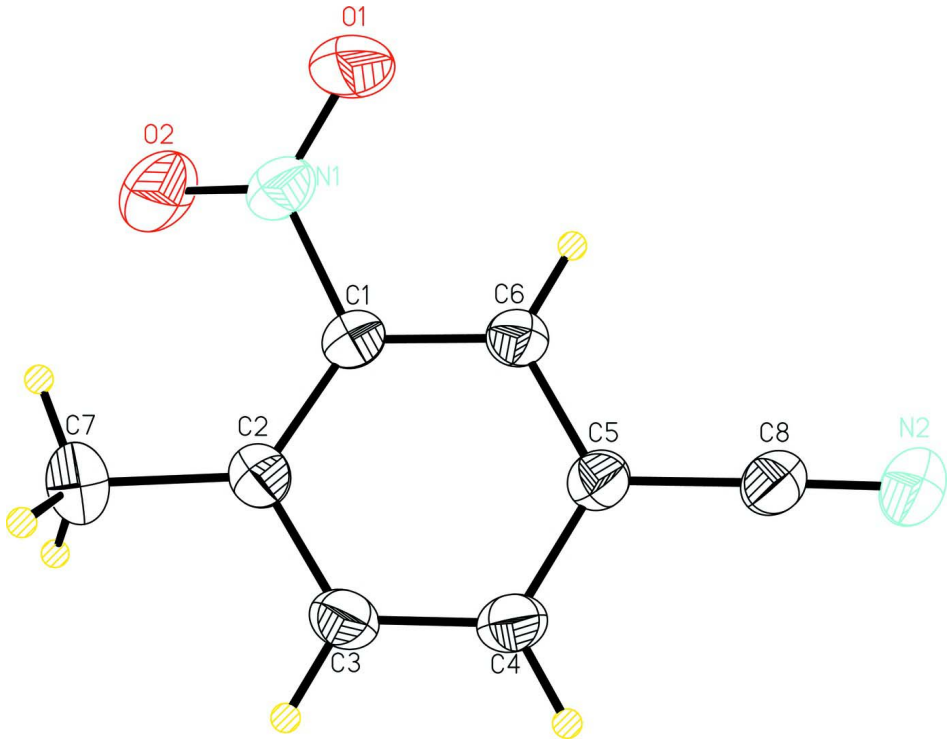

Figure 1

A view of the molecular structure of the title compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by spheres of arbitrary radius.

(I)

Crystal data

$C_8H_6N_2O_2$
$M_r = 162.15$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 3.9088\ (8)$ Å
$b = 13.576\ (3)$ Å
$c = 14.819\ (4)$ Å
$\beta = 99.13\ (3)°$
$V = 776.4\ (3)$ Å^3
$Z = 4$
$F(000) = 336$
$D_x = 1.387$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1764 reflections
$\theta = 3.1–27.6°$
$\mu = 0.10$ mm^{-1}
$T = 298$ K
Block, colourless
0.35 × 0.30 × 0.1 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.965$, $T_{max} = 0.990$
7589 measured reflections
1761 independent reflections
1336 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -5\rightarrow5$
$k = -17\rightarrow17$
$l = -19\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.208$
$S = 1.10$
1753 reflections
109 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
$w = 1/[\sigma^2(F_o^2) + (0.1036P)^2 + 0.2336P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ 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}
O1	1.0921 (7)	0.79875 (18)	0.59741 (14)	0.1001 (9)
O2	1.3658 (7)	0.89476 (18)	0.52048 (17)	0.0932 (8)
N1	1.1627 (5)	0.82762 (16)	0.52533 (14)	0.0584 (6)
N2	0.5214 (8)	0.45178 (18)	0.38967 (18)	0.0803 (8)
C1	1.0021 (5)	0.77768 (15)	0.44045 (14)	0.0444 (5)
C8	0.6195 (7)	0.53049 (18)	0.38358 (16)	0.0568 (6)
C2	0.9631 (5)	0.82620 (16)	0.35611 (15)	0.0462 (5)
C6	0.8914 (6)	0.68242 (16)	0.45126 (14)	0.0470 (5)
H6	0.9185	0.6535	0.5088	0.056*
C4	0.6963 (6)	0.67560 (17)	0.28898 (15)	0.0530 (6)
H4	0.5942	0.6412	0.2374	0.064*
C5	0.7388 (6)	0.63055 (16)	0.37444 (15)	0.0463 (5)
C3	0.8057 (7)	0.77130 (18)	0.28090 (16)	0.0559 (6)
H3	0.7738	0.8004	0.2234	0.067*
C7	1.0660 (8)	0.93151 (18)	0.3406 (2)	0.0672 (7)
H7A	1.1700	0.9601	0.3976	0.101*
H7B	0.8641	0.9687	0.3157	0.101*
H7C	1.2293	0.9326	0.2985	0.101*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.145 (2)	0.1075 (18)	0.0430 (11)	−0.0405 (15)	0.0006 (12)	−0.0087 (11)
O2	0.0966 (17)	0.0881 (15)	0.0906 (16)	−0.0397 (13)	0.0017 (12)	−0.0237 (12)
N1	0.0605 (12)	0.0593 (12)	0.0523 (12)	−0.0039 (10)	−0.0011 (9)	−0.0117 (9)

N2	0.106 (2)	0.0562 (14)	0.0755 (16)	−0.0203 (13)	0.0039 (14)	−0.0061 (11)
C1	0.0410 (10)	0.0476 (12)	0.0436 (11)	0.0013 (9)	0.0041 (8)	−0.0064 (9)
C8	0.0662 (15)	0.0501 (13)	0.0521 (14)	−0.0036 (11)	0.0029 (11)	−0.0063 (10)
C2	0.0447 (11)	0.0456 (11)	0.0496 (12)	0.0061 (9)	0.0119 (9)	0.0026 (9)
C6	0.0517 (12)	0.0478 (12)	0.0402 (11)	0.0010 (9)	0.0034 (9)	0.0011 (9)
C4	0.0619 (14)	0.0521 (13)	0.0417 (12)	0.0062 (10)	−0.0014 (10)	−0.0048 (9)
C5	0.0483 (12)	0.0446 (11)	0.0452 (12)	0.0015 (9)	0.0049 (8)	−0.0036 (9)
C3	0.0708 (16)	0.0543 (13)	0.0415 (12)	0.0083 (11)	0.0058 (10)	0.0059 (9)
C7	0.0707 (17)	0.0504 (14)	0.0807 (19)	−0.0005 (12)	0.0125 (14)	0.0096 (12)

Geometric parameters (Å, º)

O1—N1	1.210 (3)	C6—C5	1.390 (3)
O2—N1	1.218 (3)	C6—H6	0.9300
N1—C1	1.478 (3)	C4—C3	1.379 (3)
N2—C8	1.144 (3)	C4—C5	1.392 (3)
C1—C6	1.381 (3)	C4—H4	0.9300
C1—C2	1.400 (3)	C3—H3	0.9300
C8—C5	1.450 (3)	C7—H7A	0.9600
C2—C3	1.400 (3)	C7—H7B	0.9600
C2—C7	1.513 (3)	C7—H7C	0.9600
O1—N1—O2	122.4 (2)	C3—C4—H4	120.0
O1—N1—C1	118.5 (2)	C5—C4—H4	120.0
O2—N1—C1	119.1 (2)	C6—C5—C4	119.7 (2)
C6—C1—C2	123.55 (19)	C6—C5—C8	120.1 (2)
C6—C1—N1	115.43 (19)	C4—C5—C8	120.2 (2)
C2—C1—N1	121.0 (2)	C4—C3—C2	122.4 (2)
N2—C8—C5	178.9 (3)	C4—C3—H3	118.8
C3—C2—C1	115.6 (2)	C2—C3—H3	118.8
C3—C2—C7	118.4 (2)	C2—C7—H7A	109.5
C1—C2—C7	125.9 (2)	C2—C7—H7B	109.5
C1—C6—C5	118.75 (19)	H7A—C7—H7B	109.5
C1—C6—H6	120.6	C2—C7—H7C	109.5
C5—C6—H6	120.6	H7A—C7—H7C	109.5
C3—C4—C5	119.9 (2)	H7B—C7—H7C	109.5
O1—N1—C1—C6	−23.2 (3)	N1—C1—C6—C5	−179.76 (19)
O2—N1—C1—C6	155.4 (2)	C1—C6—C5—C4	−0.9 (3)
O1—N1—C1—C2	155.8 (2)	C1—C6—C5—C8	−179.9 (2)
O2—N1—C1—C2	−25.6 (3)	C3—C4—C5—C6	0.0 (3)
C6—C1—C2—C3	−0.8 (3)	C3—C4—C5—C8	179.1 (2)
N1—C1—C2—C3	−179.68 (19)	C5—C4—C3—C2	0.5 (4)
C6—C1—C2—C7	177.4 (2)	C1—C2—C3—C4	−0.1 (3)
N1—C1—C2—C7	−1.4 (3)	C7—C2—C3—C4	−178.5 (2)
C2—C1—C6—C5	1.3 (3)		