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2-Methyl-5-nitrobenzonitrile

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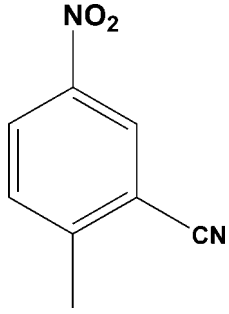
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.050; wR factor = 0.141; data-to-parameter ratio = 16.2.

In the title compound, $C_8H_6N_2O_2$, the nitro group is rotated by 10.2 (2)° 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).



Experimental

Crystal data

$C_8H_6N_2O_2$
M_r = 162.15
Monoclinic, $P2_1/n$
a = 3.8946 (8) Å
b = 7.6350 (15) Å
c = 26.180 (5) Å
β = 91.65 (3)°
V = 778.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.4 × 0.35 × 0.2 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.93, T_{max} = 0.98
7390 measured reflections
1761 independent reflections
1273 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.141
S = 1.04
1761 reflections
109 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Data collection: *CrystalClear* (Rigaku/MSC, 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2137).

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supporting information

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S1. Comment

Nitrile derivatives have found 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). And nitrile compounds are the precursor of tetrazole complexes (Dunica *et al.,* 1991), which we have focused on for the design of noncentrosymmetric bulk materials, based on axial-chiral ligand 5-(3-methyl-4-nitrophenyl)-2*H*-tetrazole (Xiong *et al.,* 2002). Recently, we have reported a few benzonitrile compounds (Fu & Zhao, 2007). As an extension of our work on the structural characterization, we report here the crystal structure of title compound. The crystal data show that in the title compound, the benzene ring and the nitro group are nearly planar, they are only twisted to each other by a torsion angles of O2—N1—C1—C2 (-10.4 (2)°) and O1—N1—C1—C6 (-9.9 (2)°), the nitrile group C7—N2 bond length of 1.137 (2)Å is within the normal range (Fig.1).

S2. Experimental

The title compound was purchased from Aldrich and was dissolved (3 mmol, 486.44 mg) in ethanol (20 ml) and evaporated in air affording colorless block crystals suitable for X-ray analysis.

S3. Refinement

Positional parameters of all the H atoms bonded to C atoms were calculated geometrically and were allowed to ride on the C atoms to which they are bonded, with C—H = 0.93Å (aromatic) and with U_{iso}(H) = 1.2$_{eq}$(C) or 0.96Å (methyl) and U_{iso}(H) = 1.5U_{eq}(C).

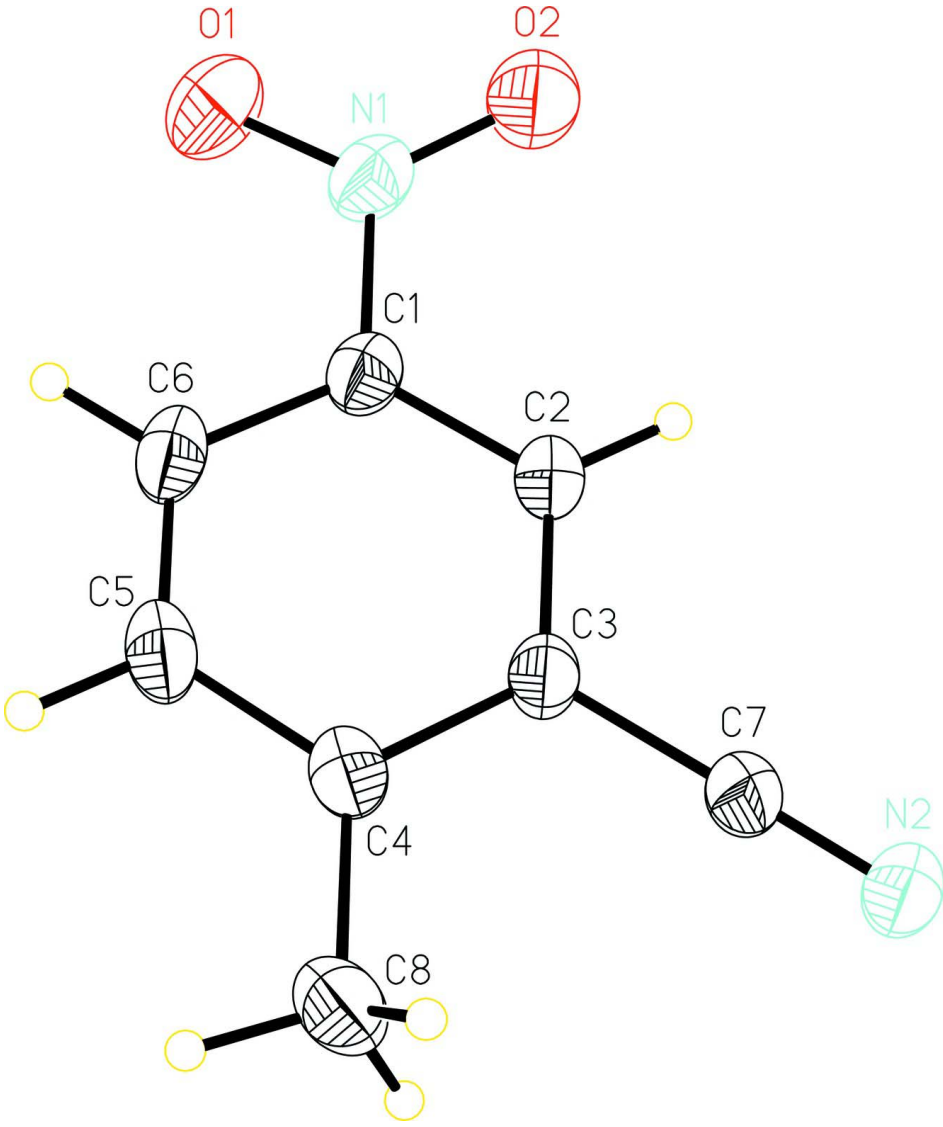

Figure 1

A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level.

2-Methyl-5-nitrobenzonitrile

Crystal data

$C_8H_6N_2O_2$
M_r = 162.15
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 3.8946 (8) Å
b = 7.6350 (15) Å
c = 26.180 (5) Å
β = 91.65 (3)°
V = 778.1 (3) Å^3
Z = 4

$F(000)$ = 336
D_x = 1.384 Mg m^{-3}
Melting point = 349–350 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1763 reflections
θ = 3.1–27.7°
μ = 0.10 mm^{-1}
T = 293 K
Block, colourless
0.4 × 0.35 × 0.2 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} = 0.93, T_{max} = 0.98
7390 measured reflections
1761 independent reflections
1273 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −5→4
k = −9→9
l = −33→33

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.141
S = 1.04
1761 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
$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2 + 0.1332P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	0.8171 (4)	0.3298 (2)	0.18614 (5)	0.0590 (4)
C3	0.8617 (4)	0.6612 (2)	0.08273 (6)	0.0450 (4)
C2	0.7935 (4)	0.5051 (2)	0.10776 (5)	0.0451 (4)
H2A	0.6877	0.4120	0.0907	0.054*
C7	0.7618 (5)	0.6787 (2)	0.02938 (6)	0.0534 (4)
C4	1.0183 (4)	0.8045 (2)	0.10793 (6)	0.0489 (4)
C1	0.8882 (4)	0.4929 (2)	0.15883 (6)	0.0469 (4)
N2	0.6808 (5)	0.6958 (2)	−0.01239 (6)	0.0745 (5)
C5	1.1068 (4)	0.7835 (2)	0.15941 (7)	0.0569 (5)
H5A	1.2101	0.8762	0.1770	0.068*
O1	0.9413 (5)	0.3114 (2)	0.22899 (6)	0.0954 (6)
O2	0.6345 (4)	0.2205 (2)	0.16517 (6)	0.0838 (5)
C6	1.0461 (4)	0.6299 (2)	0.18501 (6)	0.0550 (5)
H6A	1.1100	0.6182	0.2193	0.066*
C8	1.0878 (5)	0.9721 (2)	0.08010 (7)	0.0636 (5)
H8A	1.1998	1.0535	0.1030	0.095*

H8B	0.8748	1.0213	0.0676	0.095*
H8C	1.2333	0.9487	0.0519	0.095*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0639 (9)	0.0679 (10)	0.0450 (8)	0.0035 (8)	−0.0017 (7)	0.0075 (7)
C3	0.0453 (8)	0.0507 (9)	0.0387 (8)	−0.0026 (7)	−0.0039 (6)	−0.0050 (6)
C2	0.0460 (8)	0.0481 (9)	0.0407 (8)	−0.0017 (7)	−0.0045 (6)	−0.0051 (6)
C7	0.0660 (11)	0.0465 (9)	0.0473 (9)	−0.0131 (8)	−0.0079 (8)	−0.0006 (7)
C4	0.0438 (8)	0.0519 (9)	0.0509 (9)	−0.0024 (7)	−0.0011 (7)	−0.0091 (7)
C1	0.0445 (8)	0.0559 (10)	0.0401 (8)	0.0037 (7)	−0.0011 (6)	−0.0006 (7)
N2	0.1069 (14)	0.0667 (10)	0.0486 (9)	−0.0268 (9)	−0.0196 (9)	0.0072 (7)
C5	0.0547 (10)	0.0629 (11)	0.0525 (10)	−0.0062 (8)	−0.0072 (8)	−0.0186 (8)
O1	0.1169 (13)	0.1119 (13)	0.0559 (8)	−0.0133 (10)	−0.0234 (8)	0.0294 (8)
O2	0.1135 (13)	0.0681 (9)	0.0688 (9)	−0.0226 (9)	−0.0121 (9)	0.0108 (7)
C6	0.0540 (10)	0.0721 (12)	0.0385 (8)	0.0022 (8)	−0.0078 (7)	−0.0093 (7)
C8	0.0640 (11)	0.0545 (10)	0.0721 (12)	−0.0136 (9)	−0.0039 (9)	−0.0046 (9)

Geometric parameters (Å, º)

N1—O2	1.217 (2)	C4—C5	1.391 (2)
N1—O1	1.2168 (19)	C4—C8	1.501 (2)
N1—C1	1.467 (2)	C1—C6	1.385 (2)
C3—C4	1.407 (2)	C5—C6	1.375 (3)
C3—C2	1.390 (2)	C5—H5A	0.9300
C3—C7	1.445 (2)	C6—H6A	0.9300
C2—C1	1.380 (2)	C8—H8A	0.9600
C2—H2A	0.9300	C8—H8B	0.9600
C7—N2	1.137 (2)	C8—H8C	0.9600
O2—N1—O1	123.27 (16)	C2—C1—N1	118.73 (14)
O2—N1—C1	118.58 (14)	C6—C1—N1	119.18 (14)
O1—N1—C1	118.15 (15)	C6—C5—C4	121.98 (15)
C4—C3—C2	122.14 (14)	C6—C5—H5A	119.0
C4—C3—C7	118.83 (14)	C4—C5—H5A	119.0
C2—C3—C7	119.02 (13)	C5—C6—C1	118.89 (15)
C1—C2—C3	117.73 (14)	C5—C6—H6A	120.6
C1—C2—H2A	121.1	C1—C6—H6A	120.6
C3—C2—H2A	121.1	C4—C8—H8A	109.5
N2—C7—C3	178.63 (19)	C4—C8—H8B	109.5
C5—C4—C3	117.16 (15)	H8A—C8—H8B	109.5
C5—C4—C8	121.71 (15)	C4—C8—H8C	109.5
C3—C4—C8	121.12 (15)	H8A—C8—H8C	109.5
C2—C1—C6	122.09 (15)	H8B—C8—H8C	109.5
C4—C3—C2—C1	−0.7 (2)	O1—N1—C1—C2	170.40 (16)
C7—C3—C2—C1	−179.26 (14)	O2—N1—C1—C6	169.28 (16)

C2—C3—C4—C5	0.6 (2)	O1—N1—C1—C6	−9.9 (2)
C7—C3—C4—C5	179.19 (15)	C3—C4—C5—C6	0.2 (2)
C2—C3—C4—C8	−179.73 (15)	C8—C4—C5—C6	−179.50 (16)
C7—C3—C4—C8	−1.1 (2)	C4—C5—C6—C1	−0.8 (3)
C3—C2—C1—C6	0.0 (2)	C2—C1—C6—C5	0.7 (3)
C3—C2—C1—N1	179.64 (13)	N1—C1—C6—C5	−178.91 (15)
O2—N1—C1—C2	−10.4 (2)		