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2-Methyl-4-nitrophenol

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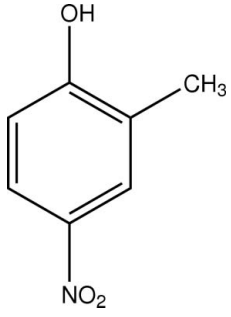
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.054; wR factor = 0.181; data-to-parameter ratio = 12.2.

The molecule of the title compound, $C_7H_7NO_3$, is nearly planar [maximum deviation 0.112 (3) Å for one of the notro O atoms]. In the crystal structure, intermolecular O—H···O and C—H···O interactions link the molecules into a three-dimensional network.

Related literature

For a related structure, see: Ahmed & Ashwini (2004). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_7H_7NO_3$
M_r = 153.14
Monoclinic, $P2_1/n$
a = 5.6210 (11) Å
b = 8.7420 (17) Å>
c = 14.300 (3) Å
β = 100.71 (3)°
V = 690.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 294 K
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.966, T_{max} = 0.988
1378 measured reflections
1245 independent reflections
870 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.181
S = 1.01
1245 reflections
102 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O2^{i}	0.82	2.10	2.770 (4)	138
C7—H7C···O1^{ii}	0.96	2.57	3.505 (5)	165

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2688).

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supplementary materials

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2-Methyl-4-nitrophenol

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Comment

Some derivatives of benzoic acids are important chemical materials. We report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Ring A (C1-C6) is, of course, planar. Atoms O1, O2, O3, N and C7 are 0.112 (3), 0.023 (3), 0.049 (3), 0.026 (4) and -0.042 (3) Å away from the ring plane, respectively. So, the molecule is nearly planar.

In the crystal structure, intermolecular O-H···O and C-H···O interactions (Table 1) link the molecules into a network, in which they may be effective in the stabilization of the structure.

Experimental

For the preparation of the title compound, ethyl acetate (150 ml), 2-methyl-phenol (5.9 g) and zinc chloride (7.4 g) are placed in an ultrasonic cleaning bath equipped with a round botton flask, and then nitric acid (5.9 g) was added dropwise in 3 min. After the reaction was completed, water (200 ml) was added. After evaporation of the organic layer, the obtained product (Ahmed & Ashwini, 2004) was crystallized by slow evaporation of a methanol solution.

Refinement

H atoms were positioned geometrically, with O-H = 0.82 Å (for OH) and C-H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,O)$, where x = 1.2 for aromatic H and x = 1.5 for all other H atoms.

Figures

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Fig. 2. A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

2-Methyl-4-nitrophenol

Crystal data

$C_7H_7NO_3$	F_{000} = 320
M_r = 153.14	D_x = 1.473 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation

	λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 25 reflections
a = 5.6210 (11) Å	θ = 9–13º
b = 8.7420 (17) Å	μ = 0.12 mm^{-1}
c = 14.300 (3) Å	T = 294 K
β = 100.71 (3)º	Block, colorless
V = 690.4 (2) $Å^3$	0.30 × 0.20 × 0.10 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.027
Radiation source: fine-focus sealed tube	θ_{max} = 25.3º
Monochromator: graphite	θ_{min} = 2.7º
T = 294 K	h = 0→6
ω/2θ scans	k = 0→10
Absorption correction: ψ scan (North *et al.*, 1968)	l = −17→16
T_{min} = 0.966, T_{max} = 0.988	3 standard reflections
1378 measured reflections	every 120 min
1245 independent reflections	intensity decay: 1%
870 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.054	$w = 1/[\sigma^2(F_o^2) + (0.08P)^2 + 0.74P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.181	$(\Delta/\sigma)_{max} < 0.001$
S = 1.01	$\Delta\rho_{max}$ = 0.25 e $Å^{-3}$
1245 reflections	$\Delta\rho_{min}$ = −0.24 e $Å^{-3}$
102 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.017 (4)
Secondary atom site location: difference Fourier map	

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}
O1	−0.3440 (5)	0.6807 (3)	0.9304 (2)	0.0769 (9)
O2	−0.0576 (5)	0.7542 (3)	0.8605 (2)	0.0682 (8)
O3	0.0480 (4)	0.0536 (3)	0.81980 (17)	0.0567 (7)
H3A	−0.0372	−0.0079	0.8417	0.085*
N	−0.1770 (5)	0.6536 (3)	0.8896 (2)	0.0490 (8)
C1	0.0652 (6)	0.4640 (4)	0.8248 (2)	0.0478 (9)
H1A	0.1525	0.5429	0.8034	0.057*
C2	0.1146 (6)	0.3143 (4)	0.8076 (2)	0.0487 (9)
H2A	0.2352	0.2908	0.7734	0.058*
C3	−0.0137 (6)	0.1979 (4)	0.8410 (2)	0.0417 (8)
C4	−0.1941 (5)	0.2284 (3)	0.8932 (2)	0.0410 (8)
C5	−0.2457 (6)	0.3796 (4)	0.9085 (2)	0.0415 (8)
H5A	−0.3678	0.4038	0.9418	0.050*
C6	−0.1175 (5)	0.4950 (4)	0.8747 (2)	0.0413 (8)
C7	−0.3278 (6)	0.1019 (4)	0.9313 (3)	0.0531 (9)
H7A	−0.2143	0.0360	0.9707	0.080*
H7B	−0.4172	0.0441	0.8793	0.080*
H7C	−0.4375	0.1443	0.9684	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.093 (2)	0.0485 (16)	0.104 (2)	0.0137 (14)	0.0576 (18)	−0.0051 (15)
O2	0.0861 (19)	0.0303 (13)	0.097 (2)	−0.0030 (12)	0.0392 (16)	0.0063 (13)
O3	0.0661 (15)	0.0341 (13)	0.0802 (17)	0.0000 (11)	0.0405 (13)	−0.0053 (11)
N	0.0594 (18)	0.0337 (15)	0.0567 (17)	0.0039 (13)	0.0180 (14)	0.0005 (13)
C1	0.0539 (19)	0.0371 (17)	0.059 (2)	−0.0036 (14)	0.0281 (17)	0.0044 (15)
C2	0.0496 (19)	0.0413 (18)	0.063 (2)	−0.0036 (15)	0.0302 (17)	−0.0024 (16)
C3	0.0438 (17)	0.0339 (15)	0.0503 (18)	−0.0019 (14)	0.0168 (14)	−0.0029 (14)
C4	0.0389 (16)	0.0397 (17)	0.0473 (18)	−0.0032 (13)	0.0156 (14)	−0.0012 (14)
C5	0.0403 (16)	0.0407 (17)	0.0469 (17)	0.0021 (14)	0.0171 (14)	0.0005 (14)
C6	0.0461 (17)	0.0312 (16)	0.0500 (18)	0.0009 (13)	0.0177 (14)	−0.0006 (13)
C7	0.054 (2)	0.045 (2)	0.068 (2)	−0.0034 (15)	0.0285 (17)	0.0007 (16)

Geometric parameters (Å, °)

O3—C3	1.357 (4)	C2—H2A	0.9300
O3—H3A	0.8200	C3—C4	1.393 (4)
N—O1	1.217 (3)	C4—C5	1.379 (4)
N—O2	1.225 (4)	C4—C7	1.496 (4)
N—C6	1.451 (4)	C5—C6	1.379 (4)
C1—C2	1.370 (5)	C5—H5A	0.9300

C1—C6	1.382 (4)	C7—H7A	0.9600
C1—H1A	0.9300	C7—H7B	0.9600
C2—C3	1.382 (4)	C7—H7C	0.9600
C3—O3—H3A	109.5	C5—C4—C7	121.1 (3)
O1—N—O2	122.9 (3)	C3—C4—C7	121.2 (3)
O1—N—C6	118.4 (3)	C6—C5—C4	120.5 (3)
O2—N—C6	118.7 (3)	C6—C5—H5A	119.8
C2—C1—C6	118.4 (3)	C4—C5—H5A	119.8
C2—C1—H1A	120.8	C5—C6—C1	121.6 (3)
C6—C1—H1A	120.8	C5—C6—N	119.9 (3)
C1—C2—C3	120.4 (3)	C1—C6—N	118.5 (3)
C1—C2—H2A	119.8	C4—C7—H7A	109.5
C3—C2—H2A	119.8	C4—C7—H7B	109.5
O3—C3—C2	115.9 (3)	H7A—C7—H7B	109.5
O3—C3—C4	122.7 (3)	C4—C7—H7C	109.5
C2—C3—C4	121.5 (3)	H7A—C7—H7C	109.5
C5—C4—C3	117.7 (3)	H7B—C7—H7C	109.5
O1—N—C6—C5	−1.5 (5)	O3—C3—C4—C5	−178.4 (3)
O2—N—C6—C5	178.6 (3)	C2—C3—C4—C5	1.8 (5)
O1—N—C6—C1	177.3 (3)	O3—C3—C4—C7	1.4 (5)
O2—N—C6—C1	−2.6 (5)	C2—C3—C4—C7	−178.3 (3)
C6—C1—C2—C3	−1.0 (5)	C3—C4—C5—C6	−1.5 (5)
C2—C1—C6—C5	1.2 (5)	C7—C4—C5—C6	178.6 (3)
C2—C1—C6—N	−177.5 (3)	C4—C5—C6—C1	0.0 (5)
C1—C2—C3—O3	179.7 (3)	C4—C5—C6—N	178.8 (3)
C1—C2—C3—C4	−0.5 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3A···O2^{i}	0.82	2.10	2.770 (4)	138
C7—H7C···O1^{ii}	0.96	2.57	3.505 (5)	165

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

Fig. 1

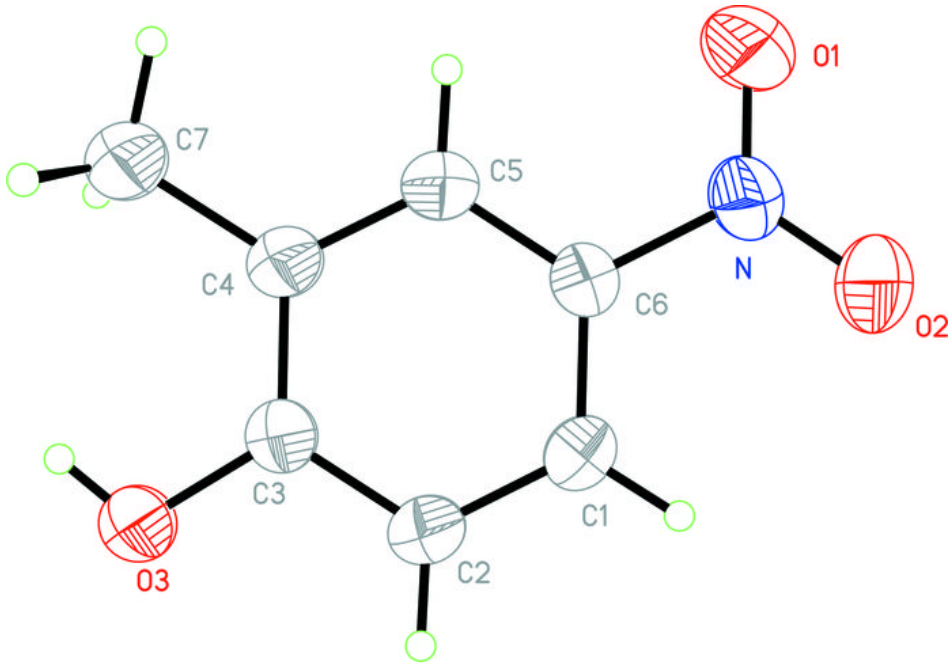

Fig. 2