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# 2-Methyl-4-nitrophenol

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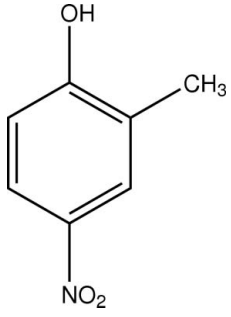
Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.054; $wR$ factor = 0.181; data-to-parameter ratio = 12.2.

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
$\beta$ = 100.71 (3)°
$V$ = 690.4 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.12 mm$^{-1}$
$T$ = 294 K
0.30 × 0.20 × 0.10 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ 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—H3$A$···O2$^{i}$ | 0.82 | 2.10 | 2.770 (4) | 138 |
| C7—H7$C$···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).

## References

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# supporting information

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## 2-Methyl-4-nitrophenol

**Sheng Bi, Yong-Zhong Wu, Yi-Xin Zhou, Jian-Guo Tang and Cheng Guo**

### S1. 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.

### S2. 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.

### S3. 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.

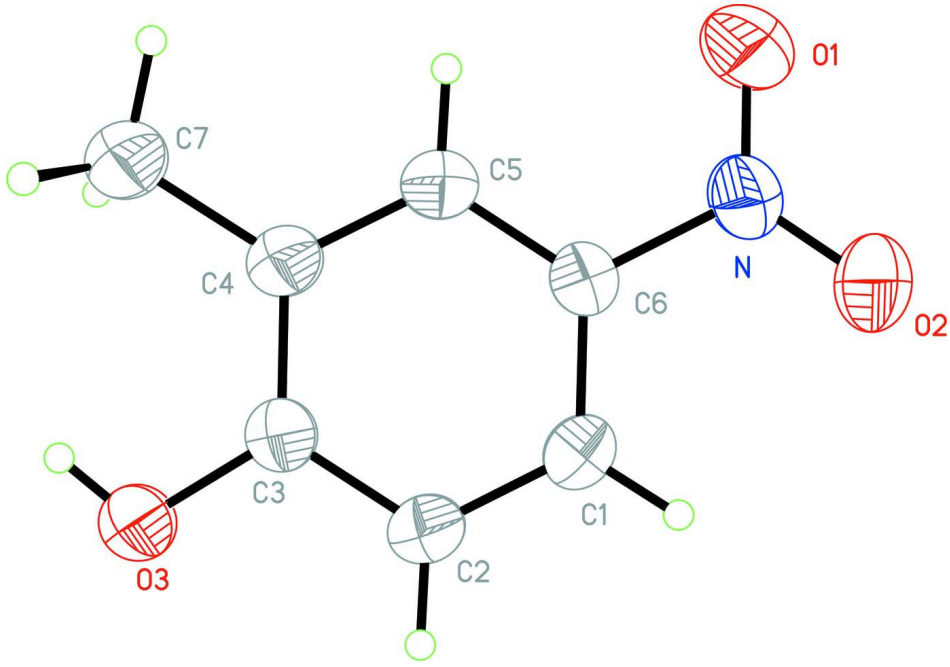


**Figure 1**

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

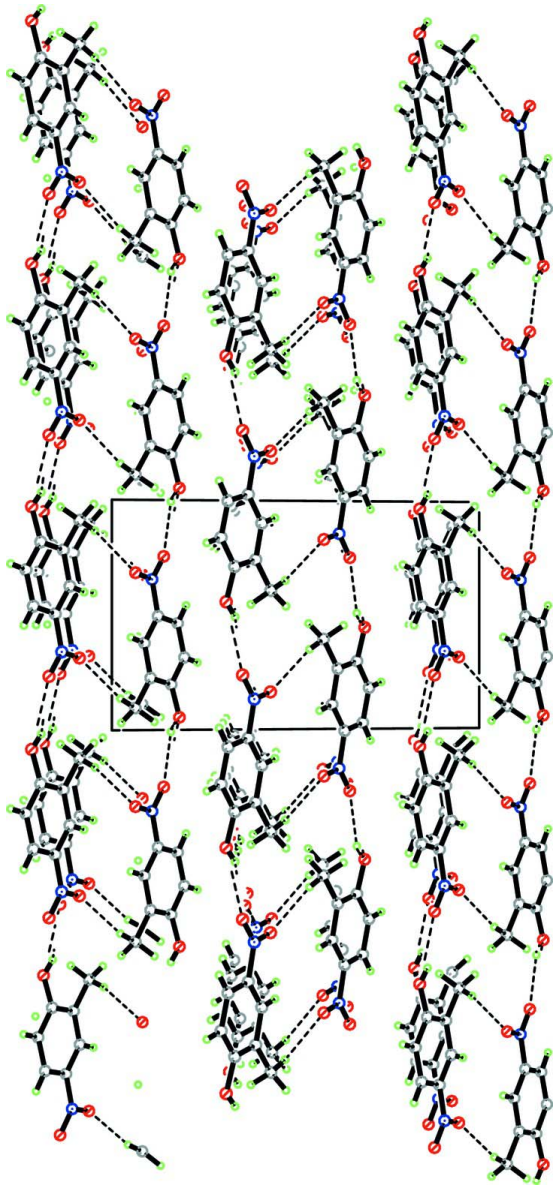

**Figure 2**

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

### 2-Methyl-4-nitrophenol

*Crystal data*

$C_7H_7NO_3$
$M_r = 153.14$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 5.6210\ (11)$ Å
$b = 8.7420\ (17)$ Å
$c = 14.300\ (3)$ Å
$\beta = 100.71\ (3)°$
$V = 690.4\ (2)$ Å$^3$
$Z = 4$

$F(000) = 320$
$D_x = 1.473$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9–13°$
$\mu = 0.12$ mm$^{-1}$
$T = 294$ K
Block, colorless
0.30 × 0.20 × 0.10 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ 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
$\theta_{max}$ = 25.3°, $\theta_{min}$ = 2.7°
$h$ = 0→6
$k$ = 0→10
$l$ = −17→16
3 standard reflections every 120 min
intensity decay: 1%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.181
$S$ = 1.01
1245 reflections
102 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
$w = 1/[\sigma^2(F_o^2) + (0.08P)^2 + 0.74P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.017 (4)

*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 | −0.3440 (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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H3*A*···O2$^{i}$ | 0.82 | 2.10 | 2.770 (4) | 138 |
| C7—H7*C*···O1$^{ii}$ | 0.96 | 2.57 | 3.505 (5) | 165 |

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