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# 6-Methylnicotinic acid

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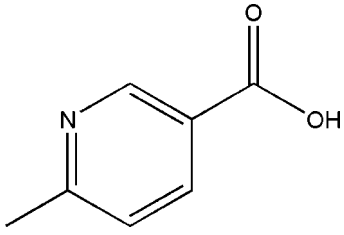
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.049; $wR$ factor = 0.126; data-to-parameter ratio = 8.3.

All non-H atoms of the title compound, $C_7H_7NO_2$, are nearly coplaner, the r.m.s. deviation being 0.0087 Å. In the crystal, the partially overlapped arrangement and the face-to-face distance of 3.466 (17) Å between parallel pyridine rings of neighboring molecules indicates the existence of $\pi$–$\pi$ stacking. Intermolecular O—H···N hydrogen bonding and weak C—H···O hydrogen bonding are present in the crystal structure.

## Related literature

The title compound is an intermediate of the drug etoricoxib (systematic name: 5-chloro-6′-methyl-3-[4-(methylsulfonyl)-phenyl]- 2,3′-bipyridine). For the structure of etoricoxibium picrate, see: Jasinski *et al.* (2011).




## Experimental

### Crystal data

$C_7H_7NO_2$ $M_r$ = 137.14
Monoclinic, $P2_1$
$a$ = 3.8788 (8) Å
$b$ = 13.634 (3) Å
$c$ = 6.1094 (12) Å
$\beta$ = 90.51 (3)°
$V$ = 323.07 (12) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 293 K
0.20 × 0.20 × 0.20 mm

### Data collection

Rigaku SCXmini diffractometer
3358 measured reflections
763 independent reflections
634 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.059

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.126
$S$ = 1.05
763 reflections
92 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···N1$^{i}$ | 0.82 | 1.87 | 2.664 (4) | 163 |
| C4—H4$A$···O2$^{ii}$ | 0.93 | 2.54 | 3.350 (4) | 146 |

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

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: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *SHELXL97*.

This work was supported by the National Natural Science Foundation of China (Ppoject 20671019)

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5270).

## References

Brandenburg, K. & Putz, H. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Jasinski, J. P., Butcher, R. J., Siddegowda, M. S., Yathirajan, H. S. & Ramesha, A. R. (2011). *Acta Cryst.* E**67**, o107–o108.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2011). E**67**, o2345 [doi:10.1107/S1600536811031837]

## 6-Methylnicotinic acid

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### S1. Comment

The title compound is the drug intermediate of etoricoxib (a non- steroidal anti-inflammatory drug for the treatment of arthritis and osteoarthritis) (Jasinski *et al.*, 2011). As part of our interest in the intermediate, we report here the crystal structure of the title compound.

The molecular structure of the title compound is shown in Fig. 1. All the non-H atoms are almost located in one plane as the atoms O1 and O2 are shifted 0.0377 and 0.0236 Å out of the pyridine ring plane, respectively.

The crystal structure is stabilized by intermolecular O—H···N and C—H···O hydrogen bonds (Table 1). $\pi\cdots\pi$ stacking is present between pyridine rings of the neighboring molecules.

### S2. Experimental

6-Methyl-nicotinic acid was purchased commercially. Crystals suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution.

### S3. Refinement

All H atoms were fixed geometrically and treated as riding with C—H ($CH_3$) = 0.96 Å or C—H (CH) = 0.93 Å and O—H = 0.82 Å with $U_{iso}$(H) =1.5 $U_{eq}$(C,O) for methyl and carboxyl H atoms and $U_{iso}$(H) = 1.2$U_{eq}$(C) for the others. Friedel pairs were merged as no significant anomalous scatterings.

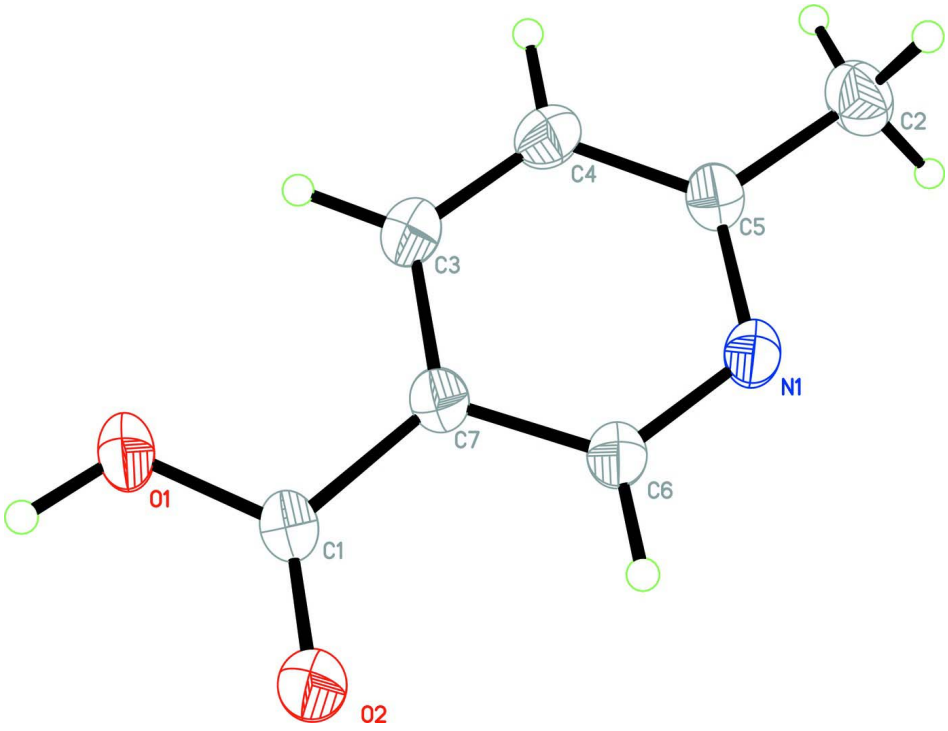


**Figure 1**

The molecular structure of the title compound with atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

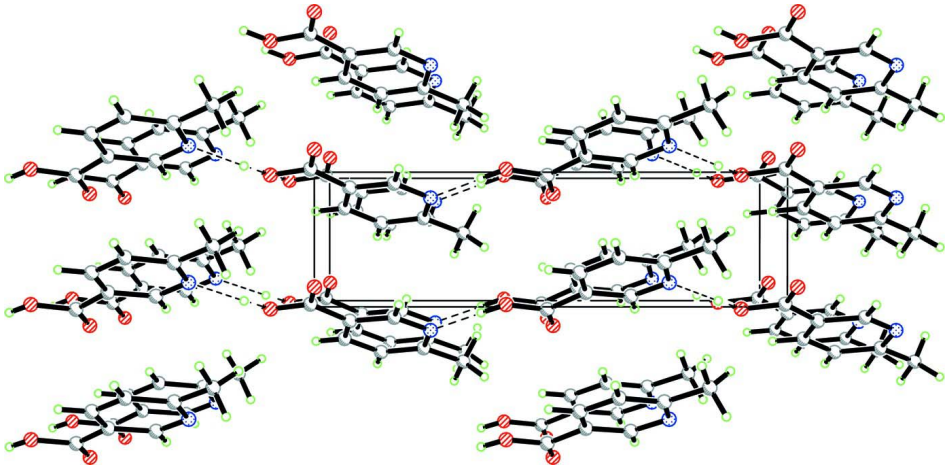

**Figure 2**

Packing diagram.

### 6-Methylnicotinic acid

*Crystal data*

$C_7H_7NO_2$
$M_r = 137.14$
Monoclinic, $P2_1$
Hall symbol: P 2yb

$a = 3.8788\ (8)$ Å
$b = 13.634\ (3)$ Å
$c = 6.1094\ (12)$ Å
$\beta = 90.51\ (3)°$

$V$ = 323.07 (12) Å$^3$
$Z$ = 2
$F$(000) = 144
$D_x$ = 1.410 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 764 reflections

$\theta$ = 3.3–27.5°
$\mu$ = 0.11 mm$^{-1}$
$T$ = 293 K
Prism, colorless
0.20 × 0.20 × 0.20 mm

*Data collection*

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm$^{-1}$
CCD_Profile_fitting scans
3358 measured reflections

763 independent reflections
634 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.059
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 3.3°
$h$ = −5→4
$k$ = −17→17
$l$ = −7→7

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.126
$S$ = 1.05
763 reflections
92 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
$w = 1/[\sigma^2(F_o^2) + (0.0712P)^2 + 0.0005P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 | 0.0195 (8) | 0.40438 (18) | 0.9514 (4) | 0.0631 (8) |
| H1 | −0.0573 | 0.3629 | 1.0349 | 0.095* |
| O2 | −0.1535 (7) | 0.50696 (18) | 1.2089 (4) | 0.0675 (8) |
| C1 | −0.0216 (7) | 0.4918 (2) | 1.0367 (5) | 0.0440 (7) |
| C2 | 0.4505 (10) | 0.8121 (3) | 0.5202 (7) | 0.0574 (9) |
| H2A | 0.5640 | 0.8578 | 0.6162 | 0.086* |
| H2B | 0.2546 | 0.8431 | 0.4526 | 0.086* |
| H2C | 0.6080 | 0.7911 | 0.4092 | 0.086* |
| C3 | 0.2600 (8) | 0.5539 (3) | 0.6920 (6) | 0.0465 (8) |
| H3A | 0.2823 | 0.4902 | 0.6394 | 0.056* |
| C4 | 0.3724 (8) | 0.6311 (3) | 0.5713 (5) | 0.0482 (8) |
| H4A | 0.4753 | 0.6202 | 0.4366 | 0.058* |

| | | | | |
|---|---|---|---|---|
| C5 | 0.3345 (9) | 0.7257 (3) | 0.6479 (5) | 0.0423 (7) |
| C6 | 0.0802 (8) | 0.6670 (2) | 0.9593 (5) | 0.0439 (8) |
| H6A | −0.0207 | 0.6796 | 1.0940 | 0.053* |
| N1 | 0.1857 (8) | 0.74310 (17) | 0.8408 (4) | 0.0453 (7) |
| C7 | 0.1119 (9) | 0.5709 (2) | 0.8942 (5) | 0.0395 (7) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.1000 (19) | 0.0295 (13) | 0.0602 (16) | −0.0059 (12) | 0.0191 (14) | 0.0014 (11) |
| O2 | 0.107 (2) | 0.0408 (16) | 0.0551 (13) | −0.0023 (14) | 0.0297 (14) | −0.0016 (11) |
| C1 | 0.0556 (18) | 0.0312 (16) | 0.0452 (16) | −0.0007 (15) | 0.0018 (14) | 0.0039 (14) |
| C2 | 0.063 (2) | 0.048 (2) | 0.0615 (19) | −0.0032 (17) | 0.0127 (17) | 0.0114 (17) |
| C3 | 0.054 (2) | 0.0369 (18) | 0.0483 (15) | 0.0028 (14) | 0.0021 (14) | −0.0069 (14) |
| C4 | 0.0549 (17) | 0.047 (2) | 0.0432 (16) | 0.0036 (15) | 0.0089 (13) | −0.0069 (15) |
| C5 | 0.0446 (16) | 0.0364 (17) | 0.0460 (16) | 0.0002 (14) | 0.0013 (13) | 0.0022 (14) |
| C6 | 0.0542 (19) | 0.0347 (18) | 0.0431 (16) | 0.0006 (14) | 0.0076 (15) | 0.0002 (13) |
| N1 | 0.0578 (16) | 0.0310 (16) | 0.0472 (14) | 0.0019 (12) | 0.0085 (13) | −0.0009 (10) |
| C7 | 0.0437 (16) | 0.0338 (17) | 0.0409 (15) | 0.0005 (11) | −0.0005 (13) | 0.0026 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.311 (4) | C3—C7 | 1.387 (4) |
| O1—H1 | 0.8200 | C3—H3A | 0.9300 |
| O2—C1 | 1.192 (3) | C4—C5 | 1.380 (5) |
| C1—C7 | 1.482 (4) | C4—H4A | 0.9300 |
| C2—C5 | 1.485 (5) | C5—N1 | 1.337 (4) |
| C2—H2A | 0.9600 | C6—N1 | 1.332 (4) |
| C2—H2B | 0.9600 | C6—C7 | 1.375 (5) |
| C2—H2C | 0.9600 | C6—H6A | 0.9300 |
| C3—C4 | 1.359 (5) | | |
| | | | |
| C1—O1—H1 | 109.5 | C3—C4—C5 | 120.3 (3) |
| O2—C1—O1 | 124.3 (3) | C3—C4—H4A | 119.9 |
| O2—C1—C7 | 123.2 (3) | C5—C4—H4A | 119.9 |
| O1—C1—C7 | 112.6 (2) | N1—C5—C4 | 120.8 (3) |
| C5—C2—H2A | 109.5 | N1—C5—C2 | 117.2 (3) |
| C5—C2—H2B | 109.5 | C4—C5—C2 | 121.9 (3) |
| H2A—C2—H2B | 109.5 | N1—C6—C7 | 123.8 (3) |
| C5—C2—H2C | 109.5 | N1—C6—H6A | 118.1 |
| H2A—C2—H2C | 109.5 | C7—C6—H6A | 118.1 |
| H2B—C2—H2C | 109.5 | C6—N1—C5 | 118.6 (3) |
| C4—C3—C7 | 119.4 (3) | C6—C7—C3 | 117.1 (3) |
| C4—C3—H3A | 120.3 | C6—C7—C1 | 119.4 (3) |
| C7—C3—H3A | 120.3 | C3—C7—C1 | 123.5 (3) |
| | | | |
| C7—C3—C4—C5 | −1.0 (4) | N1—C6—C7—C1 | −178.6 (3) |
| C3—C4—C5—N1 | −0.3 (5) | C4—C3—C7—C6 | 1.4 (4) |

| | | | |
|---|---|---|---|
| C3—C4—C5—C2 | −179.4 (4) | C4—C3—C7—C1 | 179.3 (3) |
| C7—C6—N1—C5 | −0.7 (5) | O2—C1—C7—C6 | −1.0 (5) |
| C4—C5—N1—C6 | 1.2 (5) | O1—C1—C7—C6 | 178.6 (3) |
| C2—C5—N1—C6 | −179.7 (4) | O2—C1—C7—C3 | −178.8 (3) |
| N1—C6—C7—C3 | −0.6 (5) | O1—C1—C7—C3 | 0.7 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···N1$^{i}$ | 0.82 | 1.87 | 2.664 (4) | 163 |
| C4—H4*A*···O2$^{ii}$ | 0.93 | 2.54 | 3.350 (4) | 146 |

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