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5-Methyl-2-pyridone

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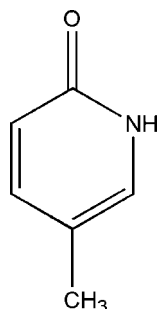
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.054; wR factor = 0.163; data-to-parameter ratio = 18.8.

The crystal structure of the title compound, $\text{C}_6\text{H}_7\text{NO}$, is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, resulting in inversion dimers. The structure is further consolidated by weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For related structures, see: Boris-Marko *et al.* (2008); Vovk *et al.* (2003).



Experimental

Crystal data

$\text{C}_6\text{H}_7\text{NO}$
 $M_r = 109.13$
Monoclinic, $C2/c$

$a = 12.965$ (3) Å
 $b = 9.7154$ (19) Å
 $c = 10.908$ (2) Å

$\beta = 118.96$ (3)°
 $V = 1202.3$ (4) Å³
 $Z = 8$
Mo $K\alpha$ radiation

$\mu = 0.08$ mm⁻¹
 $T = 293$ K
 $0.30 \times 0.23 \times 0.20$ mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan
(*CrystalClear*; Rigaku, 2005)
 $T_{\min} = 0.977$, $T_{\max} = 0.984$

5961 measured reflections
1369 independent reflections
670 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.049$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$
 $wR(F^2) = 0.163$
 $S = 0.99$
1369 reflections

73 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.12$ e Å⁻³
 $\Delta\rho_{\min} = -0.17$ e Å⁻³

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|-------|-------------|-------------|---------------|
| $\text{N1}-\text{H1A}\cdots\text{O1}^{\text{i}}$ | 0.86 | 1.94 | 2.800 (2) | 173 |
| $\text{C3}-\text{H3A}\cdots\text{O1}^{\text{ii}}$ | 0.93 | 2.46 | 3.334 (3) | 157 |
| $\text{C5}-\text{H5A}\cdots\text{O1}^{\text{iii}}$ | 0.93 | 2.33 | 3.260 (3) | 178 |

Symmetry codes: (i) $-x + \frac{1}{2}, -y + \frac{3}{2}, -z$; (ii) $x, -y + 2, z + \frac{1}{2}$; (iii) $x + \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$.

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2442).

References

- Boris-Marko, K., Popović, Z., Pavlović, G. & Rajić-Linarić, M. (2008). *J. Mol. Struct.* **882**, 47–55.
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supplementary materials

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5-Methyl-2-pyridone

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Comment

The title compound is characterized by an enol-keto tautomerism due to the labile hydrogen atom of OH-group in α -position to the basic pyridine N atom which can easily migrate to N atom (Boris-Marko *et al.*, 2008) resulting in a zwitterionic molecule (Fig. 1).

The O1 and C6 atoms located on the pyridine ring are conplanar with the ring, deviating by 0.015 (3) and 0.35 (4) Å, respectively, from the ring plane. The crystal structure is stabilized by intermolecular N—H \cdots O hydrogen bonds and further consolidated by C—H \cdots O interactions (Fig. 2 and Tab. 1).

Experimental

To a solution of the title compound (0.2 g) in acetone (2 ml) and ethanol (10 ml) was added was prepared by stirred at room temperature and then placed in a dark place. Colourless single crystals suitable for X-ray diffraction study were obtained by slow evaporation of the solution over a period of 8 d.

Refinement

Positional parameters of all H atoms were calculated geometrically and refined using a riding model, with N—H = 0.086 Å and C—H = 0.93 and 0.96 Å for aryl and methyl type H-atoms, respectively, and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{N/C-aryl})$ or $1.5 U_{\text{eq}}(\text{C-methyl})$.

Figures

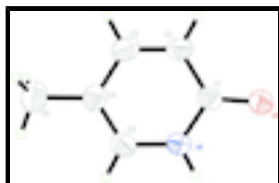


Fig. 1. An ORTEP view of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

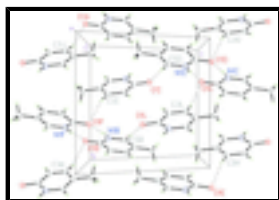


Fig. 2. Unit cell packing of the title compound showing H-bonding interactions.

5-Methyl-2-pyridone

Crystal data

| | |
|--------------------------------|---|
| C_6H_7NO | $F(000) = 464$ |
| $M_r = 109.13$ | $D_x = 1.206 \text{ Mg m}^{-3}$ |
| Monoclinic, $C2/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| Hall symbol: $-C 2yc$ | Cell parameters from 1369 reflections |
| $a = 12.965 (3) \text{ \AA}$ | $\theta = 3.6\text{--}27.5^\circ$ |
| $b = 9.7154 (19) \text{ \AA}$ | $\mu = 0.08 \text{ mm}^{-1}$ |
| $c = 10.908 (2) \text{ \AA}$ | $T = 293 \text{ K}$ |
| $\beta = 118.96 (3)^\circ$ | Prism, colourless |
| $V = 1202.3 (4) \text{ \AA}^3$ | $0.30 \times 0.23 \times 0.20 \text{ mm}$ |
| $Z = 8$ | |

Data collection

| | |
|---|--|
| Rigaku SCXmini diffractometer | 1369 independent reflections |
| Radiation source: fine-focus sealed tube graphite | 670 reflections with $I > 2\sigma(I)$ |
| Detector resolution: $13.6612 \text{ pixels mm}^{-1}$ | $R_{\text{int}} = 0.049$ |
| CCD_Profile_fitting scans | $\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.6^\circ$ |
| Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku, 2005) | $h = -16 \rightarrow 16$ |
| $T_{\text{min}} = 0.977$, $T_{\text{max}} = 0.984$ | $k = -12 \rightarrow 12$ |
| 5961 measured reflections | $l = -14 \rightarrow 14$ |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.054$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.163$ | H-atom parameters constrained |
| $S = 0.99$ | $w = 1/[\sigma^2(F_o^2) + (0.0734P)^2]$ |
| 1369 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 73 parameters | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| 0 restraints | $\Delta\rho_{\text{max}} = 0.12 \text{ e \AA}^{-3}$ |
| | $\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$ |

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|---------------|----------------------------------|
| N1 | 0.28530 (13) | 0.79540 (16) | 0.17990 (16) | 0.0616 (5) |
| H1A | 0.3148 | 0.7521 | 0.1353 | 0.074* |
| O1 | 0.11700 (11) | 0.82537 (15) | -0.02634 (14) | 0.0730 (5) |
| C1 | 0.17371 (17) | 0.8437 (2) | 0.1049 (2) | 0.0600 (6) |
| C2 | 0.13100 (19) | 0.9133 (2) | 0.1852 (2) | 0.0718 (7) |
| H2A | 0.0549 | 0.9488 | 0.1410 | 0.086* |
| C5 | 0.35432 (18) | 0.8107 (2) | 0.3216 (2) | 0.0672 (6) |
| H5A | 0.4300 | 0.7740 | 0.3655 | 0.081* |
| C4 | 0.3147 (2) | 0.8781 (2) | 0.3988 (2) | 0.0665 (6) |
| C3 | 0.1989 (2) | 0.9291 (2) | 0.3250 (2) | 0.0750 (7) |
| H3A | 0.1679 | 0.9755 | 0.3743 | 0.090* |
| C6 | 0.3897 (2) | 0.8989 (2) | 0.5532 (3) | 0.0978 (9) |
| H6A | 0.4652 | 0.8566 | 0.5840 | 0.147* |
| H6B | 0.3520 | 0.8578 | 0.6013 | 0.147* |
| H6C | 0.4000 | 0.9956 | 0.5734 | 0.147* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|-------------|-------------|-------------|--------------|-------------|--------------|
| N1 | 0.0493 (10) | 0.0718 (12) | 0.0626 (11) | 0.0060 (8) | 0.0263 (9) | -0.0035 (8) |
| O1 | 0.0544 (9) | 0.1007 (12) | 0.0615 (11) | 0.0047 (7) | 0.0262 (8) | 0.0016 (8) |
| C1 | 0.0469 (12) | 0.0662 (13) | 0.0683 (15) | 0.0002 (9) | 0.0290 (12) | 0.0079 (11) |
| C2 | 0.0635 (13) | 0.0820 (16) | 0.0773 (17) | 0.0145 (11) | 0.0401 (14) | 0.0034 (12) |
| C5 | 0.0574 (13) | 0.0666 (14) | 0.0704 (15) | -0.0003 (10) | 0.0252 (12) | -0.0006 (11) |
| C4 | 0.0713 (15) | 0.0644 (14) | 0.0624 (15) | -0.0024 (11) | 0.0312 (13) | -0.0048 (11) |
| C3 | 0.0834 (17) | 0.0739 (15) | 0.0807 (18) | 0.0098 (12) | 0.0500 (15) | -0.0020 (12) |
| C6 | 0.109 (2) | 0.102 (2) | 0.0722 (18) | -0.0037 (14) | 0.0354 (17) | -0.0110 (13) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------|-----------|--------|-----------|
| N1—C1 | 1.355 (2) | C5—H5A | 0.9300 |
| N1—C5 | 1.368 (2) | C4—C3 | 1.406 (3) |
| N1—H1A | 0.8600 | C4—C6 | 1.496 (3) |
| O1—C1 | 1.266 (2) | C3—H3A | 0.9300 |
| C1—C2 | 1.414 (3) | C6—H6A | 0.9600 |
| C2—C3 | 1.351 (3) | C6—H6B | 0.9600 |
| C2—H2A | 0.9300 | C6—H6C | 0.9600 |
| C5—C4 | 1.350 (3) | | |

supplementary materials

| | | | |
|-----------|-------------|------------|-----------|
| C1—N1—C5 | 124.56 (18) | C5—C4—C3 | 115.9 (2) |
| C1—N1—H1A | 117.7 | C5—C4—C6 | 122.1 (2) |
| C5—N1—H1A | 117.7 | C3—C4—C6 | 122.0 (2) |
| O1—C1—N1 | 119.97 (19) | C2—C3—C4 | 122.6 (2) |
| O1—C1—C2 | 125.48 (19) | C2—C3—H3A | 118.7 |
| N1—C1—C2 | 114.55 (19) | C4—C3—H3A | 118.7 |
| C3—C2—C1 | 121.1 (2) | C4—C6—H6A | 109.5 |
| C3—C2—H2A | 119.4 | C4—C6—H6B | 109.5 |
| C1—C2—H2A | 119.4 | H6A—C6—H6B | 109.5 |
| C4—C5—N1 | 121.30 (19) | C4—C6—H6C | 109.5 |
| C4—C5—H5A | 119.3 | H6A—C6—H6C | 109.5 |
| N1—C5—H5A | 119.3 | H6B—C6—H6C | 109.5 |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------------|-------|-------------|-------------|---------------|
| N1—H1A \cdots O1 ⁱ | 0.86 | 1.94 | 2.800 (2) | 173 |
| C3—H3A \cdots O1 ⁱⁱ | 0.93 | 2.46 | 3.334 (3) | 157 |
| C5—H5A \cdots O1 ⁱⁱⁱ | 0.93 | 2.33 | 3.260 (3) | 178 |

Symmetry codes: (i) $-x+1/2, -y+3/2, -z$; (ii) $x, -y+2, z+1/2$; (iii) $x+1/2, -y+3/2, z+1/2$.

Fig. 1

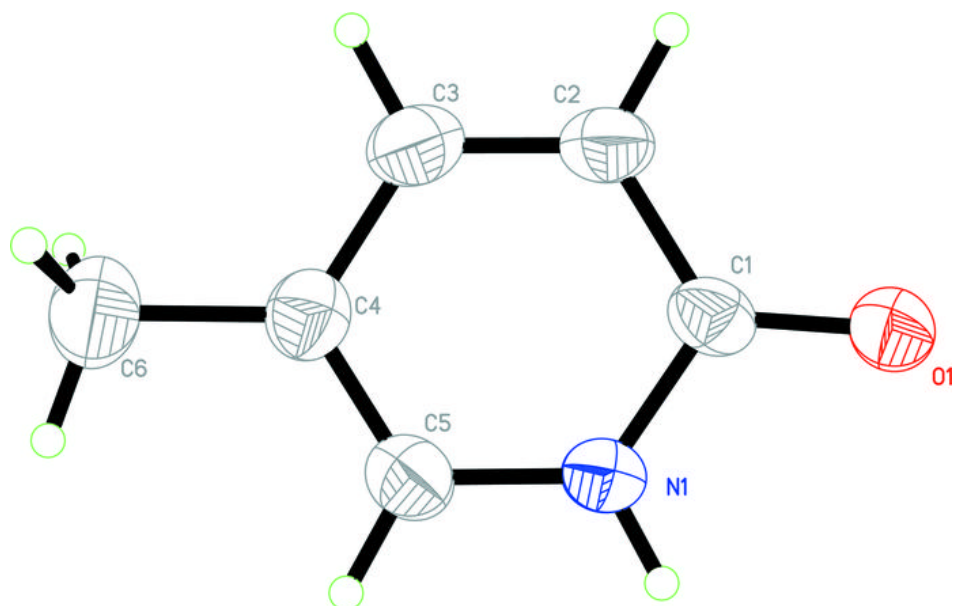


Fig. 2

