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Ethyl 6-(hydroxymethyl)picolinate

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The title complex, $C_9H_{11}NO_3$, was synthesized from dimethyl pyridine-2,6-dicarboxylate. A single weak intermolecular O—H···N hydrogen bond links molecules into a one-dimensional zigzag chain.

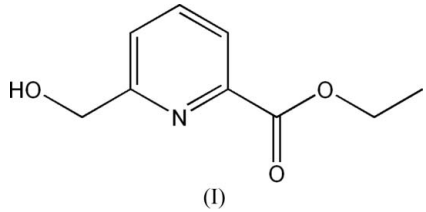
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.153
Data-to-parameter ratio = 17.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Pyridine derivatives are important intermediates widely used in the synthesis of drugs (Wachter *et al.*, 1998; Jew *et al.*, 2003) and pesticides (Li *et al.*, 2006; Mu *et al.*, 2003). 2,6-Disubstituted pyridine derivatives are very useful ligands for the construction of metal complexes (Mohamed & El-Gamel, 2005; Alcock *et al.*, 2005; Joensson *et al.*, 2004). The title compound, (I), can be used directly to coordinate transition-metal atoms (Kapoor *et al.*, 2004; Goher *et al.*, 2003; Swiatek-Kozlowska *et al.*, 2002). We report here its crystal structure.



(I)

The molecular structure of (I) is shown in Fig. 1. Molecules are linked into a one-dimensional supramolecular zigzag chain through a single weak intermolecular O—H···N hydrogen bond (Table 1 and Fig. 2).

Experimental

To dimethyl pyridine-2,6-dicarboxylate (3.68 g, 0.019 mol) was added ethanol (50 ml). After the reaction mixture had been cooled to 273 K,

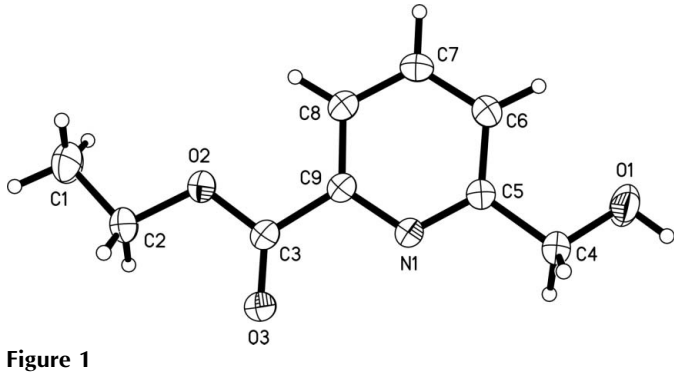


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level and H atoms shown as small spheres of arbitrary radius.

$NaBH_4$ (0.72 g, 0.019 mol) was added portionwise over 10 min. The mixture was stirred for 30 min at room temperature and then refluxed for 10 h. After cooling to room temperature, the solvent was removed by distillation at reduced pressure. Acetone (15 ml) was added to the residue and the mixture was refluxed for 1 h. After concentration, aqueous K_2CO_3 (15 ml) was added and the mixture was refluxed for 1 h. The mixture was then cooled to room temperature and extracted with EtOAc (10 × 10 ml). The organic layer was dried with anhydrous Na_2SO_4 and evaporated *in vacuo* to give a residue. The crude product was purified by column chromatography (SiO_2–EtOAc) to afford the title compound as a colorless solid (yield 72%).

Crystal data

$C_9H_{11}NO_3$
M_r = 181.19
Monoclinic, $P2_1/c$
a = 6.8871 (14) Å
b = 9.0494 (18) Å
c = 15.250 (4) Å
β = 106.86 (3)°
V = 909.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.38 × 0.32 × 0.25 mm

Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.963, T_{max} = 0.975
8654 measured reflections
2083 independent reflections
1120 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.153
S = 0.98
2083 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1E···N1^{i}	0.84	2.05	2.833 (2)	154

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

All H atoms were positioned geometrically and allowed to ride on their respective parent atoms, with C—H = 0.95–0.99 Å, O—H = 0.84 Å and U_{iso}(H) = 1.2U_{eq}(C), 1.5U_{eq}(methyl C) or 1.5U_{eq}(O).

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*b*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*b*); molecular graphics: *SHELXTL* (Sheldrick, 1997*a*); software used to prepare material for publication: *SHELXTL*.

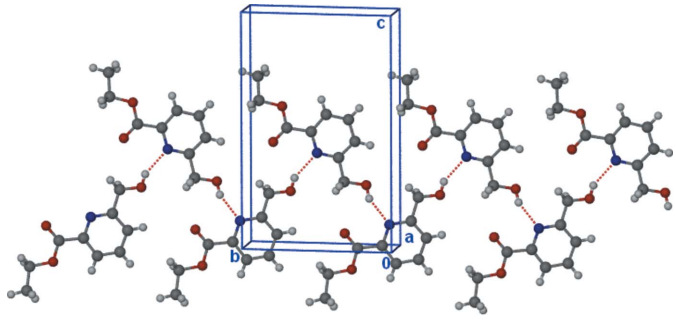


Figure 2
A view of the one-dimensional zigzag chain. Hydrogen bonds are indicated by dashed lines.

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