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Dimethyl pyridine-2,6-dicarboxylate

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The title molecule, $C_9H_9NO_4$, possesses crystallographically imposed twofold rotation symmetry. In the crystal structure, the molecules are stacked into ladders extended along the *c* axis, with a short intermolecular O···C contact of 3.297 (2) Å. The crystal packing is stabilized by carbonyl dipolar interactions and van der Waals forces.

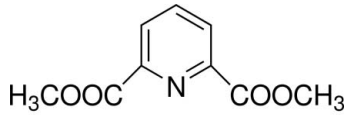
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.117
Data-to-parameter ratio = 15.6

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-Substituted pyridine derivatives are very powerful 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 title molecule (Fig. 1) possesses crystallographically imposed twofold rotation symmetry and shows normal values for bond lengths and angles. In the crystal structure, the molecules are stacked into ladders extended along the *c* axis with a short intermolecular O2···C4^{i} contact of 3.297 (2) Å [symmetry code: (i) $1-x, -y, 1-z$], indicating a significant carbonyl–carbonyl dipolar interaction (Desiraju, 1996). The crystal packing (Fig. 2) is further stabilized by van der Waals forces.

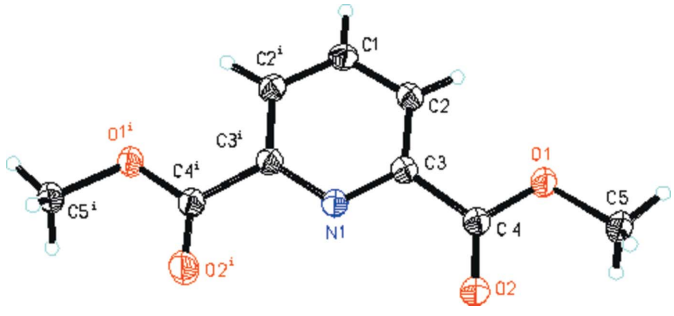


Figure 1
View of (I), showing displacement ellipsoids drawn at the 30% probability level and the atomic numbering. [Symmetry code: (i) $-x+1, y, -z+\frac{3}{2}$.]

Experimental

Pyridine-2,6-dicarboxylic acid (1.67 g, 10 mmol) and anhydrous methanol (30 ml) were stirred in a round-bottomed flask, and $SOCl_2$ (2.2 ml, 30 mmol) was added dropwise at 273 K. The reaction mixture was heated to 298 K and stirred for another 24 h. After removal of the solvent *in vacuo*, the residue was dissolved in EtOAc, washed with aqueous NaOH (5%), and then dried with anhydrous Na_2SO_4. After removal of the solvent *in vacuo*, the solid was recrystallized from water to give the desired product (yield 86%) within 4 d.

Crystal data

$C_9H_9NO_4$
M_r = 195.17
Monoclinic, $C2/c$
a = 13.345 (3) Å
b = 6.817 (1) Å
c = 11.033 (2) Å
β = 118.49 (3)°
V = 882.2 (4) Å^3
Z = 4
D_x = 1.470 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 293 (2) K
Block, colourless
0.43 × 0.32 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.956, T_{max} = 0.981
4148 measured reflections
1011 independent reflections
743 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.118
S = 1.10
1011 reflections
65 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0701P)^2 + 0.0632P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

All H atoms were positioned geometrically, with C—H = 0.93–0.96 Å, and allowed to ride on their parent atoms, with U_{iso} = 1.2–1.5U_{eq}(C).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *CrystalStructure* and *PLATON* (Spek, 2003).

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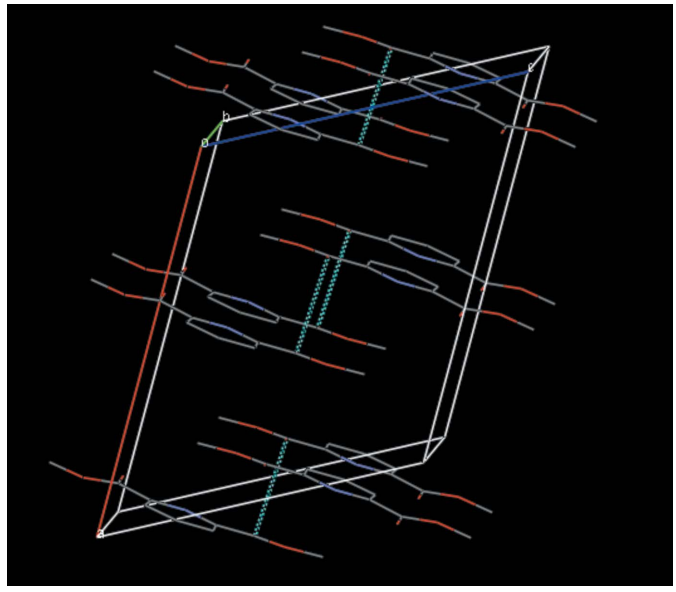

Figure 2
The packing, viewed along the *b* axis, showing the short intermolecular C···O contacts as dashed lines.

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