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Methyl 3-(3-pyridylmethylene)carbazate

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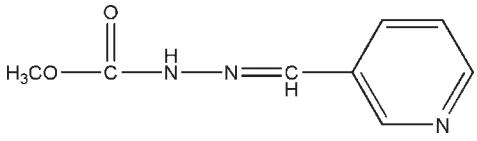
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.128; data-to-parameter ratio = 16.8.

In the crystal of the title compound, $C_8H_9N_3O_2$, molecules are linked by N—H···N hydrogen bonds, forming $S(7)$ chains propagating in [010].

Related literature

For background to Schiff bases, see: Cimerman *et al.* (1997).



Experimental

Crystal data

$C_8H_9N_3O_2$
M_r = 179.18
Orthorhombic, *Pbca*
a = 10.585 (2) Å
b = 10.019 (2) Å
c = 16.311 (3) Å
V = 1729.8 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.26 × 0.21 × 0.19 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
15411 measured reflections
1984 independent reflections
1794 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.128
S = 1.08
1984 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N4^{i}	0.86	2.12	2.9751 (14)	171

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5196).

References

Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cimerman, Z., Galic, N. & Bosner, B. (1997). *Anal. Chim. Acta*, **343**, 145–153.
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supporting information

Acta Cryst. (2009). E**65**, o2959 [https://doi.org/10.1107/S1600536809045024]

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S1. Experimental

A mixture of nicotinaldehyde (0.1 mol), and methyl carbazate (0.1 mol) was stirred in refluxing ethanol (20 mL) for 4 h to afford the title compound (0.082 mol, yield 82%). Colourless blocks of (I) were obtained by recrystallization from ethanol at room temperature.

S2. Refinement

H atoms were fixed geometrically and allowed to ride on their attached atoms.

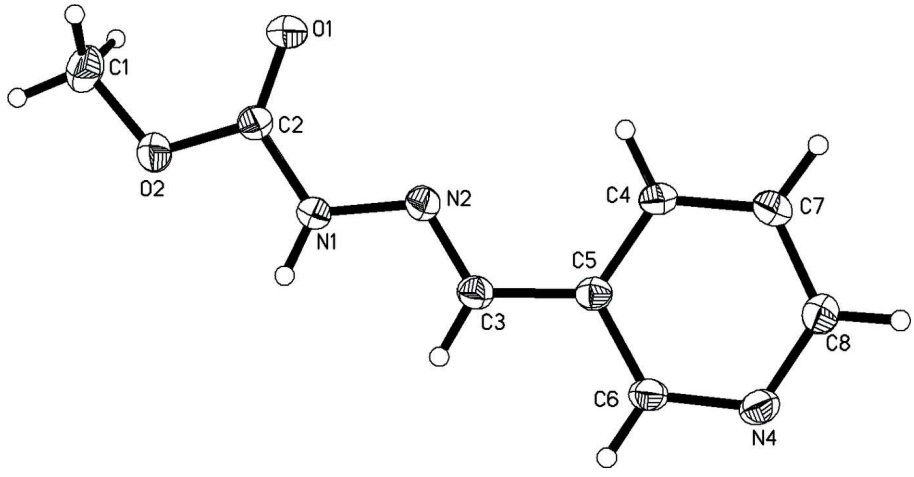

Figure 1

The structure of the title compound showing 30% probability displacement ellipsoids.

Methyl 3-(3-pyridylmethylene)carbazate

Crystal data

$C_8H_9N_3O_2$
$M_r = 179.18$
Orthorhombic, *Pbca*
$a = 10.585$ (2) Å
$b = 10.019$ (2) Å
$c = 16.311$ (3) Å
$V = 1729.8$ (6) Å^3
$Z = 8$
$F(000) = 752$
$D_x = 1.376$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1985 reflections
$\theta = 3.4$–27.5°
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Block, colourless
0.26 × 0.21 × 0.19 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
15411 measured reflections
1984 independent reflections
1794 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -13 \rightarrow 13$
$k = -13 \rightarrow 12$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.128$
$S = 1.08$
1984 reflections
118 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
$w = 1/[\sigma^2(F_o^2) + (0.0867P)^2 + 0.1822P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.18815 (8)	0.11348 (8)	0.57072 (5)	0.0433 (2)
C3	0.35300 (9)	−0.17778 (10)	0.74434 (7)	0.0343 (3)
H3A	0.4286	−0.1375	0.7291	0.041*
N4	0.48145 (8)	−0.43908 (10)	0.88319 (6)	0.0390 (3)
C5	0.35393 (9)	−0.28611 (10)	0.80449 (6)	0.0311 (2)
N1	0.26042 (8)	−0.03820 (9)	0.65555 (6)	0.0372 (2)
H1A	0.3336	−0.0124	0.6391	0.045*
C4	0.24493 (9)	−0.34567 (12)	0.83549 (7)	0.0377 (3)
H4B	0.1656	−0.3156	0.8194	0.045*
N2	0.24948 (8)	−0.13809 (9)	0.71265 (5)	0.0345 (2)
C2	0.15392 (9)	0.01936 (10)	0.62537 (6)	0.0339 (3)
O1	0.04701 (7)	−0.00686 (10)	0.64392 (6)	0.0541 (3)
C6	0.46946 (9)	−0.33613 (11)	0.83129 (6)	0.0358 (3)
H6A	0.5428	−0.2957	0.8120	0.043*
C8	0.37535 (11)	−0.49405 (11)	0.91219 (7)	0.0393 (3)
H8A	0.3819	−0.5651	0.9486	0.047*
C7	0.25615 (10)	−0.44962 (12)	0.89025 (7)	0.0414 (3)

H7A	0.1845	−0.4896	0.9123	0.050*
C1	0.08717 (14)	0.19038 (13)	0.53648 (8)	0.0523 (3)
H1B	0.1209	0.2546	0.4987	0.078*
H1C	0.0430	0.2359	0.5796	0.078*
H1D	0.0298	0.1322	0.5082	0.078*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0420 (5)	0.0450 (5)	0.0429 (5)	0.0031 (3)	0.0027 (3)	0.0115 (3)
C3	0.0289 (5)	0.0385 (5)	0.0355 (5)	−0.0040 (4)	−0.0007 (4)	0.0006 (4)
N4	0.0315 (5)	0.0440 (5)	0.0415 (5)	0.0086 (4)	−0.0001 (4)	0.0016 (4)
C5	0.0289 (5)	0.0341 (5)	0.0302 (5)	−0.0005 (4)	−0.0009 (3)	−0.0034 (4)
N1	0.0277 (4)	0.0426 (5)	0.0413 (5)	−0.0042 (3)	−0.0005 (3)	0.0102 (4)
C4	0.0257 (5)	0.0467 (6)	0.0407 (6)	−0.0008 (4)	−0.0037 (4)	0.0042 (4)
N2	0.0325 (4)	0.0364 (5)	0.0346 (4)	−0.0039 (3)	−0.0018 (3)	0.0033 (3)
C2	0.0324 (5)	0.0363 (5)	0.0330 (5)	−0.0018 (4)	−0.0015 (4)	0.0005 (4)
O1	0.0284 (4)	0.0685 (6)	0.0656 (6)	−0.0020 (4)	−0.0018 (4)	0.0220 (5)
C6	0.0263 (5)	0.0430 (6)	0.0380 (5)	0.0009 (4)	0.0026 (4)	−0.0003 (4)
C8	0.0400 (6)	0.0373 (5)	0.0407 (5)	0.0030 (4)	−0.0004 (4)	0.0038 (4)
C7	0.0312 (5)	0.0465 (6)	0.0463 (6)	−0.0069 (4)	0.0005 (4)	0.0064 (5)
C1	0.0603 (8)	0.0478 (6)	0.0489 (7)	0.0117 (6)	−0.0049 (6)	0.0102 (5)

Geometric parameters (Å, º)

O2—C2	1.3472 (13)	N1—H1A	0.8600
O2—C1	1.4312 (15)	C4—C7	1.3771 (16)
C3—N2	1.2752 (13)	C4—H4B	0.9300
C3—C5	1.4631 (14)	C2—O1	1.2005 (13)
C3—H3A	0.9300	C6—H6A	0.9300
N4—C8	1.3373 (14)	C8—C7	1.3850 (15)
N4—C6	1.3403 (14)	C8—H8A	0.9300
C5—C6	1.3920 (13)	C7—H7A	0.9300
C5—C4	1.3940 (13)	C1—H1B	0.9600
N1—C2	1.3586 (13)	C1—H1C	0.9600
N1—N2	1.3719 (12)	C1—H1D	0.9600
C2—O2—C1	115.73 (9)	O2—C2—N1	108.28 (9)
N2—C3—C5	120.59 (9)	N4—C6—C5	123.96 (9)
N2—C3—H3A	119.7	N4—C6—H6A	118.0
C5—C3—H3A	119.7	C5—C6—H6A	118.0
C8—N4—C6	117.44 (9)	N4—C8—C7	122.77 (10)
C6—C5—C4	117.33 (9)	N4—C8—H8A	118.6
C6—C5—C3	118.92 (8)	C7—C8—H8A	118.6
C4—C5—C3	123.73 (8)	C4—C7—C8	119.29 (10)
C2—N1—N2	119.05 (8)	C4—C7—H7A	120.4
C2—N1—H1A	120.5	C8—C7—H7A	120.4
N2—N1—H1A	120.5	O2—C1—H1B	109.5

C7—C4—C5	119.18 (9)	O2—C1—H1C	109.5
C7—C4—H4B	120.4	H1B—C1—H1C	109.5
C5—C4—H4B	120.4	O2—C1—H1D	109.5
C3—N2—N1	115.47 (8)	H1B—C1—H1D	109.5
O1—C2—O2	124.99 (10)	H1C—C1—H1D	109.5
O1—C2—N1	126.73 (10)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N4^{i}	0.86	2.12	2.9751 (14)	171

Symmetry code: (i) −*x*+1, *y*+1/2, −*z*+3/2.