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1,4-Dimethyl-1,5,6,7-tetrahydro-2*H*-cyclopenta[*b*]pyridin-2-one

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In the pyridone ring of the title compound, $C_{10}H_{13}NO$, single and double bonds alternate, though allowing some degree of delocalization.

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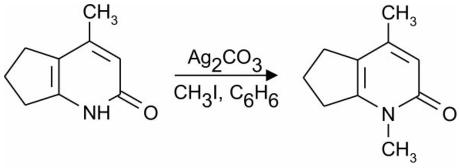
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.103
Data-to-parameter ratio = 15.7

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

Comment

In the course of our systematic study of the size effect of cycloalkane fragments on the reactivity of pyridine–based heterocycles, we have described earlier the crystal structure of 4-methyl-1,5,6,7-tetrahydro-2*H*-cyclopenta[*b*]pyridin-2-one, (1) (Albov, Mazina *et al.*, 2004). Our attempt to increase the yield in the reaction of *O*-methylation (Albov, Rybakov *et al.*, 2004), using excess methyl iodide, caused the subsequent methylation at the N atom and led to the title compound, (2) (Fig. 1).



(1) (2)

In the planar pyridone ring (N1/C9) of (2) the single and double bonds alternate, though allowing some degree of delocalization. Atom C7 is displaced from the plane of the pyridone ring by 0.179 (2) Å. Methylation of the N atom excludes hydrogen bonding and greatly changes the packing, but, in general, the structure of the bicyclic ring systems in (1) and (2) are identical.

Experimental

1,5,6,7-Tetrahydro-2*H*-cyclopenta[*b*]pyridin-2-one (6.48 g), (1), methyl iodide (12.35 g) and silver carbonate (6.00 g) were boiled in benzene (70 ml) for 50 h. The reaction flask was protected against light. The mixture was then filtered and the solvent was evaporated (yield 3.14 g, 38%). The product was recrystallized from benzene (m.p. 383 K). ^{1}H NMR (DMSO-d_6, 400 MHz, p.p.m.): 2.05 (*s*, 3H, 10-CH_3), 2.10 (*m*, 2H, 7-CH_2), 2.68 (*t*, 2H, 6-CH_2), 2.90 (*t*, 3H, 8-CH_3), 3.31 (*s*, 3H, 11-CH_3), 5.96 (*s*, 1H, 3-CH).

Crystal data

$C_{10}H_{13}NO$
M_r = 163.21
Monoclinic, $P2_1/c$
a = 9.7125 (15) Å
b = 6.8262 (16) Å
c = 15.285 (3) Å
β = 121.233 (11)°
V = 866.5 (3) Å^3
Z = 4

D_x = 1.251 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 30–33°
μ = 0.64 mm^{-1}
T = 293 (2) K
Prism, colourless
0.43 × 0.40 × 0.36 mm

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Data collection

Enraf–Nonius CAD-4 diffractometer
Non-profiled ω scans
Absorption correction: none
1740 measured reflections
1740 independent reflections
1183 reflections with $I > 2\sigma(I)$

$\theta_{\max} = 74.9°$
$h = -12 \rightarrow 10$
$k = 0 \rightarrow 8$
$l = 0 \rightarrow 16$
1 standard reflection every 200 reflections intensity decay: 2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.103$
$S = 0.87$
1740 reflections
111 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0733P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C9	1.3666 (16)	C4—C10	1.4940 (19)
N1—C2	1.4027 (18)	C5—C9	1.3490 (17)
N1—C11	1.4574 (17)	C5—C6	1.5052 (18)
C2—O2	1.2469 (16)	C6—C7	1.537 (2)
C2—C3	1.427 (2)	C7—C8	1.525 (2)
C3—C4	1.3568 (19)	C8—C9	1.5044 (18)
C4—C5	1.4232 (18)		
C9—N1—C2	120.81 (10)	C9—C5—C4	119.64 (11)
C9—N1—C11	120.91 (12)	C9—C5—C6	111.04 (12)
C2—N1—C11	118.28 (11)	C4—C5—C6	129.21 (12)
O2—C2—N1	119.67 (13)	C5—C6—C7	103.41 (11)
O2—C2—C3	124.94 (14)	C8—C7—C6	107.84 (12)
N1—C2—C3	115.38 (11)	C9—C8—C7	102.93 (11)
C4—C3—C2	123.92 (13)	C5—C9—N1	122.57 (12)
C3—C4—C5	117.55 (12)	C5—C9—C8	112.87 (11)
C3—C4—C10	122.49 (13)	N1—C9—C8	124.55 (11)
C5—C4—C10	119.93 (12)		

In (2), H atoms were included in calculated positions and refined as riding atoms. Calculated C—H bond lengths are in the range 0.93–0.97 Å. For methyl H atoms, $U_{\rm iso}$ values were set equal to $1.5U_{\rm eq}$ of the carrier atoms; for other H atoms, $U_{\rm iso}$ values were set to $1.2U_{\rm eq}$ of the carrier atoms.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

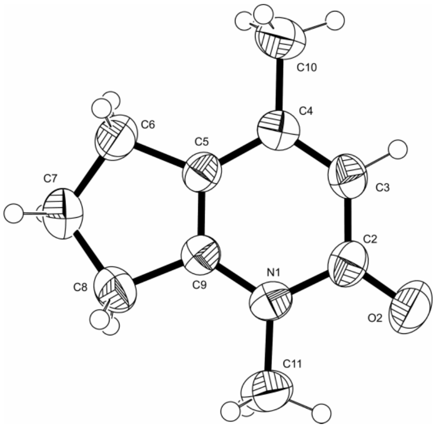

Figure 1
ORTEP-3 (Farrugia, 1997) view of (2), with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

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