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## Structure Reports

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## Key indicators

Single-crystal X-ray study
$T=293 \mathrm{~K}$
Mean $\sigma(\mathrm{C}-\mathrm{C})=0.002 \AA$
$R$ factor $=0.045$
$w R$ 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.

In the pyridone ring of the title compound, $\mathrm{C}_{10} \mathrm{H}_{13} \mathrm{NO}$, single and double bonds alternate, though allowing some degree of delocalization.

## 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-2H-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 ( $\mathrm{N} 1 / \mathrm{C} 9$ ) 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) $\AA$. 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 $3.14 \mathrm{~g}, 38 \%$ ). The product was recrystallized from benzene (m.p. 383 K ). ${ }^{1} \mathrm{H}$ NMR (DMSO- $d_{6}, 400 \mathrm{MHz}$, p.p.m.): 2.05 ( $s, 3 \mathrm{H}, 10-$ $\mathrm{CH}_{3}$ ), $2.10\left(\mathrm{~m}, 2 \mathrm{H}, 7-\mathrm{CH}_{2}\right), 2.68\left(t, 2 \mathrm{H}, 6-\mathrm{CH}_{2}\right), 2.90\left(t, 3 \mathrm{H}, 8-\mathrm{CH}_{3}\right)$, $3.31\left(s, 3 H, 11-\mathrm{CH}_{3}\right), 5.96(s, 1 \mathrm{H}, 3-\mathrm{CH})$.

## Crystal data

$$
\begin{aligned}
& \mathrm{C}_{10} \mathrm{H}_{13} \mathrm{NO} \\
& M_{r}=163.21 \\
& \text { Monoclinic, } P 2_{1} / c \\
& a=9.7125(15) \AA \\
& b=6.8262(16) \AA \\
& c=15.285(3) \AA \\
& \beta=121.233(11)^{\circ} \\
& V=866.5(3) \AA^{3} \\
& Z=4
\end{aligned}
$$

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## Data collection

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

## Refinement

Refinement on $F^{2}$
$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.045$
$w R\left(F^{2}\right)=0.103$
$S=0.87$
1740 reflections
111 parameters

$$
\begin{aligned}
& \theta_{\max }=74.9^{\circ} \\
& h=-12 \rightarrow 10 \\
& k=0 \rightarrow 8 \\
& l=0 \rightarrow 16 \\
& 1 \text { standard reflection } \\
& \quad \text { every } 200 \text { reflections } \\
& \text { intensity decay: } 2 \%
\end{aligned}
$$

H -atom parameters constrained
$w=1 /\left[\sigma^{2}\left(F_{o}{ }^{2}\right)+(0.0733 P)^{2}\right]$
where $P=\left(F_{o}{ }^{2}+2 F_{c}{ }^{2}\right) / 3$
$(\Delta / \sigma)_{\max }<0.001$
$\Delta \rho_{\max }=0.18 \mathrm{e} \mathrm{A}^{-3}$
$\Delta \rho_{\min }=-0.16 \mathrm{e}^{-3}$

Table 1
Selected geometric parameters $\left(\AA^{\circ},^{\circ}\right)$.

| 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 $\mathrm{C}-\mathrm{H}$ bond lengths are in the range $0.93-$ $0.97 \AA$. For methyl H atoms, $U_{\text {iso }}$ values were set equal to $1.5 U_{\text {eq }}$ of the carrier atoms; for other H atoms, $U_{\text {iso }}$ values were set to $1.2 U_{\text {eq }}$ of the carrier atoms.

Data collection: CAD-4 EXPRESS (Enraf-Nonius, 1994); cell refinement: CAD-4 EXPRESS; data reduction: XCAD4 (Harms \& Wocadlo, 1995); program(s) used to solve structure: SHELXS97


Figure 1
ORTEP-3 (Farrugia, 1997) view of (2), with the atom numbering scheme. Displacement ellipsoids are drawn at the $50 \%$ probability level.
(Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

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