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4-Methyl-1-(3-nitrophenacyl)-5,6,7,8-tetrahydroquinolin-2(1*H*)-one

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In the pyridone ring of the title compound, $C_{18}H_{18}N_2O_4$, single and double bonds alternate, showing some degree of conjugation.

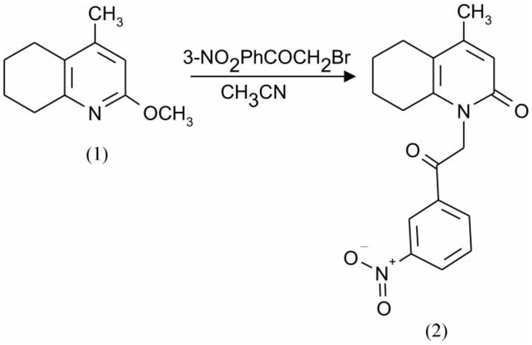
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.129
Data-to-parameter ratio = 14.2

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 effect of the size of cycloalkane fragments on the reactivity of pyridine-based heterocycles, we have previously described the crystal structure of 2-methoxy-4-methyl-5,6,7,8-tetrahydroquinoline, (1) (Albov *et al.*, 2004*a*). We report here the crystal structure of 4-methyl-1-(3-nitrophenacyl)-5,6,7,8-tetrahydroquinolin-2(1*H*)-one, (2) (Fig. 1).



In the planar pyridone ring N1—C10 of (2), the single and double bonds alternate, showing some degree of delocalization. Atoms C6, C7 and C8 are displaced from this plane by −0.144 (4), 0.258 (4) and 0.332 (5) Å, respectively. Atoms C12, C13, O13, N2 and O21 lie in the plane of the benzene ring; only atom O22 is displaced from the plane by 0.136 (3) Å, and the torsion angle O13—C13—C14—C15 is 0.0 (2)°. It is evident that the 3-nitrobenzoyl fragment is completely conjugated. The dihedral angle between the benzene and pyridone rings is 85.45 (6)°. These angles are almost the same as in the 4-chlorophenacyl relative, but do not agree with cycloheptene and cyclooctene derivatives (Albov *et al.*, 2004*b*,*c*).

Experimental

Compound (1) (4.00 g) and 3-nitrophenacyl bromide (4.10 g) were boiled in acetonitrile for 6 h. When thin-layer chromatography showed only traces of the source compounds in the solution, the solvent was evaporated and the product washed with acetone (yield 3.83 g, 52%). The product was recrystallized from acetone (m.p. 441–443 K). ^{1}H NMR (DMSO-d_6, 400 MHz, p.p.m.): 1.73 (*m*, 4H, 7-CH_2 + 8-CH_2), 2.12 (*s*, 3H, 11-CH_3), 2.48 (*m*, 4H, 6-CH_2 + 9-CH_2), 5.56 (*s*, 2H, 12-CH_2), 6.13 (*s*, 1H, 3-CH), 7.84 (*t*, 1H, 16-CH), 8.49 (*m*, 2H, 15-CH + 17-CH), 8.80 (*s*, 1H, 19-CH).

Crystal data

$C_{18}H_{18}N_2O_4$
$M_r = 326.34$
Triclinic, $P\overline{1}$
$a = 9.115$ (3) Å
$b = 9.271$ (3) Å
$c = 11.248$ (3) Å
$\alpha = 92.00$ (2)°
$\beta = 105.09$ (2)°
$\gamma = 118.82$ (2)°
$V = 789.5$ (5) Å^3

$Z = 2$
$D_x = 1.373$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 12$–14°
$\mu = 0.10$ mm^{-1}
$T = 293$ (2) K
Prism, light yellow
0.25 × 0.24 × 0.22 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Non-profiled ω scans
Absorption correction: none
3103 measured reflections
3103 independent reflections
1936 reflections with $I > 2\sigma(I)$

$\theta_{\max} = 26.0°$
$h = -11 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = 0 \rightarrow 13$
1 standard reflection every 200 reflections
intensity decay: 8%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.129$
$S = 1.06$
3103 reflections
218 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0704P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.15$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C2	1.391 (3)	C7—C8	1.526 (4)
N1—C10	1.399 (2)	C8—C9	1.493 (4)
N1—C12	1.450 (2)	C9—C10	1.533 (3)
C2—O2	1.225 (3)	C12—C13	1.509 (3)
C2—C3	1.414 (2)	C13—O13	1.210 (3)
C3—C4	1.356 (3)	C13—C14	1.475 (2)
C4—C5	1.434 (3)	C18—N2	1.454 (3)
C4—C11	1.495 (3)	N2—O22	1.202 (2)
C5—C10	1.351 (3)	N2—O21	1.233 (2)
C5—C6	1.517 (3)		
C6—C7	1.531 (4)		
C2—N1—C10	123.62 (14)	C9—C8—C7	122.5 (2)
C2—N1—C12	115.07 (15)	C8—C9—C10	112.8 (2)
C10—N1—C12	121.23 (16)	C5—C10—N1	120.12 (17)
O2—C2—N1	121.02 (16)	C5—C10—C9	124.37 (18)
O2—C2—C3	125.00 (18)	N1—C10—C9	115.50 (16)
N1—C2—C3	113.90 (16)	N1—C12—C13	114.26 (15)
C4—C3—C2	123.90 (18)	O13—C13—C14	121.47 (15)
C3—C4—C5	119.34 (17)	O13—C13—C12	120.32 (16)
C3—C4—C11	120.02 (19)	C14—C13—C12	118.21 (14)
C5—C4—C11	120.63 (19)	C17—C18—N2	118.21 (15)
C10—C5—C4	118.61 (17)	C19—C18—N2	119.15 (15)
C10—C5—C6	123.68 (19)	O22—N2—O21	121.65 (18)
C4—C5—C6	117.71 (17)	O22—N2—C18	120.14 (18)
C5—C6—C7	113.9 (2)	O21—N2—C18	118.20 (14)
C8—C7—C6	118.4 (2)		

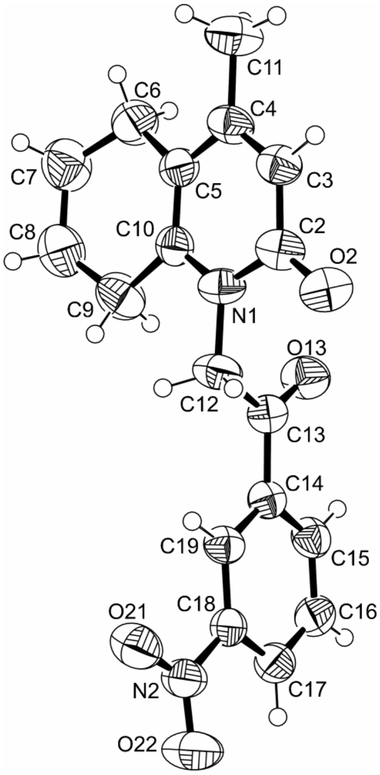


Figure 1
ORTEP-3 view (Farrugia, 1997) of (2) with the atom-numbering scheme. Atomic displacement ellipsoids are drawn at the 50% probability level.

All H atoms were positioned geometrically and refined as riding (C—H = 0.93–0.97 Å), with $U_{\rm iso}$(H) = 1.2 or $1.5U_{\rm eq}$(C). The methyl group was allowed to rotate but not to tip.

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).

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References

Albov, D. V., Rybakov, V. B., Babaev, E. V. & Aslanov, L. A. (2004*a*). *Crystallogr. Rep.* **49**, 430–436.
Albov, D. V., Rybakov, V. B., Babaev, E. V. & Aslanov, L. A. (2004*b*). *Acta Cryst.* E**60**, o894–o895.
Albov, D. V., Rybakov, V. B., Babaev, E. V. & Aslanov, L. A. (2004*c*). *Acta Cryst.* E**60**, o1219–o1221.
Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Enraf–Nonius (1994). *CAD*-4 *EXPRESS*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Harms, K. & Wocadlo, S. (1995). *XCAD*4. University of Marburg, Germany.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Acta Cryst. (2004). E**60**, o1952–o1953 Dmitry V. Albov *et al.* • $C_{18}H_{18}N_2O_4$ **o1953**