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1-Acetyl-3-ethyl-*r*-2,*c*-6-di-2-furylpiperidin-4-one

S. Balamurugan,[a] A. Thiruvalluvar,[a]* A. Manimekalai,[b] K. Selvaraju[b] and T. Maruthavanan[b]

[a]Department of Physics, Rajah Serfoji Govt College (Autonomous), Thanjavur 613 005, Tamil Nadu, India, and [b]Department of Chemistry, Annamalai University, Annamalai Nagar 608 002, Tamil Nadu, India

Correspondence e-mail: athiru@vsnl.net

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.166
Data-to-parameter ratio = 13.4

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

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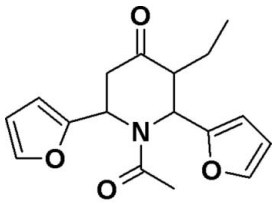
In the title molecule, $C_{17}H_{19}NO$, the piperidine ring adopts a chair conformation. The acetyl group in the 1-position and ethyl group in the 3-position each have an equatorial orientation. The furyl rings at positions 2 and 6 have axial orientations.

Comment

Electron-withdrawing groups (–NO, –CHO, $–NCOCH_3$ and –CONH-phenyl) attached to the heterocycle profoundly affect its conformation and the orientation of the substituents in 2,6-dialkyl- and 2,6-diaryl-substituted piperidines. In the title compound, (I), the N-substituted piperidine ring contains the furyl rings in positions 2 and 6. Saturated six-membered rings normally adopt a chair conformation with equatorial orientations for the majority of the substituents (Manimekalai *et al.*, 2000; Bhavani *et al.*, 2000; Krishnapillay *et al.*, 2000; Srinivasan *et al.*, 2004). The present X-ray crystal structure determination has been undertaken to establish the conformation of the N-substituted piperidine ring in (I).



(I)

In (I) (Fig. 1), all bond lengths and angles are normal. The piperidine ring adopts a chair conformation. The mean plane of atoms C2/C3/C5/C6 and the furyl rings attached to C2 and C6 make dihedral angles of 80.1 (1) and 74.53 (1)°, respectively. The dihedral angle between the two furyl rings is 25.9 (1)°. The acetyl group at N1 is oriented in an equatorial position. The furyl rings are both in axial positions.

Experimental

A mixture of 3-ethyl-r-2,c-6-di-2′-furylpiperidin-4-one (3.01 g, 0.01 mol), acetic acid (3 ml, 0.03 mol) and triethylamine (3 ml, 0.03 mol) was refluxed for 6–8 h. The reaction mixture was cooled to room temperature and poured into ice-cold water. The solid mass which separated was filtered off, dried and recrystallized from petroleum ether (333–353 K). The yield of the isolated product was 1.5 g (50%) (m.p. 353 K).

Crystal data

$C_{17}H_{19}NO_4$
M_r = 301.33
Monoclinic, $P2_1/n$
a = 8.036 (4) Å
b = 8.5608 (15) Å
c = 22.180 (7) Å
β = 91.05 (3)°
V = 1525.5 (9) Å^3
Z = 4
D_x = 1.312 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Prism, colourless
0.30 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.973, T_{max} = 0.982
2881 measured reflections
2676 independent reflections
1866 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 25.0°
2 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.166
S = 1.04
2676 reflections
200 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.095P)^2 + 0.4568P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.008 (2)

The H atoms were positioned geometrically and allowed to ride on their parent atoms with C–H = 0.93–0.98 Å and U_{iso} = 1.2–1.5 U_{eq}(parent atom).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1997); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2004); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

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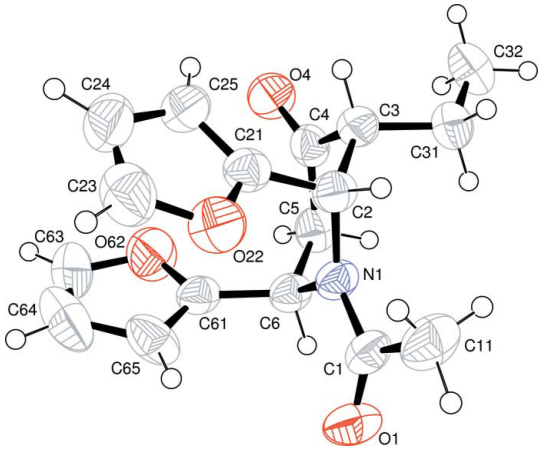

Figure 1
View of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

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1-Acetyl-3-ethyl-*r*-2,*c*-6-di-2-furylpiperidin-4-one. Corrigendum

S. Balamurugan,[a] A. Thiruvalluvar,[a]* A. Manimekalai,[b] K. Selvaraju[b] and T. Maruthavanan[b]

[a]Department of Physics, Rajah Serfoji Govt College (Autonomous), Thanjavur 613 005, Tamil Nadu, India, and [b]Department of Chemistry, Annamalai University, Annamalai Nagar 608 002, Tamil Nadu, India

Correspondence e-mail: athiru@vsnl.net

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In the paper by Balamurugan, Thiruvalluvar, Manimekalai, Selvaraju & Maruthavanan [*Acta Cryst.* (2006), E**62**, o2005–o2006], the two first sentences in the *Abstract* contain errors. The correct text is "In the title molecule, $C_{17}H_{19}NO_4$, the piperidine ring adopts a chair conformation. The acetyl group in the 1-position and the ethyl group in the 3-position have equatorial and axial orientations, respectively".