

1,3-Dimethyl-2-oxo-4,6-diphenyl-1,2,3,4-tetrahydropyridine-3-carbonitrile

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The crystal structure of the title compound, C₂₀H₁₈N₂O, reveals a distorted half-chair conformation of the central tetrahydropyridine (THP) ring, with the cyano- and adjacent phenyl-substituted C atoms displaced by 0.329 (1) and -0.315 (1) Å, respectively, from the THP best plane. Steric interactions force the phenyl rings out of the THP plane by 49.21 (9) and 65.76 (5)°. The cyano moiety is coplanar with the THP plane.

Comment

In order to study the influence of substituents of different sizes upon the structural parameters of the molecule, we report here the crystal structure of 1,3-dimethyl-2-oxo-4,6-diphenyl-1,2,3,4-tetrahydropyridine-3-carbonitrile, (I). The crystal structures of the analogous diethyl and dibenzyl derivatives of tetrahydropyridine have been reported previously (Patel *et al.*, 2001, 2002).

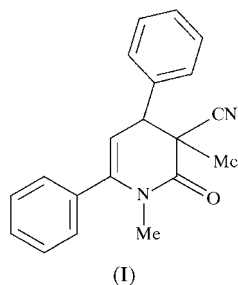


Fig. 1 depicts the structure of the molecule of (I), and selected bond lengths and angles are given in Table 1. The structure of (I) has the same characteristic molecular dimensions as are observed for similar compounds of this class (Patel

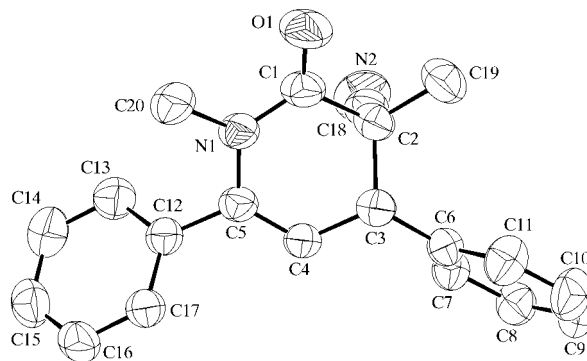


Figure 1

A view of the molecular structure of (I) showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

et al., 2001, 2002). The bonds C1—C2, C2—C3 and C3—C4 [1.548 (2), 1.554 (2) and 1.494 (2) Å, respectively] have predominantly single-bond character, whereas the C1—N1 distance of 1.361 (2) Å suggests a partial double bond. The lengthening of C2—C3 and C3—C4, and the contraction of the C2—C3—C4 angle [107.9 (1)°], may be attributed to the comparatively heavy substituent at C3 (a phenyl ring). These values are similar to those found in the other derivatives of THP that we have reported recently (Patel *et al.*, 2001, 2002).

The triple-bond character of C18—N2 [1.135 (3) Å], and the C2—C18—N2 angle of 177.8 (2)° defining the linearity of the cyano moiety, are typical of this group of 3-cyano-2-pyridine compounds (Black *et al.*, 1992; Hussain *et al.*, 1996).

The methyl group at C2 is out of the plane of the THP ring by 0.627 (3) Å, whereas that at N1 is coplanar with the THP plane. Both the phenyl rings are planar within themselves. Steric interactions force the phenyl rings out of the THP plane by 49.21 (9) and 65.76 (5)°. However, these dihedral angles are in a much smaller range than those reported for similar compounds (Patel *et al.*, 2001, 2002; Hursthouse *et al.*, 1992).

The torsion angles about C2—C18 are as follows, with values for the diethyl and dibenzyl substituents, respectively, given inside the brackets: C1—C2—C18—N2 = 107 (5)° [-126 (8) and -164 (2)°] and C3—C2—C18—N2 = -136 (5)° [113 (8) and 74 (2)°]. These observations reveal that the molecular conformation in all these compounds differs significantly about the C2—C18 bond.

In summary, these results show that, although the molecule of (I) preserves the same characteristic molecular dimensions as analogous compounds, the molecular conformation is influenced by the size of the substituents. As usual in heterocyclic compounds, weak van der Waals forces are responsible for the stability of the structure.

Experimental

Compound (I) was synthesized according to the method of Shah (2000). Full details of the synthesis will be published elsewhere. Thin needle-shaped crystals of (I) were grown from a chloroform–ethanol solution by slow evaporation. The crystal density was measured by flotation in an aqueous potassium iodide solution.

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Crystal data

$C_{20}H_{18}N_2O$	$D_m = 1.204 \text{ Mg m}^{-3}$
$M_r = 302.36$	D_m measured by flotation
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation
$a = 13.738 (3) \text{ \AA}$	Cell parameters from 25 reflections
$b = 7.4751 (16) \text{ \AA}$	$\theta = 25\text{--}35^\circ$
$c = 17.1566 (18) \text{ \AA}$	$\mu = 0.60 \text{ mm}^{-1}$
$\beta = 110.117 (13)^\circ$	$T = 293 (2) \text{ K}$
$V = 1654.4 (5) \text{ \AA}^3$	Needle, colourless
$Z = 4$	$0.2 \times 0.1 \times 0.1 \text{ mm}$
$D_x = 1.214 \text{ Mg m}^{-3}$	

Data collection

Enraf–Nonius CAD-4 diffractometer	2548 reflections with $I > 2\sigma(I)$
$\omega/2\theta$ scans	$\theta_{\text{max}} = 68^\circ$
Absorption correction: empirical via ψ scan (North <i>et al.</i> , 1968)	$h = 0 \rightarrow 16$
$T_{\text{min}} = 0.931$, $T_{\text{max}} = 0.942$	$k = 0 \rightarrow 8$
3141 measured reflections	2 standard reflections
3141 independent reflections	frequency: 60 min
	intensity decay: 1%

Refinement

Refinement on F^2	$(\Delta/\sigma)_{\text{max}} = 0.034$
$R[F^2 > 2\sigma(F^2)] = 0.046$	$\Delta\rho_{\text{max}} = 0.36 \text{ e \AA}^{-3}$
$wR(F^2) = 0.141$	$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
$S = 1.06$	Extinction correction: <i>SHELXL97</i>
3010 reflections	(Sheldrick, 1997)
220 parameters	Extinction coefficient: 0.0042 (5)
H-atom parameters constrained	

H atoms were treated as riding, with C–H = 0.93–0.98 Å, and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H and $1.2U_{\text{eq}}(\text{C})$ for all others.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Table 1

Selected geometric parameters (Å, °).

O1–C1	1.212 (2)	C5–C12	1.482 (2)
N1–C1	1.361 (2)	C3–C6	1.512 (2)
N1–C5	1.421 (2)	C2–C18	1.470 (3)
N1–C20	1.461 (2)	C2–C19	1.522 (3)
N2–C18	1.135 (3)	C2–C1	1.548 (2)
C1–N1–C5	121.87 (14)	C18–C2–C19	109.14 (16)
C5–C4–C3	121.28 (16)	C1–C2–C3	107.49 (13)
C4–C3–C2	107.90 (13)	N2–C18–C2	177.8 (2)
C5–N1–C1–O1	−174.80 (19)	N1–C5–C12–C13	53.8 (2)
C18–C2–C1–O1	−102.1 (2)	C2–C3–C6–C7	−82.3 (2)

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: DE1177). Services for accessing these data are described at the back of the journal.

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