

***r*-2,*c*-6-Bis(3-fluorophenyl)-*t*-3,*t*-5-dimethylpiperidin-4-one**R. Ramachandran,^a P. Parthiban,^a Adinarayana Doddi,^b V. Ramkumar^b and S. Kabilan^{a*}^aDepartment of Chemistry, Annamalai University, Annamalai Nagar 608 002, Tamilnadu, India, and ^bDepartment of Chemistry, IIT Madras, Chennai, Tamilnadu, India

Correspondence e-mail: prskabilan@rediffmail.com

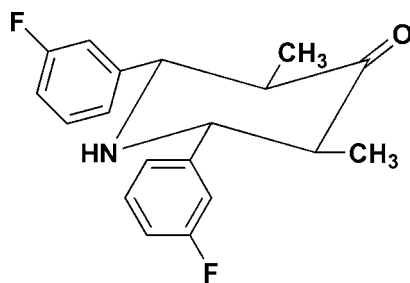
Received 19 October 2007; accepted 29 October 2007

Key indicators: single-crystal X-ray study; *T* = 298 K; mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$; disorder in main residue; *R* factor = 0.047; *wR* factor = 0.161; data-to-parameter ratio = 12.0.

The F atoms in the title compound, $\text{C}_{19}\text{H}_{17}\text{F}_2\text{NO}$, attached to the *meta* positions of the two phenyl rings, are disordered with site occupancy factors of 0.5. The crystal is stabilized by strong intermolecular $\text{N}-\text{H}\cdots\text{O}$ and van der Waals interactions.

Related literature

For related literature, see: Buxton & Roberts (1996); Dunitz & Taylor (1997); Evans & Seddon (1997); Ganellin & Spickett (1965); Kalsi (1997); Noller & Baliah (1948); Pham *et al.* (1998).

**Experimental***Crystal data*

$\text{C}_{19}\text{H}_{17}\text{F}_2\text{NO}$
 $M_r = 313.34$
 Monoclinic, $C2/c$
 $a = 22.2891 (4) \text{ \AA}$
 $b = 7.0516 (1) \text{ \AA}$
 $c = 23.4565 (4) \text{ \AA}$
 $\beta = 117.711 (2)^\circ$

$V = 3263.89 (9) \text{ \AA}^3$
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.09 \text{ mm}^{-1}$
 $T = 298 (2) \text{ K}$
 $0.28 \times 0.25 \times 0.23 \text{ mm}$

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 1999)
 $T_{\min} = 0.924$, $T_{\max} = 0.983$
 18121 measured reflections
 2795 independent reflections
 2337 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.161$
 $S = 1.09$
 2795 reflections
 232 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.26 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.18 \text{ e \AA}^{-3}$

Table 1Hydrogen-bond geometry (\AA , $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O1}^i$	0.95 (2)	2.34 (2)	3.2785 (18)	169.7 (16)

Symmetry code: (i) $x, y - 1, z$.

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2; data reduction: SAINT (Bruker, 2004); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

The authors acknowledge the Department of Chemistry, IIT Madras, for the X-ray data collection. We are thankful to Dr Babu Varghese, SAIF, IIT Madras, for his valuable suggestions.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2176).

References

- Bruker (1999). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Bruker (2004). *APEX2* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Buxton, S. R. & Roberts, S. M. (1996). *Guide to Organic Stereochemistry*. London: Longman.
 Dunitz, J. D. & Taylor, R. (1997). *Chem. Eur. J.* **3**, 89–98.
 Evans, T. A. & Seddon, K. R. (1997). *J. Chem. Soc. Chem. Commun.* pp. 2023–2024.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Ganellin, C. R. & Spickett, R. G. W. (1965). *J. Med. Chem.* **8**, 619–625.
 Kalsi, P. S. (1997). *Spectrochemistry: Conformation and Mechanism*. New Delhi: New Age International.
 Noller, C. R. & Baliah, V. (1948). *J. Am. Chem. Soc.* **70**, 3853–3855.
 Pham, M., Gdaniec, M. & Polonski, T. (1998). *J. Org. Chem.* **63**, 3731–3734.
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E63, o4559 [doi:10.1107/S1600536807054165]

***r*-2,*c*-6-Bis(3-fluorophenyl)-*t*-3,*t*-5-dimethylpiperidin-4-one**

R. Ramachandran, P. Parthiban, A. Doddi, V. Ramkumar and S. Kabilan

Comment

Substituted piperidin-4-ones are important synthetic intermediates for the preparation of various alkaloids and pharmaceuticals (Ganellin & Spickett, 1965). Biological activities of the synthesized piperidin-4-one derivatives mainly depends on the substituents on the phenyl rings flanked either side of the secondary nitrogen. Only *ortho* fluoro substituted piperidin-4-one have been reported (Pham *et al.*, 1998), which possess chair conformation.

The biological activities mainly depend on the stereochemistry (Buxton & Roberts, 1996) and the intramolecular and intermolecular hydrogen bonds with the fluorine atoms of the synthesized compound (Dunitz & Taylor, 1997; Evans & Seddon, 1997). In this study, we have incorporated the fluoro substituents at the one of the *meta* positions of the each phenyl groups on either side of the heterocyclic nitrogen to establish the stereochemistry and hydrogen bonding.

In the title compound C₁₉H₁₇F₂NO, the six membered heterocycle adopts a distorted chair conformation. The torsion angles deviate from the value of 56° expected for a perfect chair conformation (Kalsi, 1997). The equatorial dispositions of both methyl and phenyl rings which contain *meta* fluoro substituents are identified by their torsion angles. The absolute configurations of the chiral atoms C1, C2, C4 and C5 are found to be *R*, *S*, *R* and *S* respectively.

According to the modified Mannich reaction reported by Noller & Baliah (1948), we expected to obtain 2,6-bis(3-fluorophenyl)piperidin-4-one by using 3-fluorobenzaldehyde, but the crystal structure reveals that the fluorine atoms occupy either side of the *meta* positions of each phenyl ring with a disordered site-occupancy factor of 0.5 (Fig.1).

In the crystal structure the molecules are inter linked through a strong N—H···O hydrogen bonding (Table 1, Fig.2), and also the molecules are held together by weak van der Waals interactions.

Experimental

The title compound was prepared by the condensation of pentan-3-one, 3-fluorobenzaldehyde and ammonium acetate in 1: 2: 1 molar ratio in ethanol as reported by Noller for the similar type of Mannich bases (Noller & Baliah, 1948). Diffraction quality crystal was obtained by recrystallization of the crude sample from ethanol.

Refinement

The *meta* fluoro part of the molecule is disordered over two positions, the disorder refining to a 0.50:0.50 ratio. Nitrogen H atoms were located in a difference Fourier map and refined isotropically. Other hydrogen atoms were fixed geometrically and allowed to ride on the parent carbon atoms, with aromatic C—H = 0.93 Å, aliphatic C—H = 0.98 Å and methyl C—H = 0.96 Å. The displacement parameters were set for phenyl and aliphatic H atoms at $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and for methyl H atoms at $1.5U_{\text{eq}}(\text{C})$.

Figures

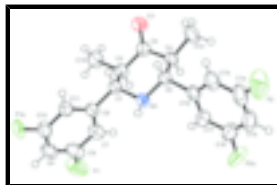


Fig. 1. ORTEP of the molecule with atoms represented as 50% probability ellipsoids. Hydrogen atoms are shown as atoms of arbitrary size.

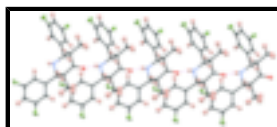


Fig. 2. Packing of molecules showing N—H...O interactions.

r-2,c-6-Bis(3-fluorophenyl)t-3,t-5-dimethylpiperidin-4-one

Crystal data

$C_{19}H_{17}F_2NO$

$M_r = 313.34$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 22.2891\ (4)\ \text{\AA}$

$b = 7.05160\ (10)\ \text{\AA}$

$c = 23.4565\ (4)\ \text{\AA}$

$\beta = 117.711\ (2)^\circ$

$V = 3263.89\ (9)\ \text{\AA}^3$

$Z = 8$

$F_{000} = 1312$

$D_x = 1.275\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 8210 reflections

$\theta = 3.1\text{--}28.2^\circ$

$\mu = 0.09\ \text{mm}^{-1}$

$T = 298\ (2)\ \text{K}$

Block, colourless

$0.28 \times 0.25 \times 0.23\ \text{mm}$

Data collection

Bruker APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298\ (2)\ \text{K}$

φ and ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 1999)

$T_{\min} = 0.924$, $T_{\max} = 0.983$

18121 measured reflections

2795 independent reflections

2337 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 25.0^\circ$

$\theta_{\min} = 2.1^\circ$

$h = -25 \rightarrow 22$

$k = -8 \rightarrow 8$

$l = -27 \rightarrow 27$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.047$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of

	independent and constrained refinement
$wR(F^2) = 0.161$	$w = 1/[\sigma^2(F_o^2) + (0.0988P)^2 + 1.2426P]$
	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{\max} < 0.001$
2795 reflections	$\Delta\rho_{\max} = 0.26 \text{ e } \text{\AA}^{-3}$
232 parameters	$\Delta\rho_{\min} = -0.18 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.10456 (8)	0.8562 (2)	0.14454 (8)	0.0382 (4)	
H1	0.1258	0.8697	0.1915	0.046*	
C2	0.09171 (8)	1.0563 (2)	0.11377 (9)	0.0445 (4)	
H2	0.0751	1.0404	0.0674	0.053*	
C3	0.15962 (9)	1.1548 (2)	0.14083 (8)	0.0443 (4)	
C4	0.21485 (9)	1.0504 (2)	0.13318 (9)	0.0467 (4)	
H4	0.2019	1.0467	0.0871	0.056*	
C5	0.21931 (8)	0.8427 (2)	0.15674 (8)	0.0389 (4)	
H5	0.2371	0.8430	0.2036	0.047*	
C6	0.03966 (8)	0.7444 (2)	0.12237 (8)	0.0411 (4)	
C7	-0.00105 (10)	0.7053 (3)	0.05773 (9)	0.0555 (5)	
H7	0.0122	0.7434	0.0273	0.067*	
C8	-0.06142 (10)	0.6095 (3)	0.03868 (11)	0.0664 (6)	
C9	-0.08187 (10)	0.5475 (3)	0.08220 (11)	0.0624 (6)	
H9	-0.1224	0.4821	0.0689	0.075*	
C10	-0.04097 (10)	0.5845 (3)	0.14551 (11)	0.0616 (6)	
C11	0.01918 (9)	0.6832 (2)	0.16639 (10)	0.0503 (5)	
H11	0.0457	0.7082	0.2100	0.060*	
C12	0.26636 (9)	0.7275 (2)	0.14005 (9)	0.0435 (4)	
C13	0.33343 (9)	0.6997 (3)	0.18524 (11)	0.0568 (5)	
H13	0.3495	0.7472	0.2268	0.068*	
C14	0.37635 (10)	0.6011 (3)	0.16827 (13)	0.0693 (6)	
C15	0.35459 (12)	0.5283 (3)	0.10790 (14)	0.0726 (7)	
H15	0.3841	0.4628	0.0971	0.087*	

supplementary materials

C16	0.28812 (13)	0.5545 (3)	0.06381 (12)	0.0701 (6)	
C17	0.24403 (10)	0.6536 (3)	0.07888 (10)	0.0563 (5)	
H17	0.1992	0.6708	0.0479	0.068*	
C18	0.03924 (10)	1.1699 (3)	0.12326 (12)	0.0623 (6)	
H18A	0.0495	1.1658	0.1678	0.093*	
H18B	-0.0049	1.1167	0.0973	0.093*	
H18C	0.0399	1.2991	0.1107	0.093*	
C19	0.28239 (12)	1.1518 (3)	0.16720 (15)	0.0802 (8)	
H19A	0.2761	1.2842	0.1566	0.120*	
H19B	0.3134	1.0988	0.1536	0.120*	
H19C	0.3005	1.1365	0.2129	0.120*	
F1	-0.10284 (15)	0.5924 (5)	-0.01925 (14)	0.1008 (10)	0.50
F1A	-0.06167 (13)	0.5306 (4)	0.18482 (13)	0.0796 (8)	0.50
F2	0.43768 (15)	0.5665 (5)	0.21028 (18)	0.1115 (12)	0.50
F2A	0.26635 (16)	0.4710 (4)	0.00831 (14)	0.0883 (9)	0.50
N1	0.15164 (7)	0.75695 (18)	0.12719 (7)	0.0406 (4)	
O1	0.16979 (7)	1.30766 (17)	0.16775 (8)	0.0638 (4)	
H1A	0.1522 (10)	0.630 (3)	0.1400 (9)	0.060 (6)*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0348 (8)	0.0340 (8)	0.0452 (9)	0.0019 (6)	0.0181 (7)	0.0023 (6)
C2	0.0432 (9)	0.0339 (9)	0.0553 (10)	0.0061 (7)	0.0219 (8)	0.0053 (7)
C3	0.0528 (10)	0.0281 (8)	0.0564 (10)	0.0026 (7)	0.0291 (9)	0.0060 (7)
C4	0.0503 (10)	0.0349 (9)	0.0655 (11)	-0.0019 (7)	0.0358 (9)	0.0023 (7)
C5	0.0355 (8)	0.0350 (8)	0.0476 (9)	0.0001 (6)	0.0204 (7)	0.0024 (6)
C6	0.0345 (9)	0.0326 (8)	0.0544 (10)	0.0042 (6)	0.0191 (8)	0.0007 (7)
C7	0.0506 (11)	0.0536 (10)	0.0556 (11)	-0.0062 (8)	0.0189 (9)	0.0021 (8)
C8	0.0451 (11)	0.0588 (12)	0.0700 (14)	-0.0056 (9)	0.0055 (10)	-0.0035 (10)
C9	0.0373 (10)	0.0522 (11)	0.0937 (16)	-0.0067 (8)	0.0271 (11)	-0.0111 (10)
C10	0.0477 (11)	0.0570 (11)	0.0918 (16)	-0.0066 (9)	0.0423 (12)	-0.0098 (10)
C11	0.0445 (10)	0.0498 (10)	0.0611 (11)	-0.0037 (8)	0.0284 (9)	-0.0058 (8)
C12	0.0409 (9)	0.0336 (8)	0.0615 (11)	0.0008 (7)	0.0284 (8)	0.0052 (7)
C13	0.0420 (10)	0.0563 (11)	0.0719 (13)	0.0046 (8)	0.0265 (9)	0.0074 (9)
C14	0.0443 (11)	0.0614 (12)	0.1080 (19)	0.0127 (9)	0.0404 (12)	0.0151 (12)
C15	0.0716 (15)	0.0526 (11)	0.123 (2)	0.0112 (10)	0.0703 (15)	0.0056 (12)
C16	0.0767 (15)	0.0579 (12)	0.0961 (17)	0.0046 (10)	0.0574 (14)	-0.0070 (11)
C17	0.0516 (11)	0.0530 (10)	0.0689 (13)	0.0042 (8)	0.0317 (10)	-0.0066 (9)
C18	0.0498 (11)	0.0421 (10)	0.0942 (15)	0.0109 (8)	0.0328 (11)	0.0025 (9)
C19	0.0645 (14)	0.0447 (11)	0.150 (2)	-0.0121 (9)	0.0655 (15)	-0.0101 (12)
F1	0.089 (2)	0.109 (2)	0.0782 (19)	-0.0390 (18)	0.0159 (16)	-0.0186 (16)
F1A	0.0718 (16)	0.105 (2)	0.0896 (17)	-0.0439 (14)	0.0609 (14)	-0.0249 (15)
F2	0.0576 (18)	0.140 (3)	0.132 (3)	0.0327 (18)	0.0401 (18)	0.013 (2)
F2A	0.110 (2)	0.0906 (19)	0.0861 (18)	0.0161 (16)	0.0635 (17)	-0.0242 (15)
N1	0.0372 (8)	0.0291 (7)	0.0569 (9)	0.0016 (5)	0.0231 (7)	0.0009 (6)
O1	0.0676 (9)	0.0369 (7)	0.0964 (11)	-0.0052 (6)	0.0462 (8)	-0.0112 (7)

Geometric parameters (Å, °)

C1—N1	1.468 (2)	C9—H9	0.9300
C1—C6	1.511 (2)	C10—F1A	1.266 (3)
C1—C2	1.550 (2)	C10—C11	1.382 (3)
C1—H1	0.9800	C11—H11	0.9300
C2—C3	1.511 (2)	C12—C17	1.384 (3)
C2—C18	1.517 (2)	C12—C13	1.387 (3)
C2—H2	0.9800	C13—C14	1.383 (3)
C3—O1	1.216 (2)	C13—H13	0.9300
C3—C4	1.515 (2)	C14—F2	1.283 (4)
C4—C19	1.515 (3)	C14—C15	1.366 (4)
C4—C5	1.552 (2)	C15—C16	1.369 (3)
C4—H4	0.9800	C15—H15	0.9300
C5—N1	1.466 (2)	C16—F2A	1.300 (3)
C5—C12	1.515 (2)	C16—C17	1.379 (3)
C5—H5	0.9800	C17—H17	0.9300
C6—C11	1.378 (3)	C18—H18A	0.9600
C6—C7	1.385 (3)	C18—H18B	0.9600
C7—C8	1.381 (3)	C18—H18C	0.9600
C7—H7	0.9300	C19—H19A	0.9600
C8—F1	1.244 (3)	C19—H19B	0.9600
C8—C9	1.369 (3)	C19—H19C	0.9600
C9—C10	1.359 (3)	N1—H1A	0.95 (2)
N1—C1—C6	110.45 (13)	F1A—C10—C9	116.8 (2)
N1—C1—C2	107.83 (13)	F1A—C10—C11	121.0 (2)
C6—C1—C2	112.00 (13)	C9—C10—C11	122.1 (2)
N1—C1—H1	108.8	C6—C11—C10	119.79 (19)
C6—C1—H1	108.8	C6—C11—H11	120.1
C2—C1—H1	108.8	C10—C11—H11	120.1
C3—C2—C18	112.69 (14)	C17—C12—C13	118.64 (17)
C3—C2—C1	106.91 (13)	C17—C12—C5	120.78 (16)
C18—C2—C1	113.61 (15)	C13—C12—C5	120.54 (17)
C3—C2—H2	107.8	C14—C13—C12	119.7 (2)
C18—C2—H2	107.8	C14—C13—H13	120.2
C1—C2—H2	107.8	C12—C13—H13	120.2
O1—C3—C2	122.27 (15)	F2—C14—C15	117.5 (3)
O1—C3—C4	121.79 (16)	F2—C14—C13	120.5 (3)
C2—C3—C4	115.93 (14)	C15—C14—C13	121.9 (2)
C3—C4—C19	111.81 (15)	C14—C15—C16	118.05 (19)
C3—C4—C5	109.72 (13)	C14—C15—H15	121.0
C19—C4—C5	111.96 (16)	C16—C15—H15	121.0
C3—C4—H4	107.7	F2A—C16—C15	117.7 (2)
C19—C4—H4	107.7	F2A—C16—C17	120.5 (2)
C5—C4—H4	107.7	C15—C16—C17	121.6 (2)
N1—C5—C12	109.89 (13)	C16—C17—C12	120.1 (2)
N1—C5—C4	109.85 (13)	C16—C17—H17	120.0
C12—C5—C4	110.57 (13)	C12—C17—H17	120.0

supplementary materials

N1—C5—H5	108.8	C2—C18—H18A	109.5
C12—C5—H5	108.8	C2—C18—H18B	109.5
C4—C5—H5	108.8	H18A—C18—H18B	109.5
C11—C6—C7	118.76 (16)	C2—C18—H18C	109.5
C11—C6—C1	120.20 (15)	H18A—C18—H18C	109.5
C7—C6—C1	121.02 (16)	H18B—C18—H18C	109.5
C8—C7—C6	119.69 (19)	C4—C19—H19A	109.5
C8—C7—H7	120.2	C4—C19—H19B	109.5
C6—C7—H7	120.2	H19A—C19—H19B	109.5
F1—C8—C9	116.6 (2)	C4—C19—H19C	109.5
F1—C8—C7	121.2 (3)	H19A—C19—H19C	109.5
C9—C8—C7	121.8 (2)	H19B—C19—H19C	109.5
C10—C9—C8	117.82 (18)	C5—N1—C1	112.54 (12)
C10—C9—H9	121.1	C5—N1—H1A	112.6 (12)
C8—C9—H9	121.1	C1—N1—H1A	105.6 (12)
N1—C1—C2—C3	-59.72 (17)	C8—C9—C10—F1A	178.1 (2)
C6—C1—C2—C3	178.56 (14)	C8—C9—C10—C11	0.7 (3)
N1—C1—C2—C18	175.32 (15)	C7—C6—C11—C10	0.1 (3)
C6—C1—C2—C18	53.6 (2)	C1—C6—C11—C10	178.65 (15)
C18—C2—C3—O1	0.8 (2)	F1A—C10—C11—C6	-178.4 (2)
C1—C2—C3—O1	-124.69 (18)	C9—C10—C11—C6	-1.1 (3)
C18—C2—C3—C4	-179.93 (15)	N1—C5—C12—C17	40.4 (2)
C1—C2—C3—C4	54.55 (19)	C4—C5—C12—C17	-81.0 (2)
O1—C3—C4—C19	4.6 (3)	N1—C5—C12—C13	-141.82 (16)
C2—C3—C4—C19	-174.68 (17)	C4—C5—C12—C13	96.75 (19)
O1—C3—C4—C5	129.41 (17)	C17—C12—C13—C14	0.5 (3)
C2—C3—C4—C5	-49.8 (2)	C5—C12—C13—C14	-177.24 (17)
C3—C4—C5—N1	49.75 (19)	C12—C13—C14—F2	-176.8 (3)
C19—C4—C5—N1	174.51 (16)	C12—C13—C14—C15	-0.4 (3)
C3—C4—C5—C12	171.21 (14)	F2—C14—C15—C16	176.1 (3)
C19—C4—C5—C12	-64.0 (2)	C13—C14—C15—C16	-0.4 (3)
N1—C1—C6—C11	120.53 (16)	C14—C15—C16—F2A	-174.2 (2)
C2—C1—C6—C11	-119.27 (16)	C14—C15—C16—C17	0.9 (3)
N1—C1—C6—C7	-61.0 (2)	F2A—C16—C17—C12	174.2 (2)
C2—C1—C6—C7	59.2 (2)	C15—C16—C17—C12	-0.8 (3)
C11—C6—C7—C8	1.1 (3)	C13—C12—C17—C16	0.0 (3)
C1—C6—C7—C8	-177.39 (16)	C5—C12—C17—C16	177.81 (17)
C6—C7—C8—F1	171.2 (3)	C12—C5—N1—C1	176.82 (12)
C6—C7—C8—C9	-1.5 (3)	C4—C5—N1—C1	-61.31 (17)
F1—C8—C9—C10	-172.4 (3)	C6—C1—N1—C5	-170.52 (13)
C7—C8—C9—C10	0.6 (3)	C2—C1—N1—C5	66.81 (17)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A \cdots O1 ⁱ	0.95 (2)	2.34 (2)	3.2785 (18)	169.7 (16)

Symmetry codes: (i) $x, y-1, z$.

Fig. 1

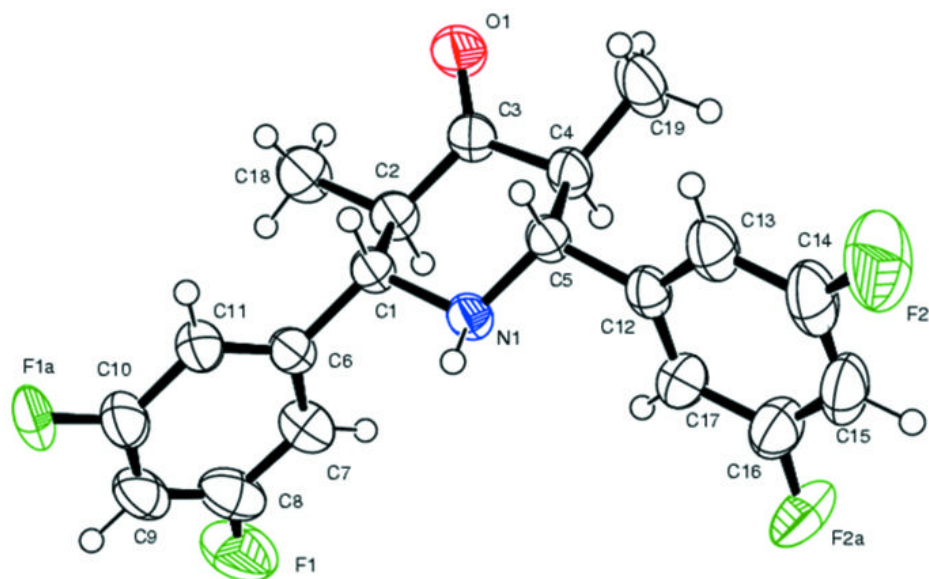


Fig. 2

