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2,4,4-Trimethyl-*N*-phenyl-2,3,4,5-tetrahydro-1*H*-1,5-benzodiazepine-1-carboxamide

A Thiruvalluvar[a]* and S Ponnuswamy[b]

[a]Department of Physics, Rajah Serfoji Government College (Autonomous), Thanjavur 613 005, Tamil Nadu, India, and [b]Department of Chemistry, Government Arts College (Autonomous), Coimbatore 613 005, Tamil Nadu, India
Correspondence e-mail: athiru@vsnl.net

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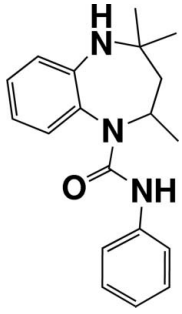
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.116; data-to-parameter ratio = 17.8.

In the title compound, $C_{19}H_{23}N_3O$, the seven-membered diazepine ring adopts a boat conformation. The phenylcarbamoyl group is coplanar with the N atom and its two attached C atoms. The methyl group at position 2 has an equatorial orientation. The dihedral angle between the two benzene rings is 81.07 (9)°. The crystal structure is stabilized by intramolecular C—H···O and intermolecular N—H···O hydrogen bonds.

Related literature

For related literature, see: Chananont *et al.* (1980); Gałdecki & Główka (1980); Gilli *et al.* (1978); Ponnuswamy *et al.* (2006).



Experimental

Crystal data

$C_{19}H_{23}N_3O$
M_r = 309.40
Orthorhombic, *Pbca*
a = 6.6010 (1) Å
b = 13.8353 (2) Å
c = 37.7572 (6) Å
V = 3448.25 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.22 × 0.20 × 0.20 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.868, T_{max} = 1.000
(expected range = 0.855–0.985)
18554 measured reflections
3834 independent reflections
2674 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.116
S = 1.03
3834 reflections
216 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···O1^{i}	0.85 (2)	2.17 (2)	3.0153 (17)	174 (2)
C2—H2A···O1	0.98	2.31	2.736 (2)	106
C116—H116···O1	0.93	2.32	2.877 (2)	118

Symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT-NT* (Bruker, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2151).

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supplementary materials

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2,4,4-Trimethyl-*N*-phenyl-2,3,4,5-tetrahydro-1*H*-1,5-benzodiazepine-1-carboxamide

A. Thiruvalluvar and S. Ponnuswamy

Comment

Benzodiazepines are a class of psychotherapeutic drugs discovered at the end of the 1950 s and now widely used owing to their broad spectrum of biological activities. They are mainly used as tranquillizers but are also of interest for their muscle relaxant, anticonvulsant and sleep-induction effects (Gilli *et al.*, 1978; Gałdecki & Główka, 1980; Chananont *et al.*, 1980). The X-ray structure analysis of the title compound was carried out to determine the crystal structure as well as to study the substituent effects on the geometry and conformation of the diazepine ring.

The conformation of the title molecule was established by NMR spectroscopy and semiempirical MO calculations by Ponnuswamy *et al.* (2006). The title molecule, $C_{19}H_{23}N_3O$, contains a benzene ring fused to a diazepine ring. The phenylcarbamoyl group is substituted at N1. The methyl groups are substituted at C2 and C4 as expected. The seven-membered diazepine ring has a boat conformation (Fig. 1). The phenylcarbamoyl group is coplanar with the C2—N1—C10 plane of the diazepine ring. The methyl group substituted on the C2 atom is in an equatorial position. The dihedral angle between the two benzene rings is 81.07 (9)°. An N—H···O intermolecular hydrogen bond exists between H5 (on N5 of the diazepine ring) and atom $O1^{i}$ [(i): $-x + 1/2$, $y + 1/2$, z] of the phenylcarbamoyl group (Fig. 2), forming an infinite one-dimensional chain, with base vector [010]. C—H···O type intramolecular interactions [C2—H2A···O1 and C116—H116···O1] are also present.

Experimental

The title compound was prepared and characterized using NMR techniques by Ponnuswamy *et al.*, 2006.

Refinement

Atoms H11 at N11 and H5 at N5 were located in a difference Fourier map and refined isotropically. Remaining 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).

Figures

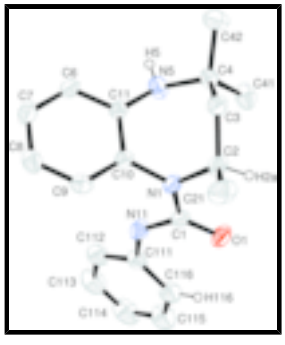

Fig. 1. The molecular structure with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. H atoms involved in hydrogen bonds are shown as small spheres of arbitrary radii.

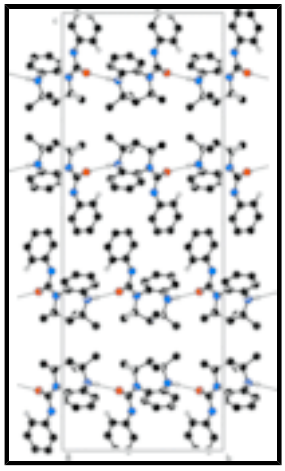

Fig. 2. The molecular packing, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

2,4,4-Trimethyl-*N*-phenyl-2,3,4,5-tetrahydro-1*H*-1,5-benzodiazepine-1-carboxamide

Crystal data

$C_{19}H_{23}N_3O$	D_x = 1.192 Mg m^{-3}
M_r = 309.40	Melting point: 440.5 K
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 5251 reflections
a = 6.6010 (1) Å	θ = 2.9–27.2º
b = 13.8353 (2) Å	μ = 0.08 mm^{-1}
c = 37.7572 (6) Å	*T* = 293 (2) K
V = 3448.25 (9) Å^3	Rectangular block, colourless
Z = 8	0.22 × 0.20 × 0.20 mm
F_{000} = 1328	

Data collection

Bruker APEXII diffractometer	3834 independent reflections
Radiation source: fine-focus sealed tube	2674 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
T = 293(2) K	θ_{max} = 27.2º
φ and ω scans	θ_{min} = 2.9º
Absorption correction: multi-scan (SADABS; Bruker, 2004)	*h* = −8→8
T_{min} = 0.868, T_{max} = 1.000	*k* = −17→17
18554 measured reflections	*l* = −48→32

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.045$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.116$	$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2 + 0.7067P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
3834 reflections	$\Delta\rho_{max} = 0.13$ e Å^{-3}
216 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.25792 (18)	−0.14773 (7)	0.13677 (3)	0.0589 (4)
N1	0.51148 (18)	−0.03994 (8)	0.14618 (3)	0.0425 (4)
N5	0.4053 (2)	0.15447 (10)	0.15438 (4)	0.0519 (5)
N11	0.3963 (2)	−0.06939 (10)	0.08966 (3)	0.0505 (4)
C1	0.3802 (2)	−0.08931 (9)	0.12488 (4)	0.0425 (4)
C2	0.4970 (3)	−0.05268 (10)	0.18463 (4)	0.0475 (5)
C3	0.5002 (2)	0.04477 (10)	0.20331 (4)	0.0453 (5)
C4	0.3515 (2)	0.12114 (10)	0.19023 (4)	0.0440 (5)
C6	0.7016 (2)	0.20114 (10)	0.12087 (4)	0.0477 (5)
C7	0.8697 (3)	0.17729 (12)	0.10145 (4)	0.0557 (6)
C8	0.9295 (3)	0.08264 (12)	0.09829 (4)	0.0552 (5)
C9	0.8157 (2)	0.01174 (11)	0.11412 (4)	0.0472 (5)
C10	0.6412 (2)	0.03434 (9)	0.13268 (4)	0.0378 (4)
C11	0.5825 (2)	0.13084 (9)	0.13702 (4)	0.0371 (4)
C21	0.6649 (3)	−0.11839 (12)	0.19792 (5)	0.0736 (7)
C41	0.1354 (3)	0.08303 (14)	0.18925 (5)	0.0658 (6)
C42	0.3633 (3)	0.20749 (12)	0.21531 (5)	0.0658 (7)
C111	0.2814 (2)	−0.10638 (11)	0.06149 (4)	0.0470 (5)
C112	0.2901 (3)	−0.05737 (14)	0.02975 (5)	0.0650 (6)
C113	0.1836 (3)	−0.08972 (18)	0.00075 (5)	0.0837 (9)
C114	0.0668 (3)	−0.1704 (2)	0.00327 (6)	0.0902 (9)
C115	0.0577 (3)	−0.21940 (17)	0.03451 (6)	0.0848 (8)
C116	0.1655 (3)	−0.18920 (13)	0.06388 (5)	0.0630 (6)
H2A	0.36710	−0.08385	0.18984	0.0569*

H3A	0.47418	0.03381	0.22827	0.0544*
H3B	0.63591	0.07108	0.20134	0.0544*
H5	0.365 (3)	0.2120 (15)	0.1507 (5)	0.081 (6)*
H6	0.66626	0.26586	0.12332	0.0573*
H7	0.94391	0.22565	0.09030	0.0668*
H8	1.04558	0.06678	0.08560	0.0662*
H9	0.85644	−0.05242	0.11234	0.0567*
H11	0.481 (3)	−0.0247 (12)	0.0847 (4)	0.061 (5)*
H21A	0.65873	−0.17909	0.18565	0.1104*
H21B	0.79383	−0.08849	0.19364	0.1104*
H21C	0.64823	−0.12913	0.22287	0.1104*
H41A	0.04631	0.13292	0.18092	0.0987*
H41B	0.12831	0.02847	0.17359	0.0987*
H41C	0.09530	0.06365	0.21264	0.0987*
H42A	0.49968	0.23151	0.21591	0.0987*
H42B	0.27407	0.25752	0.20712	0.0987*
H42C	0.32350	0.18774	0.23867	0.0987*
H112	0.36869	−0.00182	0.02792	0.0780*
H113	0.19159	−0.05639	−0.02060	0.1004*
H114	−0.00641	−0.19204	−0.01623	0.1080*
H115	−0.02290	−0.27437	0.03612	0.1018*
H116	0.16011	−0.22410	0.08491	0.0755*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0731 (8)	0.0487 (6)	0.0549 (7)	−0.0256 (6)	−0.0001 (6)	0.0033 (5)
N1	0.0550 (7)	0.0340 (6)	0.0385 (7)	−0.0098 (5)	−0.0033 (6)	0.0035 (5)
N5	0.0586 (9)	0.0495 (8)	0.0476 (8)	0.0184 (7)	0.0105 (6)	0.0130 (6)
N11	0.0569 (8)	0.0520 (7)	0.0425 (8)	−0.0177 (7)	−0.0036 (6)	0.0001 (6)
C1	0.0514 (9)	0.0317 (6)	0.0445 (8)	−0.0032 (6)	−0.0021 (7)	−0.0005 (6)
C2	0.0627 (10)	0.0402 (7)	0.0395 (8)	−0.0070 (7)	−0.0047 (8)	0.0077 (6)
C3	0.0557 (9)	0.0459 (8)	0.0343 (8)	−0.0041 (7)	−0.0057 (7)	0.0038 (6)
C4	0.0474 (8)	0.0490 (8)	0.0357 (8)	0.0008 (7)	0.0006 (7)	−0.0004 (6)
C6	0.0611 (10)	0.0353 (7)	0.0468 (9)	−0.0069 (7)	−0.0017 (8)	0.0012 (6)
C7	0.0558 (10)	0.0571 (10)	0.0542 (10)	−0.0199 (8)	0.0039 (8)	0.0053 (8)
C8	0.0429 (8)	0.0692 (10)	0.0534 (10)	−0.0027 (8)	0.0075 (8)	−0.0020 (8)
C9	0.0500 (9)	0.0423 (8)	0.0494 (9)	0.0061 (7)	−0.0009 (7)	−0.0048 (7)
C10	0.0415 (8)	0.0345 (6)	0.0373 (8)	−0.0037 (6)	−0.0043 (6)	0.0010 (6)
C11	0.0415 (8)	0.0348 (7)	0.0350 (7)	−0.0005 (6)	−0.0029 (6)	0.0031 (5)
C21	0.1081 (16)	0.0491 (9)	0.0635 (12)	0.0131 (10)	−0.0160 (11)	0.0123 (8)
C41	0.0509 (10)	0.0903 (12)	0.0562 (11)	−0.0045 (9)	0.0035 (9)	0.0037 (10)
C42	0.0811 (13)	0.0586 (10)	0.0577 (11)	0.0095 (9)	−0.0019 (10)	−0.0114 (8)
C111	0.0423 (8)	0.0542 (9)	0.0446 (9)	0.0022 (7)	−0.0024 (7)	−0.0113 (7)
C112	0.0717 (12)	0.0752 (11)	0.0481 (10)	−0.0008 (10)	−0.0028 (9)	−0.0062 (9)
C113	0.0843 (15)	0.1195 (18)	0.0473 (11)	0.0095 (14)	−0.0113 (10)	−0.0109 (12)
C114	0.0669 (13)	0.140 (2)	0.0637 (14)	−0.0025 (14)	−0.0154 (11)	−0.0363 (14)
C115	0.0680 (13)	0.1096 (16)	0.0768 (15)	−0.0270 (12)	−0.0058 (11)	−0.0325 (13)

C116	0.0581 (10)	0.0719 (11)	0.0589 (11)	−0.0140 (9)	−0.0041 (9)	−0.0146 (9)

Geometric parameters (Å, °)

O1—C1	1.2273 (17)	C6—H6	0.930
N1—C1	1.3654 (18)	C7—H7	0.930
N1—C2	1.4656 (19)	C8—H8	0.930
N1—C10	1.4315 (17)	C9—H9	0.930
N5—C4	1.473 (2)	C111—C116	1.381 (2)
N5—C11	1.3801 (19)	C111—C112	1.378 (2)
N11—C1	1.3622 (19)	C112—C113	1.376 (3)
N11—C111	1.4030 (19)	C113—C114	1.360 (3)
N5—H5	0.85 (2)	C114—C115	1.362 (3)
N11—H11	0.854 (18)	C115—C116	1.382 (3)
C2—C21	1.519 (3)	C21—H21A	0.960
C2—C3	1.522 (2)	C21—H21B	0.960
C3—C4	1.5244 (19)	C21—H21C	0.960
C4—C41	1.521 (2)	C41—H41A	0.960
C4—C42	1.526 (2)	C41—H41B	0.960
C6—C11	1.3914 (19)	C41—H41C	0.960
C6—C7	1.370 (2)	C42—H42A	0.960
C7—C8	1.373 (2)	C42—H42B	0.960
C8—C9	1.373 (2)	C42—H42C	0.960
C9—C10	1.3841 (19)	C112—H112	0.930
C10—C11	1.3998 (18)	C113—H113	0.930
C2—H2A	0.980	C114—H114	0.930
C3—H3A	0.970	C115—H115	0.930
C3—H3B	0.970	C116—H116	0.930
O1···C116	2.877 (2)	H3B···C10	2.640
O1···N5^{i}	3.0153 (17)	H3B···C11	2.590
O1···H2A	2.310	H3B···H21B	2.460
O1···H116	2.320	H3B···H42A	2.460
O1···H5^{i}	2.17 (2)	H5···H6	2.360
N1···N5	2.7967 (18)	H5···H42B	2.300
N1···C41	3.421 (2)	H5···O1^{ii}	2.17 (2)
N5···N1	2.7967 (18)	H6···H5	2.360
N5···O1^{ii}	3.0153 (17)	H6···H9^{iv}	2.550
N11···C9	3.1269 (19)	H7···C1^{iv}	3.100
N1···H41B	2.890	H7···C116^{iv}	3.010
C6···C116^{ii}	3.578 (2)	H8···C111^{vi}	3.000
C9···N11	3.1269 (19)	H9···H6^{iii}	2.550
C41···N1	3.421 (2)	H11···C9	2.524 (19)
C1···H41B	2.970	H11···C10	2.251 (16)
C1···H116	2.800	H11···C11	2.997 (16)
C1···H7^{iii}	3.100	H11···H112	2.290
C2···H41B	2.710	H21A···C6^{iii}	3.090
C6···H21A^{iv}	3.090	H21B···C10	3.030

C6···H116^{ii}	2.930	H21B···H3B	2.460
C8···H113^{v}	3.060	H21C···H3A	2.540
C9···H41B^{vi}	3.060	H41A···H42B	2.490
C9···H11	2.524 (19)	H41B···N1	2.890
C10···H3B	2.640	H41B···C1	2.970
C10···H11	2.251 (16)	H41B···C2	2.710
C10···H21B	3.030	H41B···C9^{viii}	3.060
C11···H3B	2.590	H41B···H2A	2.300
C11···H11	2.997 (16)	H41C···H42C	2.490
C113···C113^{vii}	3.470 (3)	H41C···H3A^{xi}	2.410
C116···O1	2.877 (2)	H42A···H3B	2.460
C116···C6^{i}	3.578 (2)	H42B···H5	2.300
C41···H2A	2.770	H42B···H41A	2.490
C111···H8^{viii}	3.000	H42B···H2A^{ii}	2.470
C113···H115^{ix}	3.040	H42C···H3A	2.380
C116···H7^{iii}	3.010	H42C···H41C	2.490
H2A···O1	2.310	H112···H11	2.290
H2A···C41	2.770	H113···C8^{v}	3.060
H2A···H41B	2.300	H115···C113^{xii}	3.040
H2A···H42B^{i}	2.470	H116···O1	2.320
H3A···H21C	2.540	H116···C1	2.800
H3A···H42C	2.380	H116···C6^{i}	2.930
H3A···H41C^{x}	2.410		
C1—N1—C2	118.81 (12)	C6—C7—H7	120.0
C1—N1—C10	121.94 (12)	C8—C7—H7	120.0
C2—N1—C10	118.56 (12)	C9—C8—H8	120.0
C4—N5—C11	124.50 (13)	C7—C8—H8	120.0
C1—N11—C111	128.62 (13)	C8—C9—H9	120.0
C4—N5—H5	111.6 (13)	C10—C9—H9	120.0
C11—N5—H5	114.2 (13)	N11—C111—C112	117.21 (14)
C1—N11—H11	114.3 (10)	C112—C111—C116	119.23 (15)
C111—N11—H11	116.8 (10)	N11—C111—C116	123.55 (15)
N1—C1—N11	115.10 (12)	C111—C112—C113	120.71 (18)
O1—C1—N1	122.10 (14)	C112—C113—C114	120.06 (19)
O1—C1—N11	122.79 (13)	C113—C114—C115	119.6 (2)
C3—C2—C21	111.54 (14)	C114—C115—C116	121.5 (2)
N1—C2—C21	110.59 (14)	C111—C116—C115	118.93 (17)
N1—C2—C3	110.59 (11)	C2—C21—H21A	109.0
C2—C3—C4	117.07 (13)	C2—C21—H21B	109.0
N5—C4—C3	111.06 (12)	C2—C21—H21C	109.0
N5—C4—C41	108.19 (13)	H21A—C21—H21B	109.0
N5—C4—C42	108.22 (12)	H21A—C21—H21C	109.0
C3—C4—C41	111.80 (12)	H21B—C21—H21C	109.0
C3—C4—C42	107.98 (13)	C4—C41—H41A	109.0
C41—C4—C42	109.52 (13)	C4—C41—H41B	109.0
C7—C6—C11	121.58 (13)	C4—C41—H41C	109.0

C6—C7—C8	120.60 (16)	H41A—C41—H41B	109.0
C7—C8—C9	119.11 (16)	H41A—C41—H41C	109.0
C8—C9—C10	120.97 (14)	H41B—C41—H41C	109.0
C9—C10—C11	120.34 (13)	C4—C42—H42A	109.0
N1—C10—C9	121.06 (12)	C4—C42—H42B	109.0
N1—C10—C11	118.52 (12)	C4—C42—H42C	109.0
N5—C11—C10	121.07 (12)	H42A—C42—H42B	109.0
C6—C11—C10	117.32 (13)	H42A—C42—H42C	109.0
N5—C11—C6	121.43 (12)	H42B—C42—H42C	109.0
C21—C2—H2A	108.0	C111—C112—H112	120.0
N1—C2—H2A	108.0	C113—C112—H112	120.0
C3—C2—H2A	108.0	C112—C113—H113	120.0
C2—C3—H3A	108.0	C114—C113—H113	120.0
C2—C3—H3B	108.0	C113—C114—H114	120.0
C4—C3—H3A	108.0	C115—C114—H114	120.0
C4—C3—H3B	108.0	C114—C115—H115	119.0
H3A—C3—H3B	107.0	C116—C115—H115	119.0
C7—C6—H6	119.0	C111—C116—H116	121.0
C11—C6—H6	119.0	C115—C116—H116	121.0
C2—N1—C1—O1	−3.9 (2)	C2—C3—C4—C42	173.30 (13)
C10—N1—C1—O1	−174.28 (12)	C2—C3—C4—N5	−68.20 (16)
C2—N1—C1—N11	176.52 (12)	C2—C3—C4—C41	52.76 (18)
C10—N1—C1—N11	6.17 (18)	C7—C6—C11—C10	0.0 (2)
C2—N1—C10—C9	112.01 (16)	C11—C6—C7—C8	−2.1 (2)
C1—N1—C10—C11	99.09 (16)	C7—C6—C11—N5	−175.22 (15)
C1—N1—C2—C3	−132.63 (13)	C6—C7—C8—C9	1.6 (2)
C10—N1—C2—C3	38.05 (19)	C7—C8—C9—C10	0.9 (2)
C1—N1—C2—C21	103.31 (16)	C8—C9—C10—C11	−3.0 (2)
C10—N1—C2—C21	−86.01 (15)	C8—C9—C10—N1	173.69 (14)
C1—N1—C10—C9	−77.61 (18)	N1—C10—C11—C6	−174.28 (13)
C2—N1—C10—C11	−71.29 (18)	C9—C10—C11—N5	177.72 (14)
C4—N5—C11—C10	53.8 (2)	C9—C10—C11—C6	2.4 (2)
C11—N5—C4—C3	−8.98 (19)	N1—C10—C11—N5	1.0 (2)
C11—N5—C4—C42	109.37 (16)	N11—C111—C112—C113	179.24 (17)
C4—N5—C11—C6	−131.10 (16)	C116—C111—C112—C113	0.5 (3)
C11—N5—C4—C41	−132.04 (15)	N11—C111—C116—C115	179.94 (16)
C1—N11—C111—C116	−17.8 (2)	C112—C111—C116—C115	−1.4 (3)
C111—N11—C1—N1	−178.55 (13)	C111—C112—C113—C114	0.6 (3)
C111—N11—C1—O1	1.9 (2)	C112—C113—C114—C115	−0.7 (3)
C1—N11—C111—C112	163.52 (16)	C113—C114—C115—C116	−0.3 (3)
N1—C2—C3—C4	51.20 (19)	C114—C115—C116—C111	1.3 (3)
C21—C2—C3—C4	174.72 (13)		

Symmetry codes: (i) −*x*+1/2, *y*−1/2, *z*; (ii) −*x*+1/2, *y*+1/2, *z*; (iii) −*x*+3/2, *y*−1/2, *z*; (iv) −*x*+3/2, *y*+1/2, *z*; (v) −*x*+1, −*y*, −*z*; (vi) *x*+1, *y*, *z*; (vii) −*x*, −*y*, −*z*; (viii) *x*−1, *y*, *z*; (ix) *x*+1/2, −*y*−1/2, −*z*; (x) *x*+1/2, *y*, −*z*+1/2; (xi) *x*−1/2, *y*, −*z*+1/2; (xii) *x*−1/2, −*y*−1/2, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5···O1^{ii}	0.85 (2)	2.17 (2)	3.0153 (17)	174 (2)

C2—H2A···O1	0.98	2.31	2.736 (2)	106
C116—H116···O1	0.93	2.32	2.877 (2)	118

Symmetry codes: (ii) −*x*+1/2, *y*+1/2, *z*.

Fig. 1

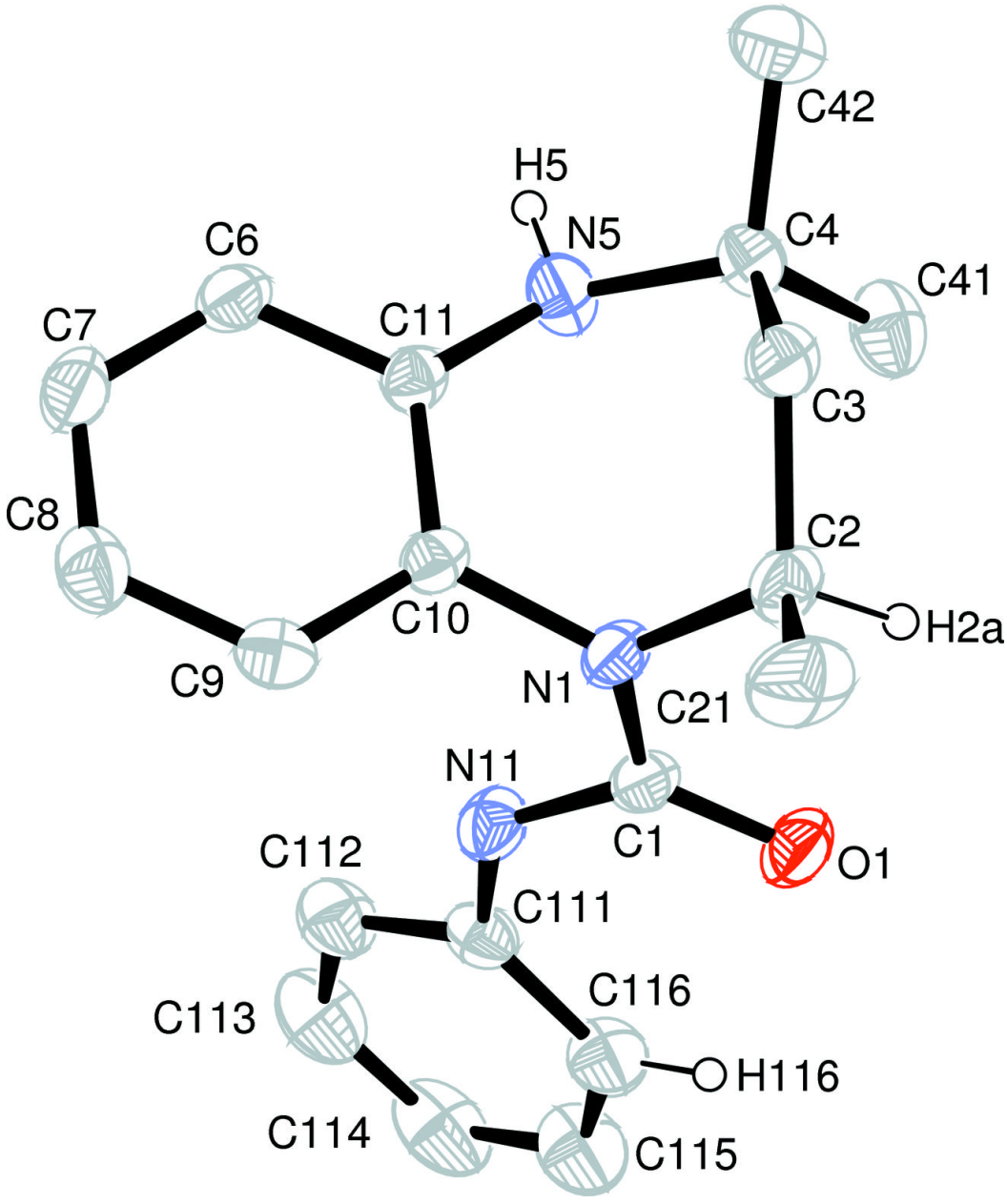
C42
H5
N5
C4
C6
C41
C7
C11
C3
C8
C2
C10
H2a
C9
N1
C21
N11
C1
O1
C112
C111
C116
C113
H116
C114
C115

Fig. 2