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2-(2,2-Dimethoxyethyl)-3-oxo-1,2,3,4,5,6-hexahydro-1,5-methano-7*H*-azocino[4,3-*b*]indole

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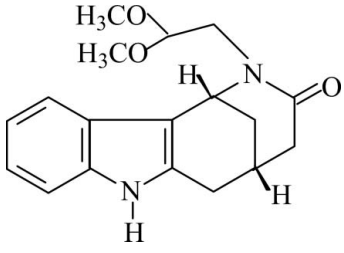
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.067; wR factor = 0.231; data-to-parameter ratio = 23.8.

The title compound, $C_{18}H_{22}N_2O_3$, consists of a tetracyclic ring system containing an azocino skeleton with a dimethoxyethyl group as a substituent. The benzene and five-membered rings are nearly coplanar, with a dihedral angle of 1.26 (8)°. In the crystal structure, intermolecular N—H···O hydrogen bonds link the molecules into chains parallel to the *b* axis.

Related literature

For general background, see: Hesse (2002); Bosch & Bonjoch (1988); Saxton (1983). For bond-length data, see: Allen *et al.* (1987). For related literature, see: Hökelek *et al.* (2004, 2006); Uludağ *et al.* (2006).



Experimental

Crystal data

$C_{18}H_{22}N_2O_3$
M_r = 314.38
Monoclinic, $P2_1/n$
a = 10.0347 (4) Å
b = 8.4616 (7) Å
c = 20.1168 (9) Å
β = 103.750 (3)°
V = 1659.16 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.35 × 0.20 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.971, T_{max} = 0.987
47331 measured reflections
5094 independent reflections
2625 reflections with $I > 2\sigma(I)$
R_{int} = 0.076

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.231
S = 1.06
5094 reflections
214 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N7—H7···O1^{i}	0.95 (2)	1.86 (2)	2.805 (2)	172 (2)

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2017).

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supplementary materials

Acta Cryst. (2007). E**63**, o3268 [**doi:10.1107/S1600536807029480**]

2-(2,2-Dimethoxyethyl)-3-oxo-1,2,3,4,5,6-hexahydro-1,5-methano-7*H*-azocino[4,3-*b*]indole

T. Hökelek, E. Sahin, N. Uludag and Ü.I. Erdogan

Comment

The hexahydro-1,5-methano-azocino[4,3-*b*]indole core structure can be considered to be synthetic precursor for most of the pentacyclic and tetracyclic indol alkaloids of biological interests (Hesse, 2002; Bosch & Bonjoch, 1988; Saxton, 1983), such as akuminicine and uleine. Most of them have the pentacyclic ring system as a common structural element and include a large group of naturally occurring compounds such as strychnine, a covulsant poison.

The structures of tricyclic, tetracyclic and pentacyclic ring systems with different substituent of azocino[4,3-*b*]indole core, have been the subject of much interest in our laboratory. These include *N*-(2-benzyloxyethyl)-4,7- dimethyl-6-(1,3-dithiolan-2-yl)-1,2,3,4,5,6-hexahydro-1,5-methano-2- azocino[4,3-*b*]indol-2-one, (II) (Hökelek *et al.*, 2004), 12-ethyl-2-methyl- 6,6-ethylenedithio-1,2,3,4,5,6-hexahydro-1,5-methano-2-azocino[4,3-*b*]indole- 3-one, (III), (Uludağ *et al.*, 2006) and 4-ethyl-6,6-ethylenedithio-2-(2- methoxymethyl)-7-methoxymethylene-2,3,4,5,6,7-hexahydro-1,5-methano-1*H*- azocino[4,3-*b*]indol-3-one, (IV), (Hökelek *et al.*, 2006). The present study was undertaken to ascertain the crystal structure of the title compound, (I).

The molecule of the title compound, (I), (Fig. 1), consists of a tetracyclic system containing an azocino skeleton with dimethoxyethyl group as substituent at position N2, in which the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The bonds N7—C6a [1.377 (3) Å] and N7—C7a [1.376 (3) Å] agree well with those in compounds (II) [1.392 (8) and 1.370 (8) Å] and (IV) [1.393 (4) and 1.386 (5) Å]. In all three structures atom N7 is substituted. The absolute configurations of C1 and C5 are *R* and S (Fig. 1), respectively.

An examination of the deviations from the least-squares planes through individual rings shows that rings A (C7a/C8/C9/C10/C11/C11*a*) and B (N7/C7a/C11*a*/C11*b*/C6a) are planar. They are also nearly co-planar with a dihedral angle of A/B = 1.25 (7)°. Rings C (C1/C11*b*/C6a/C6/C5/C12) and D (C1/N2/C3/C4/C5/C12) are, of course, not planar. Atom C12 deviates from the planes of E (C1/C5/C6/C6a/C11*b*) and F (C1/N2/C3/C4/C5) by −0.710 (2) Å and 0.7445 (2) Å, respectively, where the dihedral angle between the planes of E and F is E/F = 69.72 (6)°. On the other hand, the dihedral angles between the plane of G (C1/C5/C12) and planes of E and F are 53.93 (7)° and 69.84 (6)°, respectively.

In the crystal structure, intermolecular N–H···O hydrogen bonds (see Table) link the molecules into chains nearly parallel to *b* axis (Fig. 2), in which they may be effective in the stabilization of the structure; van der Waals interactions are also effective in the molecular packing.

Experimental

The title compound, (I), was prepared from *N*-(2',2'-Dimethoxyethyl)-6- (1,2-dithiolane-2-yl)-1,2,3,4,5,6-hexahydro-1,5-methano-3-oxo-1*H*- azocino[4,3-*b*]indole (1.0 g, 2.47 mmol) and Raney nickel (1.0 g) in ethanol (50 ml). The mixture was refluxed for 22 h, and then filtered and evaporated. The residue was purified by silica gel chromatography using ethyl acetate and crystallized from diethyl ether (yield; 0.42 g, 54%, m.p. 453 K).

Figures

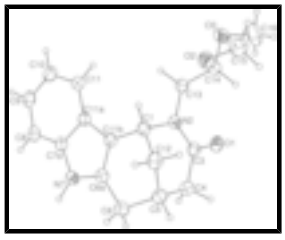

Fig. 1. The structure of the title molecule with the atom-numbering scheme. The displacement ellipsoids are drawn at the 20% probability level. The hydrogen atoms are drawn as spheres with arbitrary radius.

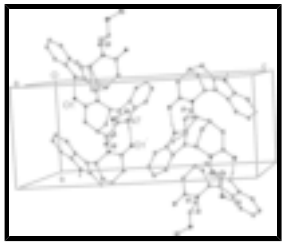

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted [symmetry code: (') 1/2 − *x*, 1/2 + *y*, 1/2 − *z*].

2-(2,2-Dimethoxyethyl)-3-oxo-1,2,3,4,5,6-hexahydro-1,5-methano- 7*H*-azocino[4,3-*b*]indole

Crystal data

$C_{18}H_{22}N_2O_3$	F_{000} = 672
M_r = 314.38	D_x = 1.259 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 6164 reflections
a = 10.0347 (4) Å	θ = 2.1–30.6º
b = 8.4616 (7) Å	μ = 0.09 mm^{-1}
c = 20.1168 (9) Å	T = 294 (2) K
β = 103.750 (3)º	Prism, colorless
V = 1659.16 (17) Å^3	0.35 × 0.20 × 0.15 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID-S diffractometer	5094 independent reflections
Radiation source: fine-focus sealed tube	2625 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.076
T = 294(2) K	θ_{max} = 30.7º
ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (Blessing, 1995)	h = −14→14
T_{min} = 0.971, T_{max} = 0.987	k = −10→12
47331 measured reflections	l = −28→28

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.067$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.231$	$w = 1/[\sigma^2(F_o^2) + (0.1052P)^2 + 0.0611P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
5094 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
214 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-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 $F^2 > 2$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	0.05988 (15)	0.19313 (18)	0.09564 (7)	0.0701 (4)
O2	−0.31895 (16)	0.1229 (2)	0.14450 (8)	0.0794 (5)
O3	−0.2405 (2)	−0.12092 (19)	0.12128 (10)	0.0944 (6)
C1	−0.0680 (2)	0.3424 (2)	0.23627 (10)	0.0594 (5)
H1	−0.1476	0.3034	0.2516	0.071*
N2	−0.04095 (17)	0.2356 (2)	0.18262 (8)	0.0595 (4)
C3	0.03154 (19)	0.2844 (2)	0.13862 (10)	0.0581 (5)
C4	0.0769 (2)	0.4547 (3)	0.14005 (12)	0.0715 (6)
H4A	0.0477	0.4955	0.0938	0.086*
H4B	0.1764	0.4556	0.1519	0.086*
C5	0.0288 (2)	0.5715 (3)	0.18762 (11)	0.0702 (6)
H5	0.0053	0.6712	0.1629	0.084*
C6	0.1378 (3)	0.6059 (3)	0.25340 (12)	0.0768 (6)
H6A	0.2262	0.6213	0.2427	0.092*
H6B	0.1144	0.7019	0.2743	0.092*
C6A	0.1460 (2)	0.4708 (2)	0.30211 (10)	0.0626 (5)
C7A	0.2202 (2)	0.3180 (2)	0.39445 (10)	0.0590 (5)

N7	0.24803 (18)	0.4512 (2)	0.36095 (9)	0.0663 (5)
H7	0.315 (2)	0.529 (3)	0.3798 (12)	0.077 (7)*
C8	0.2921 (2)	0.2521 (3)	0.45622 (10)	0.0677 (6)
H8	0.3729	0.2974	0.4813	0.081*
C9	0.2393 (3)	0.1185 (3)	0.47851 (11)	0.0756 (6)
H9	0.2848	0.0724	0.5196	0.091*
C10	0.1190 (3)	0.0506 (3)	0.44087 (12)	0.0792 (7)
H10	0.0856	−0.0401	0.4574	0.095*
C11	0.0475 (2)	0.1142 (3)	0.37944 (11)	0.0673 (6)
H11	−0.0328	0.0669	0.3549	0.081*
C11A	0.0979 (2)	0.2506 (2)	0.35487 (9)	0.0560 (5)
C11B	0.0528 (2)	0.3514 (2)	0.29624 (10)	0.0570 (5)
C12	−0.1000 (2)	0.5072 (3)	0.20518 (12)	0.0705 (6)
H12A	−0.1739	0.5011	0.1642	0.085*
H12B	−0.1285	0.5765	0.2376	0.085*
C13	−0.0850 (2)	0.0703 (2)	0.18074 (10)	0.0644 (5)
H13A	−0.1020	0.0420	0.2247	0.077*
H13B	−0.0121	0.0030	0.1728	0.077*
C14	−0.2129 (2)	0.0419 (2)	0.12555 (11)	0.0636 (5)
H14	−0.2009	0.0815	0.0816	0.076*
C15	−0.4422 (3)	0.1293 (4)	0.09197 (15)	0.0976 (9)
H15A	−0.4230	0.1734	0.0513	0.146*
H15B	−0.5081	0.1943	0.1067	0.146*
H15C	−0.4784	0.0245	0.0825	0.146*
C16	−0.2419 (5)	−0.1910 (4)	0.05865 (17)	0.1358 (15)
H16A	−0.3086	−0.1393	0.0232	0.204*
H16B	−0.2651	−0.3008	0.0602	0.204*
H16C	−0.1528	−0.1814	0.0493	0.204*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0713 (9)	0.0756 (10)	0.0610 (9)	0.0142 (7)	0.0112 (7)	0.0032 (7)
O2	0.0630 (9)	0.0999 (12)	0.0721 (10)	−0.0028 (8)	0.0097 (8)	0.0025 (8)
O3	0.1162 (15)	0.0666 (10)	0.0902 (12)	−0.0259 (9)	0.0043 (11)	−0.0006 (9)
C1	0.0540 (10)	0.0674 (12)	0.0553 (11)	−0.0031 (9)	0.0100 (8)	0.0005 (9)
N2	0.0593 (9)	0.0623 (10)	0.0542 (9)	−0.0065 (7)	0.0080 (7)	−0.0011 (7)
C3	0.0506 (10)	0.0666 (12)	0.0526 (10)	0.0055 (9)	0.0037 (8)	0.0049 (9)
C4	0.0750 (14)	0.0717 (14)	0.0679 (13)	−0.0088 (11)	0.0176 (11)	0.0050 (11)
C5	0.0802 (14)	0.0586 (12)	0.0681 (13)	0.0022 (10)	0.0104 (11)	0.0093 (10)
C6	0.0919 (16)	0.0639 (13)	0.0710 (14)	−0.0125 (12)	0.0122 (12)	0.0034 (11)
C6A	0.0646 (12)	0.0637 (12)	0.0573 (11)	−0.0051 (9)	0.0101 (9)	−0.0005 (9)
C7A	0.0596 (11)	0.0642 (12)	0.0527 (10)	−0.0001 (9)	0.0122 (9)	−0.0055 (8)
N7	0.0625 (10)	0.0699 (11)	0.0622 (10)	−0.0150 (9)	0.0064 (8)	−0.0034 (8)
C8	0.0651 (12)	0.0834 (15)	0.0506 (10)	0.0062 (11)	0.0059 (9)	−0.0073 (10)
C9	0.0920 (17)	0.0815 (15)	0.0501 (11)	0.0105 (13)	0.0105 (11)	0.0059 (10)
C10	0.1020 (18)	0.0760 (15)	0.0607 (13)	−0.0012 (13)	0.0218 (13)	0.0082 (11)
C11	0.0739 (13)	0.0700 (13)	0.0579 (12)	−0.0117 (10)	0.0158 (10)	0.0005 (9)

C11A	0.0568 (11)	0.0605 (11)	0.0509 (10)	−0.0019 (8)	0.0132 (8)	−0.0023 (8)
C11B	0.0549 (10)	0.0619 (11)	0.0534 (10)	−0.0039 (9)	0.0115 (8)	−0.0005 (8)
C12	0.0682 (13)	0.0753 (14)	0.0652 (12)	0.0135 (11)	0.0101 (10)	0.0026 (10)
C13	0.0670 (12)	0.0633 (12)	0.0574 (11)	−0.0056 (10)	0.0037 (9)	0.0057 (9)
C14	0.0692 (12)	0.0615 (12)	0.0564 (11)	−0.0103 (10)	0.0074 (9)	0.0035 (9)
C15	0.0691 (15)	0.119 (2)	0.096 (2)	−0.0027 (14)	0.0021 (14)	0.0302 (16)
C16	0.190 (4)	0.087 (2)	0.098 (2)	0.014 (2)	−0.030 (2)	−0.0281 (18)

Geometric parameters (Å, °)

O1—C3	1.242 (2)	C6A—C6	1.495 (3)
O2—C14	1.393 (3)	C7A—C8	1.396 (3)
O2—C15	1.424 (3)	C7A—C11A	1.414 (3)
O3—C14	1.404 (2)	C8—C9	1.368 (3)
O3—C16	1.390 (4)	C8—H8	0.9300
N2—C3	1.338 (3)	C9—C10	1.388 (3)
N2—C13	1.464 (3)	C9—H9	0.9300
N2—C1	1.482 (2)	C10—H10	0.9300
N7—C7A	1.376 (3)	C11—C10	1.382 (3)
N7—C6A	1.378 (2)	C11—H11	0.9300
N7—H7	0.95 (2)	C11A—C11	1.397 (3)
C1—C11B	1.495 (3)	C11A—C11B	1.439 (3)
C1—C12	1.530 (3)	C12—H12A	0.9700
C1—H1	0.9800	C12—H12B	0.9700
C3—C4	1.509 (3)	C13—C14	1.503 (3)
C4—H4A	0.9700	C13—H13A	0.9700
C4—H4B	0.9700	C13—H13B	0.9700
C5—C4	1.532 (3)	C14—H14	0.9800
C5—H5	0.9800	C15—H15A	0.9600
C5—C6	1.531 (3)	C15—H15B	0.9600
C5—C12	1.519 (3)	C15—H15C	0.9600
C6—H6A	0.9700	C16—H16A	0.9600
C6—H6B	0.9700	C16—H16B	0.9600
C6A—C11B	1.362 (3)	C16—H16C	0.9600
C14—O2—C15	113.62 (19)	C9—C8—H8	121.2
C16—O3—C14	115.7 (2)	C7A—C8—H8	121.2
C3—N2—C13	119.09 (18)	C8—C9—C10	121.2 (2)
C3—N2—C1	121.07 (16)	C8—C9—H9	119.4
C13—N2—C1	119.67 (16)	C10—C9—H9	119.4
C7A—N7—C6A	108.88 (17)	C11—C10—C9	121.7 (2)
C7A—N7—H7	125.2 (14)	C11—C10—H10	119.1
C6A—N7—H7	124.6 (14)	C9—C10—H10	119.1
N7—C7A—C8	129.9 (2)	C10—C11—C11A	118.9 (2)
N7—C7A—C11A	107.72 (17)	C10—C11—H11	120.5
C8—C7A—C11A	122.4 (2)	C11A—C11—H11	120.5
C11—C11A—C7A	118.18 (19)	C6A—C11B—C11A	107.04 (17)
C11—C11A—C11B	135.28 (19)	C6A—C11B—C1	121.07 (17)
C7A—C11A—C11B	106.52 (17)	C11A—C11B—C1	131.89 (17)
N2—C1—C11B	111.41 (16)	C5—C12—C1	108.28 (17)

N2—C1—C12	108.36 (16)	C5—C12—H12A	110.0
C11B—C1—C12	109.54 (17)	C1—C12—H12A	110.0
N2—C1—H1	109.2	C5—C12—H12B	110.0
C11B—C1—H1	109.2	C1—C12—H12B	110.0
C12—C1—H1	109.2	H12A—C12—H12B	108.4
O1—C3—N2	121.26 (19)	N2—C13—C14	111.79 (16)
O1—C3—C4	119.29 (18)	N2—C13—H13A	109.3
N2—C3—C4	119.43 (18)	C14—C13—H13A	109.3
C3—C4—C5	119.29 (18)	N2—C13—H13B	109.3
C3—C4—H4A	107.5	C14—C13—H13B	109.3
C5—C4—H4A	107.5	H13A—C13—H13B	107.9
C3—C4—H4B	107.5	O2—C14—O3	110.32 (18)
C5—C4—H4B	107.5	O2—C14—C13	107.03 (17)
H4A—C4—H4B	107.0	O3—C14—C13	108.87 (17)
C12—C5—C6	109.86 (19)	O2—C14—H14	110.2
C12—C5—C4	109.05 (18)	O3—C14—H14	110.2
C6—C5—C4	113.3 (2)	C13—C14—H14	110.2
C12—C5—H5	108.2	O2—C15—H15A	109.5
C6—C5—H5	108.2	O2—C15—H15B	109.5
C4—C5—H5	108.2	H15A—C15—H15B	109.5
C6A—C6—C5	109.75 (18)	O2—C15—H15C	109.5
C6A—C6—H6A	109.7	H15A—C15—H15C	109.5
C5—C6—H6A	109.7	H15B—C15—H15C	109.5
C6A—C6—H6B	109.7	O3—C16—H16A	109.5
C5—C6—H6B	109.7	O3—C16—H16B	109.5
H6A—C6—H6B	108.2	H16A—C16—H16B	109.5
C11B—C6A—N7	109.84 (18)	O3—C16—H16C	109.5
C11B—C6A—C6	125.46 (19)	H16A—C16—H16C	109.5
N7—C6A—C6	124.68 (19)	H16B—C16—H16C	109.5
C9—C8—C7A	117.6 (2)		
C15—O2—C14—O3	−71.6 (2)	C12—C5—C6—C6A	45.2 (3)
C15—O2—C14—C13	170.10 (19)	C4—C5—C6—C6A	−77.0 (2)
C16—O3—C14—O2	123.3 (3)	C6—C5—C12—C1	−68.7 (2)
C16—O3—C14—C13	−119.5 (3)	C4—C5—C12—C1	56.0 (2)
C13—N2—C3—O1	1.3 (3)	C11B—C6A—C6—C5	−13.1 (3)
C1—N2—C3—O1	176.60 (17)	N7—C6A—C6—C5	168.7 (2)
C13—N2—C3—C4	179.79 (17)	N7—C6A—C11B—C11A	0.3 (2)
C1—N2—C3—C4	−4.9 (3)	C6—C6A—C11B—C11A	−178.1 (2)
C3—N2—C1—C11B	−80.3 (2)	N7—C6A—C11B—C1	−179.11 (18)
C13—N2—C1—C11B	95.02 (19)	C6—C6A—C11B—C1	2.5 (3)
C3—N2—C1—C12	40.3 (2)	N7—C7A—C8—C9	178.9 (2)
C13—N2—C1—C12	−144.41 (18)	C11A—C7A—C8—C9	−0.7 (3)
C3—N2—C13—C14	−81.7 (2)	N7—C7A—C11A—C11	−179.01 (18)
C1—N2—C13—C14	102.9 (2)	C8—C7A—C11A—C11	0.7 (3)
C6A—N7—C7A—C8	−178.8 (2)	N7—C7A—C11A—C11B	−0.7 (2)
C6A—N7—C7A—C11A	0.8 (2)	C8—C7A—C11A—C11B	179.03 (18)
C7A—N7—C6A—C11B	−0.7 (2)	C7A—C8—C9—C10	0.3 (3)
C7A—N7—C6A—C6	177.7 (2)	C8—C9—C10—C11	0.1 (4)
N2—C1—C11B—C6A	96.2 (2)	C11A—C11—C10—C9	−0.2 (3)

C12—C1—C11B—C6A	−23.7 (3)	C7A—C11A—C11—C10	−0.2 (3)
N2—C1—C11B—C11A	−83.0 (3)	C11B—C11A—C11—C10	−178.0 (2)
C12—C1—C11B—C11A	157.1 (2)	C11—C11A—C11B—C6A	178.2 (2)
N2—C1—C12—C5	−66.2 (2)	C7A—C11A—C11B—C6A	0.2 (2)
C11B—C1—C12—C5	55.5 (2)	C11—C11A—C11B—C1	−2.5 (4)
O1—C3—C4—C5	173.37 (19)	C7A—C11A—C11B—C1	179.5 (2)
N2—C3—C4—C5	−5.2 (3)	N2—C13—C14—O2	−67.5 (2)
C12—C5—C4—C3	−21.6 (3)	N2—C13—C14—O3	173.28 (18)
C6—C5—C4—C3	101.1 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N7—H7···O1^{i}	0.95 (2)	1.86 (2)	2.805 (2)	172 (2)

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

Fig. 1

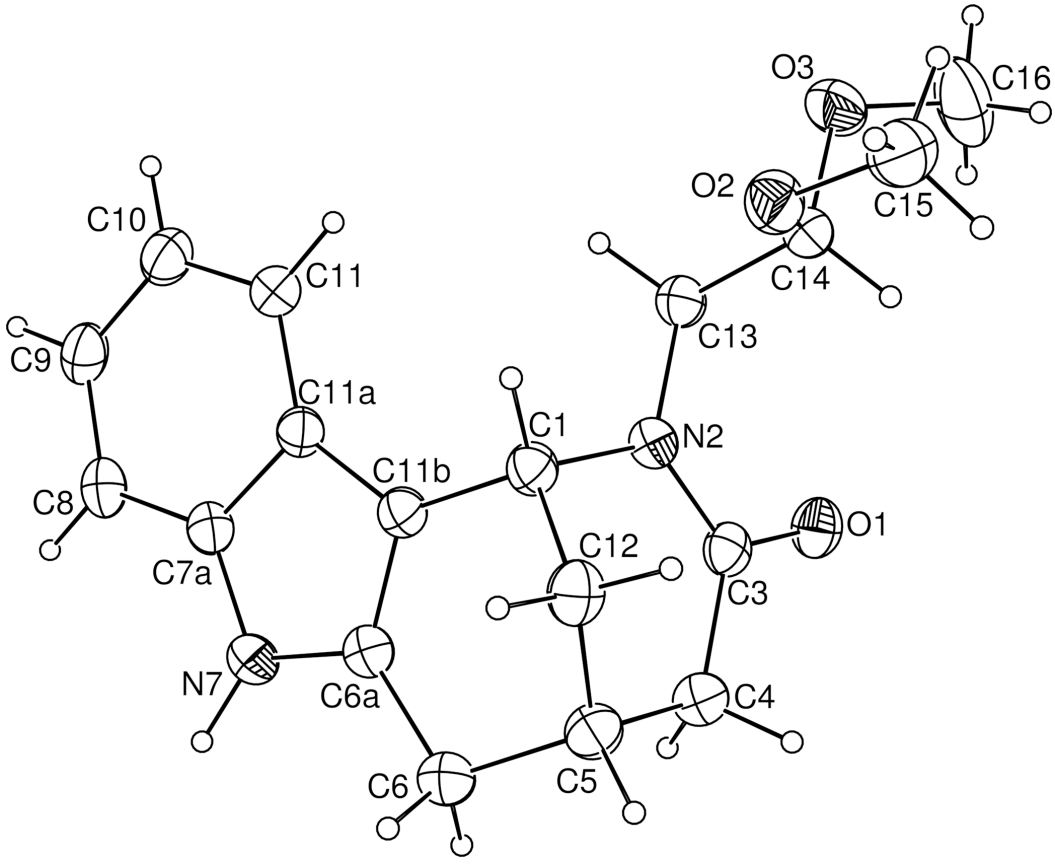
O3
C16
O2
C15
C10
C11
C14
C13
C9
C11a
C1
N2
C11b
C8
O1
C12
C7a
C3
N7
C6a
C4
C6
C5

Fig. 2