

C17	0.0265 (3)	-0.3806 (2)	0.7759 (2)	0.0224 (11)	C9—C12—C8	60.77 (15)	C24—C28—C30	137.9 (2)
C18	-0.1053 (3)	-0.3842 (3)	0.7993 (2)	0.0268 (12)	C13—C12—C8	137.0 (2)	C25—C28—C30	138.2 (2)
C19	-0.2330 (3)	-0.3553 (3)	0.7550 (3)	0.036 (2)	C14—C12—C8	139.3 (2)	C29—C28—C30	61.6 (2)
C20	-0.1295 (3)	-0.2965 (3)	0.8911 (3)	0.036 (2)	C12—C13—C14	58.9 (2)	C28—C29—C30	59.3 (2)
C21	-0.0859 (3)	-0.5087 (2)	0.7842 (2)	0.0272 (12)	C12—C14—C13	58.7 (2)	C28—C30—C29	59.1 (2)
C22	-0.1887 (3)	-0.6653 (3)	0.7098 (3)	0.038 (2)				
C23	-0.0929 (3)	-0.6080 (3)	0.8471 (3)	0.037 (2)				
C24	0.2216 (3)	-0.0702 (2)	0.7362 (2)	0.0221 (12)				
C25	0.1297 (3)	-0.0020 (2)	0.7315 (2)	0.0235 (12)				
C26	-0.0304 (3)	-0.0367 (3)	0.6533 (2)	0.0318 (14)				
C27	0.0368 (3)	0.0305 (3)	0.7924 (2)	0.0319 (14)				
C28	0.2870 (3)	0.0711 (2)	0.7309 (2)	0.0243 (12)				
C29	0.3547 (3)	0.1486 (3)	0.6588 (3)	0.035 (2)				
C30	0.4370 (3)	0.2134 (3)	0.7979 (3)	0.0337 (15)				

This work was supported in part by the Alexander von Humboldt Foundation

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71089 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HU1043]

Table 2. Bond lengths (Å) and angles (°)

C1—C3	1.482 (3)	C15—C17	1.323 (2)
C1—C2	1.526 (4)	C15—C16	1.480 (2)
C2—C3	1.480 (3)	C16—C24	1.328 (3)
C3—C4	1.455 (3)	C17—C21	1.455 (3)
C3—C7	1.507 (3)	C17—C18	1.456 (3)
C4—C5	1.469 (3)	C18—C21	1.482 (3)
C4—C6	1.480 (3)	C18—C19	1.484 (4)
C4—C7	1.494 (3)	C18—C20	1.486 (4)
C5—C6	1.523 (4)	C19—C20	1.521 (4)
C7—C16	1.511 (2)	C21—C23	1.483 (4)
C7—C8	1.526 (3)	C21—C22	1.485 (4)
C8—C9	1.500 (3)	C22—C23	1.520 (4)
C8—C12	1.507 (3)	C24—C28	1.459 (3)
C8—C15	1.510 (3)	C24—C25	1.457 (3)
C9—C12	1.458 (3)	C25—C28	1.473 (3)
C9—C11	1.477 (3)	C25—C27	1.486 (4)
C9—C10	1.475 (3)	C25—C26	1.487 (3)
C10—C11	1.521 (4)	C26—C27	1.523 (4)
C12—C13	1.478 (4)	C28—C29	1.483 (3)
C12—C14	1.482 (4)	C28—C30	1.485 (3)
C13—C14	1.533 (4)	C29—C30	1.520 (4)
C3—C1—C2	58.9 (2)	C17—C15—C16	136.97 (13)
C3—C2—C1	59.1 (2)	C17—C15—C8	132.47 (10)
C4—C3—C2	134.2 (2)	C16—C15—C8	90.51 (9)
C4—C3—C1	138.2 (2)	C24—C16—C15	136.8 (2)
C2—C3—C1	62.0 (2)	C24—C16—C7	132.2 (2)
C4—C3—C7	60.55 (15)	C15—C16—C7	90.87 (12)
C2—C3—C7	138.1 (2)	C15—C17—C21	148.6 (2)
C1—C3—C7	140.2 (2)	C15—C17—C18	150.2 (2)
C3—C4—C5	135.3 (2)	C21—C17—C18	61.2 (2)
C3—C4—C6	137.6 (2)	C17—C18—C19	59.3 (2)
C5—C4—C6	62.2 (2)	C17—C18—C19	140.7 (2)
C3—C4—C7	61.44 (15)	C21—C18—C19	138.6 (2)
C5—C4—C7	137.0 (2)	C17—C18—C20	138.0 (2)
C6—C4—C7	139.6 (2)	C21—C18—C20	135.7 (2)
C4—C5—C6	59.3 (2)	C19—C18—C20	61.6 (2)
C4—C6—C5	58.5 (2)	C18—C19—C20	59.3 (2)
C4—C7—C3	58.01 (15)	C18—C20—C19	59.1 (2)
C4—C7—C16	129.26 (9)	C17—C21—C18	59.4 (2)
C3—C7—C16	124.81 (8)	C17—C21—C23	141.6 (2)
C4—C7—C8	131.0 (2)	C18—C21—C23	137.1 (2)
C3—C7—C8	129.3 (2)	C17—C21—C22	138.2 (2)
C16—C7—C8	88.75 (9)	C18—C21—C22	135.9 (2)
C9—C8—C12	57.99 (15)	C23—C21—C22	61.6 (2)
C9—C8—C15	128.8 (2)	C21—C22—C23	59.2 (2)
C12—C8—C15	124.8 (2)	C21—C23—C22	59.2 (2)
C9—C8—C7	130.8 (2)	C16—C24—C28	147.4 (2)
C12—C8—C7	129.6 (2)	C16—C24—C25	151.5 (2)
C15—C8—C7	89.1 (2)	C28—C24—C25	60.7 (2)
C12—C9—C11	136.6 (2)	C24—C25—C28	59.7 (2)
C12—C9—C10	137.7 (2)	C24—C25—C27	141.1 (2)
C11—C9—C10	62.0 (2)	C28—C25—C27	139.2 (2)
C12—C9—C8	61.25 (15)	C24—C25—C26	137.6 (2)
C11—C9—C8	137.5 (2)	C28—C25—C26	134.4 (2)
C10—C9—C8	138.2 (2)	C27—C25—C26	61.6 (2)
C9—C10—C11	59.1 (2)	C25—C26—C27	59.2 (2)
C9—C11—C10	58.9 (2)	C25—C27—C26	59.2 (2)
C9—C12—C13	135.3 (2)	C24—C28—C25	59.6 (2)
C9—C12—C14	138.5 (2)	C24—C28—C29	141.1 (2)
C13—C12—C14	62.4 (2)	C25—C28—C29	135.6 (2)

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Structure of *N*-Nitroso-2,4-diphenyl-3-azabicyclo[3.3.1]nonane

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Abstract

The title compound adopts a twin-chair conformation. The overall conformation is similar in both the molecules of the asymmetric unit. The phenyl rings are equatorially disposed with respect to the central ring system. The plane of the nitroso group makes angles of 31.0 (4) and 33.4 (5)° with the C(2)—N(3)—C(4) plane of the piperidine ring in molecules *A* and *B*, respectively. The N(3)⋯C(7) non-bonded separation is 3.19 (7) Å for both molecules *A* and *B*.

The crystal structure is stabilized by van der Waals interactions.

Comment

The crystal structure of the title compound (III) reported here, forms part of our work on the synthesis (T. Ravindran & R. Jeyaraman, unpublished work) and X-ray studies of a series of cyclic nitrosamines (Priya, Shamala, Viswamitra, Senthil Kumar & Jeyaraman, 1992; Priya, Shamala, Viswamitra, Ravindran & Jeyaraman, 1993). This compound contains the bicyclo[3.3.1]nonane ring system which offers wide conformational flexibility (Jeyaraman & Avila, 1981).

The crystal structure has two molecules in the asymmetric unit. The overall conformation is similar in both molecules. The bicyclic compound adopts a twin-chair conformation as illustrated in Fig. 1. This is the most favoured conformation for the bicyclo[3.3.1]nonane ring system (Chakraborty, Ellis & Roberts, 1970; Epenbetov, Yanovskii, Struchkov, Omarov & Aldabergenov, 1983). In the cyclohexane ring, the displacements of the C(7) and C(9) atoms from the C(1)–C(5)–C(6)–C(8) plane are 0.62 (1) and -0.71 (1) Å, respectively, for molecule *A* and 0.59 (1) and -0.71 (1) Å, respectively, for molecule *B*. Thus, both molecules show deviation from ideal chair conformation. The C_{sp^2} – C_{sp^3} bond lengths are in the range 1.493 (11)–1.537 (10) Å for molecule *A* and 1.511 (10)–1.533 (10) Å for molecule *B*. The bond angles are in the range 110.3 (6)–112.6 (6)° for molecule *A* and 110.5 (5)–113.9 (6)° for molecule *B*, showing that the ring is flattened. The asymmetry parameter (Duax & Norton, 1975) of the cyclohexane ring for the best twofold axis passing through C(1)–C(9) and C(6)–C(7) is $\Delta C_2 = 1.65^\circ$ for molecule *A* and 3.76° for molecule *B*.

The piperidine ring is also distorted from ideal chair conformation. The sp^2 -hybridized N atom N(3) causes considerable flattening of the ring. The displacement of atom N(3) from the C(2)–C(4)–N(22) plane is 0.246 (3) Å for molecule *A* and 0.256 (4) Å for molecule *B*. The sum of the angles around N(3) is 351.8° in molecule *A* and 350.9° in molecule *B*, showing that the sp^2 -hybridized N atom exhibits pyramidal character. The asymmetry parameter for the best mirror passing through atoms N(3) and C(9) is $\Delta C_s = 4.5^\circ$ for molecule *A* and 1.27° for molecule *B*.

The phenyl rings are equatorially disposed with respect to the piperidine rings in molecules *A* and *B*. The dihedral angle between the phenyl rings is 14.0 (2)° in molecule *A* and 12.4 (2)° in molecule *B*. The orientation of the phenyl rings appears to influence the coplanarity of the nitroso group with the C(2)–N(3)–C(4) plane. In the present case, the plane

of the nitroso group makes an angle of 31.0 (4)° with the C(2)–N(3)–C(4) atom plane in molecule *A* and 33.4 (5)° in molecule *B*. The nitroso moiety tilts away from the plane probably in order to minimize the steric hindrance with the phenyl rings in the equatorial position. In our previous structure, *N*-nitroso-*r*-2,*c*-7-diphenylhexahydro-1,4-diazepin-5-one (I) (Priya, Shamala, Viswamitra, Senthil Kumar & Jeyaraman, 1992), the nitroso group prefers a coplanar orientation with the C(2)–N(1)–C(7) plane of the central ring because of lack of any steric hindrance from the phenyl rings which are in the quasi-axial position. The non-coplanarity also inhibits the resonance effect of the nitroso group. This is reflected in the N–N bond length of 1.443 (7) Å in molecule *B* which corresponds to an N–N single bond. However, the nitroso group dimensions of molecule *A* have to be treated with caution since they have high thermal parameters associated with them.

The conformational changes induced in the bicyclic system by substituting an sp^3 -hybridized N atom at the 3 position were studied by comparing the crystal structure of (III) with that of 2,4-diphenyl-3-

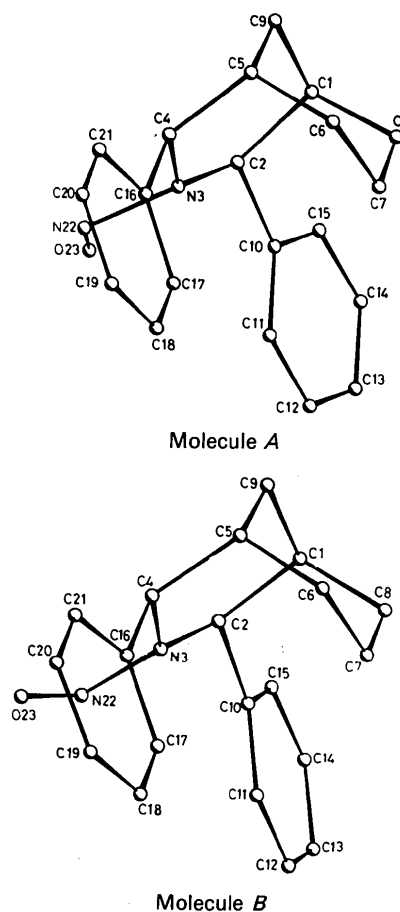


Fig. 1. View showing atomic labelling scheme and conformation of molecules *A* and *B*.

azabicyclo[3.3.1]nonane, henceforth abbreviated as ABN (Cox, McCabe, Milne & Sim, 1985). The decreased lone-pair repulsion of the sp^2 -hybridized N atom on the C(7) *endo*-H in (III) as compared to ABN is seen from the torsion angles about the bonds C(6)—C(7) and C(7)—C(8) listed in Table 3. This is in agreement with the observation that the introduction of a trigonal atom at the 3 position decreases the 3...7 repulsion (Zefirov & Palyulin, 1991). The flattening of the piperidine ring in (III) causes a marginal increase in the N(3)...C(7) separation to 3.19 (7) Å in molecules *A* and *B* as compared to 2.96 Å in ABN. On comparing the torsion angles about the phenyl rings for molecules *A* and *B*, with ABN, from Table 3, it appears that the bulky nitroso group does not have much influence on the disposition of the phenyl rings since it is essentially similar in molecules *A*, *B* and ABN. The crystal structure of the title compound is stabilized by van der Waals interactions (Fig. 2).

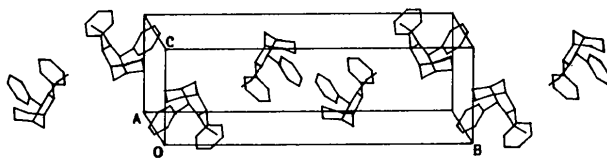


Fig. 2. Packing of the molecules in the unit cell.

Experimental

Crystal data

$C_{20}H_{22}N_2O$

$M_r = 306.36$

Monoclinic

$P2_1/c$

$a = 18.456 (2) \text{ \AA}$

$b = 24.097 (3) \text{ \AA}$

$c = 7.540 (1) \text{ \AA}$

$\beta = 91.8 (1)^\circ$

$V = 3351.5 \text{ \AA}^3$

$Z = 8$

$D_x = 1.20 \text{ Mg m}^{-3}$

Cu $K\alpha$ radiation

$\lambda = 1.5418 \text{ \AA}$

Cell parameters from 22 reflections

$\theta = 9-22^\circ$

$\mu = 0.51 \text{ mm}^{-1}$

$T = 295 \text{ K}$

Parallelepiped

$0.36 \times 0.2 \times 0.1 \text{ mm}$

Yellow

Crystal source: ethanol

Data collection

Enraf-Nonius CAD-4 diffractometer

ω - 2θ scans

Absorption correction: none

4318 measured reflections

2913 independent reflections

1925 observed reflections

$[I > 2.5\sigma(I)]$

$R_{int} = 0.014$

$\theta_{max} = 60^\circ$

$h = 0 \rightarrow 16$

$k = 0 \rightarrow 27$

$l = -8 \rightarrow 8$

3 standard reflections

frequency: 60 min

intensity variation: $< 3\%$

Refinement

Refinement on F

Final $R = 0.045$

$wR = 0.045$

$S = 1.362$

1925 reflections

296 parameters

All H-atom parameters refined

$w = 1/\sigma^2(|F|)$

$(\Delta/\sigma)_{max} = 0.006$

$\Delta\rho_{max} = 0.26 \text{ e \AA}^{-3}$

$\Delta\rho_{min} = -0.22 \text{ e \AA}^{-3}$

Atomic scattering factors

from *International Tables*

for *X-ray Crystallography*

(1974, Vol. IV)

Data collection: *SDP* (Enraf-Nonius, 1985). Program(s) used to solve structure: *MULTAN87* (Debaerdemaeker, Germain, Main, Tate & Woolfson, 1987). Program(s) used to refine structure: *SHELX400* [enhanced version of *SHELX76* (Sheldrick, 1976)].

Table 1. Fractional atomic coordinates and equivalent isotropic thermal parameters (\AA^2)

$$U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	U_{eq}
Molecule A				
C(1)	0.9683 (4)	0.1153 (3)	0.8692 (8)	0.073 (3)
C(2)	0.9470 (3)	0.0978 (2)	0.6771 (6)	0.054 (2)
N(3)	1.0126 (2)	0.0901 (1)	0.5678 (5)	0.051 (2)
C(4)	1.0873 (3)	0.0817 (2)	0.6352 (7)	0.052 (2)
C(5)	1.0984 (3)	0.1035 (3)	0.8250 (7)	0.060 (2)
C(6)	1.1101 (4)	0.1664 (3)	0.8429 (9)	0.072 (3)
C(7)	1.0413 (4)	0.1998 (3)	0.7964 (10)	0.077 (3)
C(8)	0.9786 (4)	0.1777 (3)	0.8949 (10)	0.086 (3)
C(9)	1.0353 (3)	0.0835 (3)	0.9328 (8)	0.073 (3)
C(10)	0.8912 (3)	0.1370 (2)	0.5904 (8)	0.055 (2)
C(11)	0.9034 (4)	0.1701 (2)	0.4452 (8)	0.063 (2)
C(12)	0.8496 (5)	0.2064 (2)	0.3825 (10)	0.078 (3)
C(13)	0.7851 (5)	0.2105 (3)	0.4624 (12)	0.086 (4)
C(14)	0.7727 (4)	0.1779 (3)	0.6056 (12)	0.083 (4)
C(15)	0.8246 (4)	0.1408 (3)	0.6673 (10)	0.075 (3)
C(16)	1.1443 (3)	0.1034 (2)	0.5149 (6)	0.054 (2)
C(17)	1.1358 (4)	0.1498 (2)	0.4084 (7)	0.069 (2)
C(18)	1.1944 (5)	0.1705 (3)	0.3144 (8)	0.089 (3)
C(19)	1.2610 (5)	0.1440 (4)	0.3312 (10)	0.091 (4)
C(20)	1.2695 (4)	0.0974 (4)	0.4355 (10)	0.087 (3)
C(21)	1.2120 (4)	0.0773 (3)	0.5269 (8)	0.067 (3)
N(22)	1.0164 (3)	0.0570 (3)	0.3933 (10)	0.146 (3)
O(23)	0.9544 (4)	0.0563 (2)	0.3698 (6)	0.124 (3)
Molecule B				
C(1)	0.6329 (3)	0.0978 (2)	0.3758 (7)	0.063 (2)
C(2)	0.6583 (3)	0.1231 (2)	0.1997 (7)	0.058 (2)
N(3)	0.5976 (2)	0.1501 (2)	0.0969 (5)	0.057 (2)
C(4)	0.5310 (3)	0.1728 (2)	0.1736 (7)	0.061 (2)
C(5)	0.5132 (3)	0.1431 (3)	0.3511 (7)	0.069 (3)
C(6)	0.4768 (4)	0.0862 (3)	0.3302 (10)	0.083 (3)
C(7)	0.5259 (4)	0.0417 (3)	0.2597 (10)	0.073 (3)
C(8)	0.5984 (4)	0.0404 (3)	0.3590 (10)	0.075 (3)
C(9)	0.5829 (4)	0.1384 (3)	0.4641 (8)	0.072 (3)
C(10)	0.7007 (3)	0.0823 (2)	0.0918 (7)	0.054 (2)
C(11)	0.7713 (4)	0.0703 (3)	0.1452 (8)	0.062 (3)
C(12)	0.8106 (4)	0.0311 (3)	0.0577 (10)	0.078 (3)
C(13)	0.7813 (5)	0.0034 (3)	-0.0862 (10)	0.085 (3)
C(14)	0.7115 (5)	0.0153 (3)	-0.1419 (10)	0.095 (3)
C(15)	0.6727 (4)	0.0543 (3)	-0.0550 (8)	0.074 (3)
C(16)	0.4663 (3)	0.1734 (2)	0.0456 (7)	0.059 (2)
C(17)	0.4522 (4)	0.1326 (3)	-0.0793 (8)	0.082 (3)
C(18)	0.3881 (5)	0.1333 (4)	-0.1806 (10)	0.098 (4)
C(19)	0.3380 (4)	0.1742 (4)	-0.1553 (12)	0.099 (4)
C(20)	0.3522 (5)	0.2154 (4)	-0.0345 (11)	0.088 (4)
C(21)	0.4160 (4)	0.2148 (3)	0.0652 (8)	0.071 (3)
N(22)	0.6330 (3)	0.1775 (2)	-0.0469 (7)	0.094 (2)
O(23)	0.5928 (3)	0.2111 (2)	-0.1025 (6)	0.107 (2)

Table 2. Selected geometric parameters (Å, °)

	Molecule A	Molecule B
C(1)—C(2)	1.547 (8)	1.547 (7)
C(2)—N(3)	1.497 (6)	1.491 (7)
N(3)—C(4)	1.468 (7)	1.479 (7)
C(4)—C(5)	1.532 (8)	1.562 (8)
C(5)—C(6)	1.537 (10)	1.533 (10)
C(6)—C(7)	1.534 (10)	1.511 (10)
C(7)—C(8)	1.493 (11)	1.512 (11)
C(8)—C(1)	1.527 (10)	1.526 (9)
C(1)—C(9)	1.519 (9)	1.514 (9)
C(5)—C(9)	1.519 (8)	1.524 (9)
C(2)—C(10)	1.529 (7)	1.510 (7)
C(4)—C(16)	1.504 (7)	1.511 (8)
N(3)—N(22)	1.542 (8)	1.443 (7)
N(22)—O(23)	1.152 (9)	1.167 (7)
C(10)—C(11)	1.379 (8)	1.382 (9)
C(11)—C(12)	1.394 (10)	1.373 (10)
C(12)—C(13)	1.354 (13)	1.370 (11)
C(13)—C(14)	1.361 (12)	1.372 (13)
C(14)—C(15)	1.380 (11)	1.362 (11)
C(10)—C(15)	1.378 (9)	1.382 (8)
C(16)—C(17)	1.383 (7)	1.381 (8)
C(17)—C(18)	1.403 (11)	1.387 (11)
C(18)—C(19)	1.387 (13)	1.369 (13)
C(19)—C(20)	1.377 (13)	1.367 (13)
C(20)—C(21)	1.372 (11)	1.377 (11)
C(16)—C(21)	1.399 (9)	1.374 (9)
C(11)—C(12)—C(13)	121.4 (7)	121.0 (7)
C(12)—C(13)—C(14)	118.9 (8)	118.9 (7)
C(13)—C(14)—C(15)	120.6 (7)	120.0 (7)
C(14)—C(15)—C(10)	121.3 (7)	122.2 (6)
C(15)—C(10)—C(11)	117.8 (6)	117.1 (5)
C(4)—C(16)—C(17)	124.5 (5)	123.8 (5)
C(4)—C(16)—C(21)	116.4 (4)	117.4 (5)
C(16)—C(17)—C(18)	120.4 (6)	120.4 (7)
C(17)—C(18)—C(19)	119.0 (7)	120.0 (8)
C(18)—C(19)—C(20)	120.8 (8)	120.0 (8)
C(19)—C(20)—C(21)	119.9 (8)	120.0 (8)
C(20)—C(21)—C(16)	120.8 (6)	121.2 (7)
C(21)—C(16)—C(17)	119.1 (5)	118.5 (6)
C(1)—C(2)—N(3)	111.3 (4)	112.0 (4)
C(2)—N(3)—C(4)	126.4 (4)	125.3 (4)
N(3)—C(4)—C(5)	111.9 (4)	111.4 (4)
C(4)—C(5)—C(6)	115.8 (5)	115.2 (5)
C(5)—C(6)—C(7)	112.6 (6)	113.9 (6)
C(6)—C(7)—C(8)	110.3 (6)	111.8 (6)
C(7)—C(8)—C(1)	112.5 (6)	112.5 (6)
C(8)—C(1)—C(9)	111.1 (6)	111.3 (5)
C(1)—C(9)—C(5)	107.5 (5)	108.5 (5)
C(9)—C(5)—C(4)	108.0 (5)	108.5 (5)
C(9)—C(5)—C(6)	112.0 (5)	110.5 (5)
C(2)—C(1)—C(8)	114.5 (5)	115.0 (5)
C(2)—C(1)—C(9)	109.8 (5)	109.2 (5)
C(1)—C(2)—C(10)	112.3 (5)	112.4 (4)
C(2)—N(3)—N(22)	126.4 (4)	103.9 (4)
C(4)—N(3)—N(22)	99.0 (4)	121.7 (4)
N(3)—C(4)—C(16)	114.2 (4)	113.8 (4)
C(5)—C(4)—C(16)	111.6 (4)	111.6 (4)
N(3)—N(22)—O(23)	93.8 (5)	106.8 (5)
N(3)—C(2)—C(10)	112.7 (4)	113.4 (4)
C(2)—C(10)—C(15)	117.3 (5)	124.2 (5)
C(2)—C(10)—C(11)	124.9 (5)	118.6 (5)
C(10)—C(11)—C(12)	120.0 (6)	120.8 (6)

Piperidine ring			
C(1)—C(2)—N(3)—C(4)	18.9 (6)	25.3 (6)	54.9
C(2)—N(3)—C(4)—C(5)	-22.4 (6)	-26.2 (6)	-56.7
N(3)—C(4)—C(5)—C(9)	46.1 (6)	45.3 (6)	60.0
C(4)—C(5)—C(9)—C(1)	-70.8 (6)	-68.6 (6)	-63.2
C(5)—C(9)—C(1)—C(2)	67.8 (6)	67.7 (6)	62.0
C(9)—C(1)—C(2)—N(3)	-39.6 (6)	-43.5 (6)	-57.0

About the phenyl rings			
C(5)—C(4)—C(16)—C(17)	-90.5 (6)	-91.0 (7)	-93.4
C(5)—C(4)—C(16)—C(21)	78.7 (6)	83.7 (6)	84.5
N(3)—C(4)—C(16)—C(17)	33.1 (7)	36.2 (7)	30.6
N(3)—C(4)—C(16)—C(21)	-153.1 (5)	-149.1 (5)	-151.5
C(1)—C(2)—C(10)—C(11)	115.4 (6)	-75.2 (6)	-80.6
C(1)—C(2)—C(10)—C(15)	-62.3 (7)	102.4 (6)	98.9
N(3)—C(2)—C(10)—C(11)	-11.3 (7)	156.4 (5)	155.4
N(3)—C(2)—C(10)—C(15)	171.0 (5)	-26.0 (7)	-25.1

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Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71051 (21 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: LI1040]

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Table 3. Torsion angles (°) for the title compound and ABN

	Molecule A	Molecule B	ABN
Cyclohexane ring			
C(8)—C(1)—C(9)—C(5)	-59.8 (7)	-60.4 (7)	-64.2
C(1)—C(9)—C(5)—C(6)	57.8 (7)	58.5 (7)	63.6
C(9)—C(5)—C(6)—C(7)	-54.5 (7)	-54.1 (8)	-53.9
C(5)—C(6)—C(7)—C(8)	50.5 (8)	48.7 (8)	43.6
C(6)—C(7)—C(8)—C(1)	-52.9 (8)	-49.2 (8)	-44.5
C(7)—C(8)—C(1)—C(9)	59.5 (8)	56.4 (7)	55.4