the type of interaction in which one of the components is weaker than the other. Another criterion observed is that the H atom lies in or close to the plane of the donor and the two acceptor atoms. The planarity of N(1), H(N1), Cl and O(2)[a] for the present molecule is indicated by the sum of the three angles at H(N1), which is 360°.

The short intramolecular distance of 2·923 (9) Å between N(2) and C(12) in the molecule mentioned earlier also appears to be due to a three-center hydrogen bond involving the atoms N(2), O(1)[b] ($x, y+1, z$) and C(12), the weaker component being N(2)–H(N2)···C(12) (83°). The relevant distances are H(N2)···C(12) = 2·88 and H(N2)···O(1)[b] = 1·96 Å. The angles N(2)–H(N2)···C(12) (83°), N(2)–H(N2)···O(1) (154°) and C(12)···H(N2)···O(1) (114°) at H(N2) sum to 351°.

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N-Methyl-10-azabicyclo[4.3.1]decane-8-spiro-5′-hydantoin*†

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Abstract. $C_{12}H_{19}N_3O_2$, M_r = 237·303, monoclinic, $P2_1/n$, a = 6·853 (1), b = 11·995 (1), c = 14·835 (1) Å, β = 90·58 (3)°, V = 1217·40 Å^3, Z = 4, D_x = 1·293 g cm^{-3}, μ (Mo $K\alpha$) = 0·8396 cm^{-1}. The structure was solved by direct methods and refined to an R of 0·042 for 2621 observed reflections. The bicyclo[4.3.1]decane system has a chair–boat conformation. The CH_3 group is attached in an axial position.

Introduction. The title compound was synthesized by Dr E. Martínez Muñoz of the Departamento de Química Orgánica de la Facultad de Farmacia de la Universidad Complutense de Madrid. The chemical structure could not be unequivocally established by conventional spectroscopic techniques.

The crystal used for all X-ray measurements was a transparent colourless parallelepiped of approximate dimensions 0·33 × 0·27 × 0·21 mm. An accurate determination of the cell parameters was made by a least-squares fit of the settings of 25 reflections on an automatic Enraf–Nonius CAD-4 diffractometer.

The space group $P2_1/n$ was assigned uniquely from the systematic absences. The intensities of reflections up to 2θ = 60° were collected on the diffractometer using graphite-monochromatized Mo $K\alpha$ radiation. 3486 independent reflections were recorded with the θ–2θ scan mode, 2621 of which were considered as observed [$I \geq 2\sigma(I)$ where $\sigma(I)$ was calculated from counting statistics]. The intensities were not corrected for absorption.

The structure was solved by *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). The solution was based on phases determined for 250 reflections with $E \geq 1{\cdot}90$. The E map with the best figure of merit revealed the positions of all the non-hydrogen atoms.

After full-matrix least-squares refinement with anisotropic temperature factors (R = 0·090), the H atoms were located in a difference map. Final refinement, in which the positional parameters and isotropic temperature factors of the H atoms were allowed to vary, converged at R = 0·042 and $R_w = [\sum w(|F_o| - |F_c|)^2/\sum w|F_o|^2]^{1/2}$ = 0·047. The function minimized was $\sum w(|F_o| - |F_c|)^2$ with w = 1·00. The final difference map contained no peaks >0·3 e Å^{-3}. The scattering factors were taken from *International Tables for*

* The Conformation of Heterocyclic Spiro Compounds. XI. Part X: Vilches, Florencio, Smith-Verdier & García-Blanco (1981).

† Hydantoin is 2,4-imidazolidenedione.

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Table 1. *Atomic coordinates* ($\times 10^5$ *for* C, N *and* O, $\times 10^3$ *for* H) *and thermal parameters* ($U_{eq} \times 10^4$ *for* C, N *and* O, $U_{iso} \times 10^3$ *for* H)

$U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j \cos(a_i a_j)$.

	x	y	z	U_{eq}/U_{iso} (Å^2)
C(1)	57969 (25)	33893 (16)	63381 (12)	302 (5)
C(2)	52199 (27)	31784 (18)	53433 (12)	334 (5)
C(3,5′)	30700 (25)	28133 (15)	51980 (11)	276 (5)
C(4)	24058 (26)	19676 (16)	59183 (12)	310 (5)
C(5)	30996 (26)	22384 (15)	68857 (11)	289 (5)
C(6)	19130 (27)	31896 (18)	73114 (13)	358 (6)
C(7)	29650 (30)	38625 (19)	80445 (13)	395 (6)
C(8)	47387 (30)	45329 (17)	77177 (14)	376 (6)
C(9)	50471 (30)	45121 (16)	67026 (14)	369 (6)
N(10)	52328 (21)	24478 (13)	69215 (9)	275 (4)
C(11)	63472 (33)	14266 (19)	67113 (14)	428 (7)
N(1′)	17083 (24)	37445 (14)	50544 (10)	340 (5)
C(2′)	8715 (28)	37261 (17)	42239 (12)	335 (5)
N(3′)	16229 (24)	28234 (14)	37589 (10)	340 (5)
C(4′)	29156 (26)	22264 (16)	42765 (11)	309 (5)
O(1)	−3333 (24)	43780 (13)	39146 (10)	486 (5)
O(2)	37621 (23)	13878 (13)	40607 (10)	453 (5)
H(11)	727 (3)	342 (2)	636 (1)	14 (6)
H(21)	607 (3)	259 (2)	508 (1)	10 (5)
H(22)	551 (3)	385 (2)	498 (1)	11 (5)
H(41)	289 (3)	118 (2)	572 (1)	10 (5)
H(42)	98 (3)	191 (2)	591 (1)	15 (6)
H(51)	282 (3)	153 (2)	725 (1)	9 (5)
H(61)	74 (3)	285 (2)	759 (1)	18 (6)
H(62)	140 (3)	375 (2)	684 (1)	13 (6)
H(71)	322 (3)	337 (2)	856 (2)	24 (7)
H(72)	203 (3)	437 (2)	835 (1)	17 (6)
H(81)	594 (3)	432 (2)	800 (1)	14 (6)
H(82)	458 (3)	534 (2)	789 (1)	11 (5)
H(91)	383 (3)	477 (2)	640 (1)	17 (6)
H(92)	594 (3)	509 (2)	653 (1)	18 (6)
H(111)	783 (4)	155 (2)	679 (2)	45 (9)
H(112)	621 (3)	114 (2)	607 (2)	23 (6)
H(113)	595 (4)	78 (2)	711 (2)	26 (7)
H(1′1)	137 (3)	431 (2)	544 (1)	14 (6)
H(3′1)	129 (4)	267 (2)	320 (2)	24 (7)

X-ray Crystallography (1974). The computations were made with programs of the XRAY 70 system (Stewart, Kundell & Baldwin, 1970). Final atomic coordinates are given in Table 1.*

Discussion. The crystallographic atom numbers, bond lengths and angles are given in Fig. 1 and Table 2. Distances and angles do not deviate significantly from their expected values. The molecule contains a six-membered (I) and a seven-membered (II) ring joined by a common C(1)–N(10)–C(5) bridge with a CH_3 group attached to the N atom in the axial position and a hydantoin ring substituted at the spiranic C(3,5′).

Ring I has a slightly deformed chair conformation. The asymmetry parameters (Duax & Norton, 1975), $\Delta C_s^{3,5'} = 0{\cdot}48°$, $\Delta C_2^{\{2-3,5'\}} = 8{\cdot}40°$, $\Delta C_2^{\{1-2\}} = 17{\cdot}80°$, show that there is an approximate C_s plane passing through C(3,5′) and N(10). These atoms are displaced by −0·523 (2) and 0·665 (2) Å respectively out of the plane defined by the remaining ring atoms. The seven-membered ring (II) has a boat conformation; C(1), C(5), C(6) and C(9) form the bottom of the boat. Torsional angles, Table 3, are in very good agreement with those of an ideal boat. The deviation of N(10), C(7) and C(8) from the least-squares plane through C(1), C(5), C(6) and C(9) are −0·718 (2), −1·153 (2) and −1·200 (2) Å respectively. The molecular geometry approximates to *m* [mirror plane defined by C(3,5′), N(10) and C(11)]. The atoms belonging to the hydantoin ring are approximately in this plane, only C(2′), O(1) and O(2) deviate slightly. By comparing the deformation of the cyclohexane ring (I) with that found in *N*-methyltropane-3-spiro-5′-hydantoin (Smith-

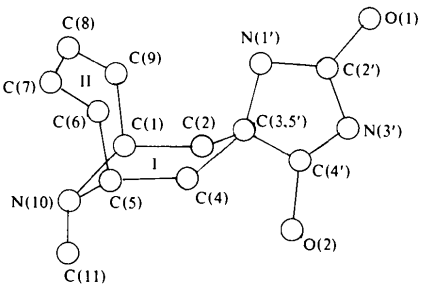

Fig. 1. Scheme and crystallographic numbering of the molecule.

Table 2. *Interatomic distances* (Å) *and angles* (°)

The e.s.d.'s are in parentheses.

C(1)–C(2)	1·545 (3)	C(6)–C(7)	1·529 (3)
C(1)–C(9)	1·541 (3)	C(7)–C(8)	1·540 (3)
C(1)–N(10)	1·477 (2)	C(8)–C(9)	1·523 (3)
C(2)–C(3,5′)	1·550 (3)	N(10)–C(11)	1·478 (3)
C(3,5′)–C(4)	1·545 (3)	N(1′)–C(2′)	1·354 (2)
C(3,5′)–N(1′)	1·470 (2)	C(2′)–N(3′)	1·386 (3)
C(3,5′)–C(4′)	1·540 (3)	C(2′)–O(1)	1·223 (3)
C(4)–C(5)	1·542 (2)	N(3′)–C(4′)	1·369 (2)
C(5)–C(6)	1·540 (3)	C(4′)–O(2)	1·206 (2)
C(5)–N(10)	1·484 (2)		
C(9)–C(1)–N(10)	111·9 (2)	C(6)–C(7)–C(8)	114·8 (2)
C(2)–C(1)–N(10)	111·6 (2)	C(7)–C(8)–C(9)	114·9 (2)
C(2)–C(1)–C(9)	113·3 (2)	C(1)–C(9)–C(8)	114·3 (2)
C(1)–C(2)–C(3,5′)	114·4 (2)	C(1)–N(10)–C(5)	111·9 (1)
C(2)–C(3,5′)–C(4′)	108·0 (2)	C(5)–N(10)–C(11)	111·3 (2)
C(2)–C(3,5′)–N(1′)	114·0 (2)	C(1)–N(10)–C(11)	111·8 (2)
C(2)–C(3,5′)–C(4)	112·1 (2)	C(3,5′)–N(1′)–C(2′)	112·5 (2)
N(1′)–C(3,5′)–C(4′)	100·4 (1)	N(1′)–C(2′)–O(1)	127·5 (2)
C(4)–C(3,5′)–C(4′)	107·2 (1)	N(1′)–C(2′)–N(3′)	108·0 (2)
C(4)–C(3,5′)–N(1′)	114·1 (2)	N(3′)–C(2′)–O(1)	124·4 (2)
C(3,5′)–C(4)–C(5)	114·5 (2)	C(2′)–N(3′)–C(4)	111·8 (2)
C(4)–C(5)–N(10)	111·3 (1)	C(3,5′)–C(4′)–N(3′)	107·3 (2)
C(4)–C(5)–C(6)	112·3 (2)	N(3′)–C(4′)–O(2)	126·7 (2)
C(6)–C(5)–N(10)	112·6 (2)	C(3,5′)–C(4′)–O(2)	126·0 (2)
C(5)–C(6)–C(7)	115·8 (2)		

* Lists of structure factors, anisotropic thermal parameters and deviations of atoms from least-squares planes have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36766 (27 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 3. *Torsional angles* (°)

C(1)–C(2)–C(3,5′)–C(4)	−41·3 (2)	C(1)–N(10)–C(5)–C(6)	−67·6 (2)
C(2)–C(3,5′)–C(4)–C(5)	41·8 (2)	N(10)–C(5)–C(6)–C(7)	−27·2 (2)
C(3,5′)–C(4)–C(5)–N(10)	−50·9 (2)	C(5)–C(6)–C(7)–C(8)	64·9 (2)
C(4)–C(5)–N(10)–C(1)	59·5 (2)	C(6)–C(7)–C(8)–C(9)	5·7 (3)
C(5)–N(10)–C(1)–C(2)	−59·5 (2)	C(7)–C(8)–C(9)–C(1)	−72·3 (2)
N(10)–C(1)–C(2)–C(3,5′)	50·3 (2)	C(8)–C(9)–C(1)–N(10)	26·1 (2)
		C(9)–C(1)–N(10)–C(5)	68·9 (2)

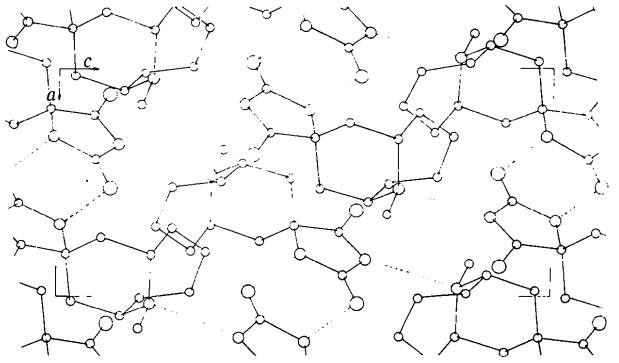

Fig. 2. Projection of the structure along **b**.

Verdier, Florencio & García-Blanco, 1977) and in *N*-methylgranatanine-3-spiro-5′-hydantoin (Florencio, Smith-Verdier & García-Blanco, 1978) it can be seen that the deformation in the present compound is smaller than in those compounds; it could be due to the boat conformation adopted by the seven-membered ring that produces a decrease in the interactions between C(3,5′) and the C(7) and C(8) atoms.

The position of the hydantoin ring on the C(3,5′) atom is similar to that found in *N*-methyltropane-3-spiro-5′-hydantoin and in *N*-methylgranatanine-3-spiro-5′-hydantoin.

The molecular packing as viewed along **b** is shown in Fig. 2. Hydrogen bonds of types N–H···O and N–H···N link the molecules together. Two N(1′)···O(1) bonds of 2·886 (1) Å and N(1′)–H···O(1) angles of 168 (2)° are formed between pairs of molecules related by a centre of symmetry, while the N(3′)···N(10) bond of 2·896 (2) Å [and N(3′)–H···N(10) angle of 170 (2)°] links the molecules forming chains along [101]. The other intermolecular contacts correspond to normal van der Waals interactions.

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