Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

N–C(1)	1·280 (4)	C(9)–C(10)	1·366 (5)
N–C(5)	1·415 (4)	C(12)–C(13)	1·390 (6)
C(1)–C(2)	1·486 (4)	C(12)–C(17)	1·397 (4)
C(1)–C(18)	1·490 (5)	C(13)–C(14)	1·386 (5)
C(2)–C(3)	1·327 (6)	C(14)–C(15)	1·383 (5)
C(2)–C(12)	1·487 (5)	C(15)–C(16)	1·372 (7)
C(3)–C(4)	1·487 (6)	C(16)–C(17)	1·376 (5)
C(5)–C(6)	1·383 (5)	C(18)–C(19)	1·395 (5)
C(5)–C(10)	1·385 (5)	C(18)–C(23)	1·379 (5)
C(6)–C(7)	1·383 (5)	C(19)–C(20)	1·386 (6)
C(7)–C(8)	1·382 (5)	C(20)–C(21)	1·364 (7)
C(8)–C(9)	1·382 (6)	C(21)–C(22)	1·373 (7)
C(8)–C(11)	1·504 (5)	C(22)–C(23)	1·381 (6)

C(1)–N–C(5)	122·4 (3)	C(2)–C(12)–C(17)	121·9 (3)
N–C(1)–C(18)	117·2 (3)	C(2)–C(12)–C(13)	120·9 (3)
N–C(1)–C(2)	125·1 (3)	C(13)–C(12)–C(17)	117·1 (4)
C(2)–C(1)–C(18)	117·7 (3)	C(12)–C(13)–C(14)	122·0 (3)
C(1)–C(2)–C(12)	116·8 (3)	C(13)–C(14)–C(15)	119·5 (4)
C(1)–C(2)–C(3)	120·4 (3)	C(14)–C(15)–C(16)	119·4 (4)
C(3)–C(2)–C(12)	122·9 (3)	C(15)–C(16)–C(17)	121·1 (3)
C(2)–C(3)–C(4)	126·0 (3)	C(12)–C(17)–C(16)	120·9 (4)
N–C(5)–C(10)	118·6 (3)	C(1)–C(18)–C(23)	121·5 (3)
N–C(5)–C(6)	122·8 (4)	C(1)–C(18)–C(19)	119·4 (4)
C(6)–C(5)–C(10)	118·3 (4)	C(19)–C(18)–C(23)	119·1 (3)
C(5)–C(6)–C(7)	119·9 (4)	C(18)–C(19)–C(20)	119·4 (4)
C(6)–C(7)–C(8)	121·8 (4)	C(19)–C(20)–C(21)	120·7 (4)
C(7)–C(8)–C(11)	121·2 (4)	C(20)–C(21)–C(22)	120·4 (5)
C(7)–C(8)–C(9)	117·5 (4)	C(21)–C(22)–C(23)	119·6 (4)
C(8)–C(9)–C(10)	121·3 (4)	C(18)–C(23)–C(22)	120·8 (4)
C(5)–C(10)–C(9)	121·2 (4)		

The two phenyl groups are synclinal with respect to the C(1)–C(2) bond, torsion angle C(18)–C(1)–C(2)–C(12), −71·4 (4)°.

In the double-bond system, the two double bonds are oriented synclinal about C(1)–C(2); the torsion angle N=C(1)–C(2)=C(3) is −69·3 (5)°. The deviations of the atoms from the best least-squares plane through N,C(1),C(2),C(3) are 0·095 (3), −0·261 (4), 0·229 (4) and −0·124 (4) Å, respectively.

The packing of the crystal is determined solely by van der Waals interactions.

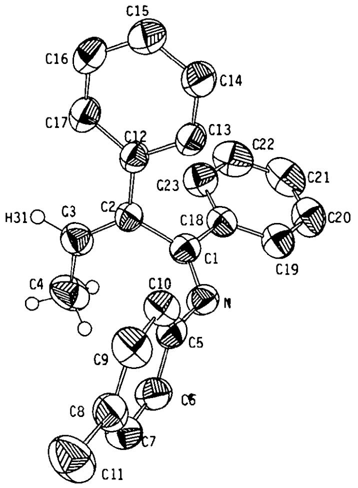

Fig. 1. *ORTEP* (Johnson, 1965) drawing of the molecule showing the atom numbering.

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Structure of 2-Benzoyl-1,2-dihydro-1-isoquinolinecarbonitrile

By E. Tykarska, M. Jaskólski and Z. Kosturkiewicz*

Department of Crystallography, Faculty of Chemistry, A. Mickiewicz University, ul. Grunwaldzka 6, 60-780 Poznań, Poland

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Abstract. $C_{17}H_{12}N_2O$, $M_r = 260{\cdot}30$, monoclinic, $P2_1/c$, $a = 7{\cdot}2105$ (9), $b = 12{\cdot}628$ (2), $c = 15{\cdot}953$ (2) Å, $\beta = 112{\cdot}26$ (1)°, $V = 1344{\cdot}3$ (3) Å^3, $D_m = 1{\cdot}285$, $D_x = 1{\cdot}286$ Mg m^{-3}, $Z = 4$, λ(Cu $K\alpha$) = 1·54178 Å, μ(Cu $K\alpha$) = 0·661 mm^{-1}, $F(000) = 554$, room temperature, $R = 0{\cdot}040$ for 1579 observed reflexions. The

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* To whom correspondence should be addressed.

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heterocyclic fragment of the molecule exhibits a 1,3-diplanar conformation. The C(3)—N(2)—C(13)—O(14) torsion angle [−165·3 (2)°] characterizes the amide bond as *anti*. The amide group and the phenyl ring are deconjugated, the corresponding dihedral angle between the planes of the two groups being 45·0 (3)°.

Introduction. The present work is the third part of an investigation into the structures of a series of Reissert compounds (Reissert, 1905). In the structure of 2-benzoyl-1,2,3,4-tetrahydro-1-isoquinilinecarbonitrile the heterocyclic ring exists in a sofa conformation (Pływaczyk, Tykarska, Jaskólski & Kosturkiewicz, 1984), while in ethyl 1-cyano-1,2,3,4-tetrahydro-2-isoquinolinecarboxylate it has a half-chair form (Gzella, Rychlewska, Jaskólski & Kosturkiewicz, 1984). In both structures the carbonyl group is disposed *anti* with respect to the C(3)—N(2) bond. In the present molecule a double bond has been introduced into the heterocyclic ring. The study was undertaken in order to determine the effects of substituents and the degree of hydrogenation on the molecular conformation.

Table 1. *Final fractional coordinates and equivalent isotropic thermal parameters* (Å^2)

$U_{\rm eq} = (U_{11}U_{22}U_{33})^{1/3}$.

	x	y	z	$U_{\rm eq}$
C(1)	0·1125 (3)	0·4560 (1)	0·1441 (1)	0·0370 (7)
N(2)	0·2559 (2)	0·3712 (1)	0·1473 (1)	0·0386 (6)
C(3)	0·3578 (3)	0·3187 (2)	0·2306 (1)	0·0404 (7)
C(4)	0·2886 (3)	0·3196 (2)	0·2964 (1)	0·0449 (7)
C(5)	0·0141 (3)	0·3647 (2)	0·3500 (1)	0·0552 (8)
C(6)	−0·1565 (3)	0·4203 (2)	0·3406 (2)	0·0601 (9)
C(7)	−0·2388 (3)	0·4884 (2)	0·2680 (2)	0·0573 (9)
C(8)	−0·1528 (3)	0·4992 (2)	0·2040 (1)	0·0477 (8)
C(9)	0·0178 (3)	0·4420 (1)	0·2137 (1)	0·0374 (7)
C(10)	0·1052 (3)	0·3749 (2)	0·2874 (1)	0·0416 (7)
C(11)	0·2134 (3)	0·5606 (2)	0·1552 (1)	0·0456 (8)
N(12)	0·2912 (3)	0·6406 (2)	0·1640 (1)	0·0670 (9)
C(13)	0·3086 (3)	0·3638 (2)	0·0731 (1)	0·0428 (7)
O(14)	0·2398 (2)	0·4275 (1)	0·0108 (1)	0·0614 (6)
C(15)	0·4497 (3)	0·2791 (2)	0·0705 (1)	0·0409 (7)
C(16)	0·6011 (3)	0·3065 (2)	0·0408 (1)	0·0495 (8)
C(17)	0·7378 (4)	0·2308 (2)	0·0379 (2)	0·065 (1)
C(18)	0·7196 (4)	0·1277 (2)	0·0624 (2)	0·068 (1)
C(19)	0·5648 (4)	0·0991 (2)	0·0883 (2)	0·064 (1)
C(20)	0·4290 (4)	0·1747 (2)	0·0928 (1)	0·0545 (8)

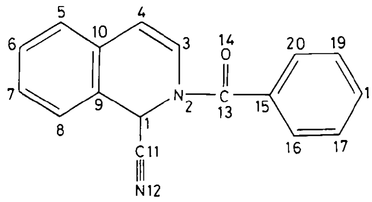
Table 2. *Bond distances* (Å) *and angles* (°)

C(1)—N(2)	1·476 (2)	C(1)—C(11)	1·486 (3)
N(2)—C(3)	1·416 (3)	C(11)—N(12)	1·139 (3)
C(3)—C(4)	1·323 (3)	N(2)—C(13)	1·376 (3)
C(4)—C(10)	1·454 (3)	C(13)—O(14)	1·228 (3)
C(10)—C(9)	1·392 (3)	C(13)—C(15)	1·488 (3)
C(9)—C(1)	1·518 (3)	C(15)—C(16)	1·389 (3)
C(10)—C(5)	1·394 (3)	C(16)—C(17)	1·386 (3)
C(5)—C(6)	1·374 (3)	C(17)—C(18)	1·380 (4)
C(6)—C(7)	1·383 (4)	C(18)—C(19)	1·376 (4)
C(7)—C(8)	1·387 (4)	C(19)—C(20)	1·389 (4)
C(8)—C(9)	1·384 (3)	C(20)—C(15)	1·389 (3)

C(1)—N(2)—C(3)	118·6 (1)	C(1)—C(11)—N(12)	179·8 (2)
N(2)—C(3)—C(4)	121·6 (2)	C(1)—N(2)—C(13)	116·0 (2)
C(3)—C(4)—C(10)	121·9 (2)	C(3)—N(2)—C(13)	124·1 (2)
C(4)—C(10)—C(9)	118·7 (2)	N(2)—C(13)—C(15)	119·2 (2)
C(10)—C(9)—C(1)	120·2 (2)	N(2)—C(13)—O(14)	119·6 (2)
C(9)—C(1)—N(2)	113·2 (2)	O(14)—C(13)—C(15)	121·3 (2)
C(10)—C(5)—C(6)	121·3 (2)	C(15)—C(16)—C(17)	120·0 (2)
C(5)—C(6)—C(7)	119·5 (2)	C(16)—C(17)—C(18)	119·8 (2)
C(6)—C(7)—C(8)	120·5 (2)	C(17)—C(18)—C(19)	120·5 (2)
C(7)—C(8)—C(9)	119·5 (2)	C(18)—C(19)—C(20)	120·2 (2)
C(8)—C(9)—C(10)	120·7 (2)	C(19)—C(20)—C(15)	119·6 (2)
C(9)—C(10)—C(5)	118·5 (2)	C(20)—C(15)—C(16)	119·9 (2)
C(9)—C(1)—C(11)	110·6 (2)	C(13)—C(15)—C(16)	117·7 (2)
N(2)—C(1)—C(11)	109·6 (2)	C(13)—C(15)—C(20)	122·3 (2)

Experimental. Suitable crystals (elongated prisms) obtained from ethanol. D_m by flotation. Crystal 0·3 × 0·3 × 0·4 mm. Syntex $P2_1$ diffractometer. Cell parameters from least-squares treatment of setting angles of 15 reflexions. Profiles measured for 1780 reflexions with $2\theta \le 115°$, $hk\pm l$. Profile analysis according to Lehmann & Larsen (1974). No significant intensity variation for two standard reflexions. No absorption or extinction corrections. 1586 observed reflexions with $I \ge 1\cdot96\sigma(I)$. Structure solved by direct methods using *SHELX*76 (Sheldrick, 1976). Full-matrix least-squares refinement on F. $w^{-1} = \sigma^2(F)$. Seven extinction-affected reflexions excluded from final refinement. H atoms located in a ΔF map and included with fixed isotropic thermal parameters. $R = 0\cdot040$, $wR = 0\cdot049$. $(\Delta/\sigma)_{\rm max} = 0\cdot005$. Largest peak in final ΔF map = 0·15, largest trough = −0·13 e Å^{-3}. Computer programs: *SHELX*76 (Sheldrick, 1976) and local programs (Jaskólski, 1982), molecular illustrations drawn using *PLUTO* (Motherwell & Clegg, 1978). Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Discussion. Atomic coordinates are in Table 1* and bond lengths and bond angles are in Table 2. The labeling sequence is shown below.



The molecule consists of a heterocyclic dihydrogenated ring condensed with an aromatic ring and two side chains: a nitrile group bonded to C(1) and a benzoyl group joined to N(2). Bond lengths and angles in the aromatic fragments of the molecule are similar to those in the tetrahydrogenated derivative (Pływaczyk,

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42406 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Tykarska, Jaskólski & Kosturkiewicz, 1984). The dimensions of the amide groups in both structures are also comparable. Each bond in the present hetero ring is of different character and their lengths vary from 1·323 (3) to 1·518 (3) Å. Five bond angles in this ring are typical for sp^2 hybridization; C(1) is bonded to two sp^2 centers and this probably accounts for the opening of the C(9)—C(1)—N(2) angle [113·2 (2)°].

A stereoview of the molecule is shown in Fig. 1, while Table 3 reports the torsion angles characterizing the molecular conformation. The torsion angles around the hetero ring are typical for a 1,3-diplanar conformation.

The corresponding asymmetry parameter (Duax & Norton, 1975) is $C_2^{1,2} = 2\cdot1°$. In the tetrahydro analogue the hetero ring is in a sofa conformation (Pływaczyk, Tykarska, Jaskólski & Kosturkiewicz, 1984). The C=O group is situated *anti* with respect to the C(3)—N(2) bond. Maximum conjugation of the amide-group electrons and the aromatic system of the isoquinoline moiety requires these groups to be coplanar. It seems to be more easily realized by an *anti* disposition as a consequence of steric hindrance between O(14) and H(C3) in the other possible isomer. The COCN amide group is planar ($\chi^2 = 3\cdot2$). The N(2) amide atom is not exactly flat [sum of C—N(2)—C angles 358·7 (3)°]. The twist angle (Winkler & Dunitz, 1971) about the N(2)—C(13) bond is 7·9 (2)°. The aromatic ring of the dihydroisoquinoline moiety is slightly distorted ($\chi^2 = 47\cdot7$) and the phenyl ring of the benzoyl group shows significant deviations from planarity ($\chi^2 = 140\cdot4$). The amide group and the phenyl ring are deconjugated; the dihedral angle between their mean planes is 45·0 (3)°. A lack of conjugation between these groups is often observed in amides with aromatic rings at their C end (Gdaniec, Jaskólski & Kosturkiewicz, 1979). In the present case this effect can be attributed to the C=O group being *anti* to the C(3)—N(2) bond and to steric hindrance between H(C16) or H(C20) and H(C3).

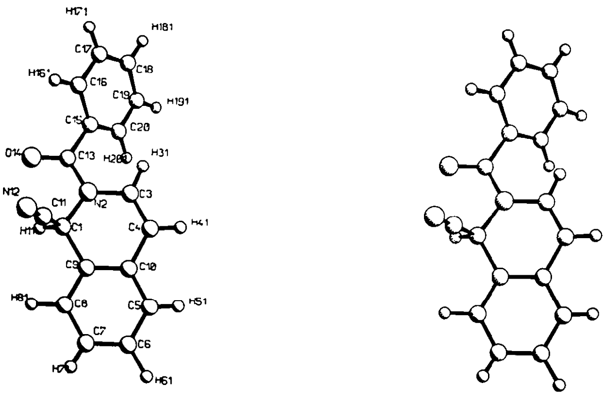

Fig. 1. Stereodrawing of the molecule.

Table 3. *Torsion angles (°) characterizing the molecular conformation*

C(9)—C(1)—N(2)—C(3)	−27·9 (2)	C(1)—N(2)—C(13)—O(14)	1·7 (2)
C(1)—N(2)—C(3)—C(4)	20·5 (2)	C(1)—N(2)—C(13)—C(15)	−178·9 (2)
N(2)—C(3)—C(4)—C(10)	−0·4 (3)	O(14)—C(13)—C(15)—C(16)	43·2 (2)
C(3)—C(4)—C(10)—C(9)	−10·2 (2)	C(11)—C(1)—N(2)—C(13)	−71·7 (2)
C(4)—C(10)—C(9)—C(1)	0·4 (2)	N(2)—C(13)—C(15)—C(20)	46·5 (2)
C(10)—C(9)—C(1)—N(2)	17·7 (2)	C(8)—C(9)—C(1)—C(11)	72·5 (2)
C(3)—N(2)—C(1)—C(11)	96·1 (2)	O(14)—C(13)—C(15)—C(20)	−134·1 (2)
C(3)—N(2)—C(13)—O(14)	−165·3 (2)	C(13)—N(2)—C(3)—C(4)	−172·8 (2)
C(3)—N(2)—C(13)—C(15)	14·1 (2)	N(2)—C(13)—C(15)—C(16)	−136·3 (2)

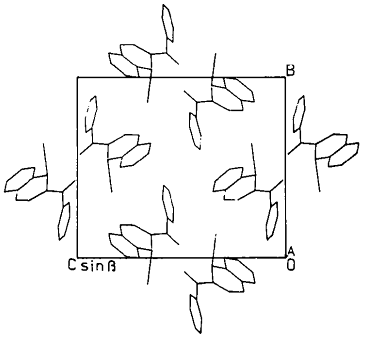

Fig. 2. Projection of the structure down **a**.

The molecular packing is shown in Fig. 2. The chiral molecules [asymmetric atom C(1)] form a racemic crystal.

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