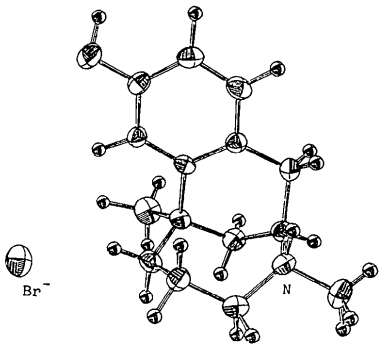

Fig. 2. *ORTEP* drawing of the molecule. Non-hydrogen atoms are depicted by 30% probability ellipsoids and H atoms are on an arbitrary scale for clarity.

Like the usual benzomorphans, the molecule is L-shaped with the N-containing *C* ring protruding from the molecular plane. In the title compound, the *C* ring of the benzomorphan is enlarged from a six-membered to a seven-membered ring. The *C* ring adopts a chair conformation with an approximate mirror plane passing through C(2) and the midpoint of N—C(6). The H atom at the cationic N atom occupies a β, axial-like position. This orientation is opposite to those of morphine (3) and 2,9β-dimethyl-6,7-benzomorphan (2). From inspection of the molecular model, an alternative chair conformation with a mirror plane through the N atom and the midpoint of C(1)—C(2) also seems to be stable, and would allow the α, axial orientation for the H atom on the cationic N atom, if the *N*-methyl group were preferably to take the equatorial configuration. The distance between the N atom and the center of the benzene ring is 4·45 Å, whereas the values in morphine (3) and (2) are 4·71 and 4·69 Å, respectively. It is noteworthy that in spite of these structural differences, compound (1) still retains an analgesic activity as strong as that of morphine. More precise and extensive stereochemical studies may be necessary for the elucidation of the structure–activity relationships in opiates. The crystalline cohesion is ensured by two hydrogen bonds N···Br 3·32 (1) Å [(N)H···Br 2·4 (1) Å] and N···Br 3·28 (1) Å [(N)H···Br 2·6 (1) Å], and by van der Waals contacts.

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1,4,5,6,7,8-Hexahydro-7-methyl-3-phenylcinnoline-1-carboxamide, $C_{16}H_{19}N_3O$

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Abstract. $M_r = 269·3$, triclinic, $P\bar{1}$, $a = 13·37$ (1), $b = 15·41$ (1), $c = 11·75$ (1) Å, $\alpha = 75·1$ (3), $\beta = 69·4$ (3), $\gamma = 94·0$ (3)°, $V = 2155$ (7) Å^3, $Z = 6$, $D_m = 1·24$, $D_x = 1·25$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 5·99$ cm^{-1}, $F(000) = 864$, $T \simeq 293$ K, final $R = 0·093$ for 2943 observed reflections. Bond distances and angles in the three independent molecules show good overall agreement. Molecules are hydrogen-

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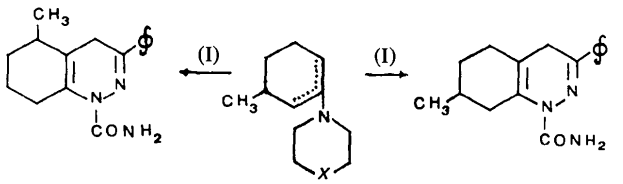
bonded through the amide group to form two crystallographically independent dimers. The methyl group is bonded in pseudo-equatorial position. Dimers lie on planes and their packing is controlled by normal van der Waals interactions.

Introduction. In the course of the investigation of the synthesis and structure of the products obtained by reaction of enamine isomers with α-haloketone derivatives, the reactions of ω-bromoacetophenone semicarbazone (I) with some 3-methylcyclohexanone enamines (II) have been examined (Cocco, Maccioni & Plumitallo, 1984).



(III) (IV)

X = CH2,O,–

(II)

Although the enamines exist as a mixture of two structural isomers Δ^1 and Δ^6, reactions always give one dihydropyridazine, to which either structure (III) or (IV) could be assigned; since spectral data did not elucidate the structural assignment an X-ray single-crystal analysis was undertaken.

Experimental. Flat prismatic crystals were obtained by evaporation of an ethanol solution; crystal used: 0·1 × 0·3 × 0·5 mm; automatic Siemens AED diffractometer, Ni-filtered Cu $K\alpha$ radiation; accurate cell dimensions and orientation matrix obtained from least-squares fit of θ, χ, φ values of 15 reflections in the range $18° \le \theta \le 30°$, measured by use of a narrow counter aperture; 4447 reflections up to $\theta = 50°$ ($\bar{1}1 \le h \le 13$, $\bar{1}4 \le k \le 15$, $0 \le l \le 10$) measured by θ–2θ scan technique; intensities of three standard reflections ($6\bar{5}2$, 142, $\bar{3}71$) measured every 200 reflections, fluctuation within 5%; intensities corrected for Lorentz and polarization factors but not for absorption; structure solved by *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) and refined isotropically by block-diagonal least squares (Immirzi, 1967) using 2943 reflections having $I \ge 2{\cdot}5\sigma(I)$; $\sum w\Delta F^2$ minimized, where $w = 1/(7{\cdot}0 + F_o + 0{\cdot}075F_o^2)$; a difference Fourier synthesis (Immirzi, 1973) in final stages of refinement indicated the positions of most H atoms; residual electron density |0·35| e Å^{-3}; H contribution in calculated positions included and held fixed in final least-squares cycles; $R = 0{\cdot}093$, $wR = 0{\cdot}108$, $S = 0{\cdot}35$, $(\Delta/\sigma)_{av} = 0{\cdot}1$, $(\Delta/\sigma)_{max} = 0{\cdot}5$; no correction for secondary extinction; geometrical calculations by *PARST* (Nardelli, 1983); atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Discussion. Refined atomic coordinates are given in Table 1.* Bond distances and angles are listed in Table 2.

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42080 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional atomic coordinates* (×10⁴) *and isotropic thermal parameters with e.s.d.'s in parentheses*

The temperature factor is of the form $T = \exp(-B\sin^2\theta/\lambda^2)$.

	x	y	z	B(Å²)
O(11)	−70 (2)	3729 (2)	−4670 (2)	4·98 (5)
N(11)	−332 (3)	4558 (2)	−3305 (3)	5·68 (7)
N(12)	−352 (2)	3003 (2)	−2557 (3)	4·26 (6)
N(13)	−419 (2)	3227 (2)	−1484 (3)	4·41 (6)
C(11)	−235 (3)	3781 (2)	−3590 (3)	4·04 (7)
C(12)	−427 (3)	2087 (2)	−2602 (3)	4·02 (7)
C(13)	−763 (3)	1857 (2)	−3625 (3)	4·25 (7)
C(14)	−1223 (3)	843 (3)	−3254 (4)	4·96 (8)
C(15)	−1368 (4)	603 (3)	−4352 (4)	5·65 (9)
C(16)	−472 (4)	274 (3)	−2770 (4)	6·18 (10)
C(17)	−396 (3)	468 (3)	−1597 (4)	5·22 (9)
C(18)	−302 (3)	1464 (2)	−1678 (3)	4·07 (7)
C(19)	−102 (3)	1686 (3)	−616 (4)	5·18 (9)
C(110)	−322 (3)	2602 (3)	−559 (4)	4·76 (8)
C(111)	−395 (3)	2899 (3)	571 (4)	4·79 (8)
C(112)	−300 (4)	2338 (3)	1600 (4)	6·45 (10)
C(113)	−378 (4)	2614 (4)	2666 (5)	7·46 (12)
C(114)	−540 (4)	3403 (4)	2725 (5)	7·67 (12)
C(115)	−809 (5)	3998 (4)	1769 (6)	10·09 (16)
C(116)	−686 (5)	3721 (4)	666 (5)	8·38 (13)
O(21)	2393 (2)	878 (2)	7986 (2)	5·44 (6)
N(21)	2616 (3)	67 (2)	6588 (3)	5·58 (7)
N(22)	2682 (2)	1622 (2)	5912 (3)	4·52 (6)
N(23)	2869 (3)	1475 (2)	4743 (3)	4·76 (6)
C(21)	2579 (3)	831 (3)	6893 (4)	4·67 (8)
C(22)	2790 (3)	2528 (3)	5980 (4)	4·97 (8)
C(23)	3216 (4)	2713 (3)	6971 (4)	6·76 (11)
C(24)	3740 (5)	3757 (4)	6492 (5)	8·34 (13)
C(25)	4088 (6)	3904 (5)	7551 (7)	11·74 (19)
C(26)	2854 (4)	4305 (4)	6247 (5)	7·89 (12)
C(27)	2770 (4)	4177 (3)	5055 (4)	6·31 (10)
C(28)	2639 (3)	3189 (3)	5105 (4)	4·81 (8)
C(29)	2364 (3)	2965 (3)	4098 (4)	5·14 (8)
C(210)	2726 (3)	2117 (3)	3884 (4)	4·64 (8)
C(211)	2983 (3)	1948 (3)	2634 (4)	4·78 (8)
C(212)	2488 (4)	2389 (3)	1825 (5)	6·86 (11)
C(213)	2697 (5)	2227 (4)	649 (5)	7·96 (12)
C(214)	3418 (4)	1645 (4)	272 (5)	7·62 (12)
C(215)	3883 (4)	1227 (3)	1074 (4)	6·57 (10)
C(216)	3665 (3)	1367 (3)	2237 (4)	5·22 (9)
O(31)	2776 (2)	−1410 (2)	−1355 (3)	6·44 (7)
N(32)	3280 (3)	−1948 (2)	322 (3)	4·82 (7)
N(33)	3504 (2)	−1687 (2)	1240 (3)	4·68 (6)
N(31)	3208 (3)	−409 (2)	−450 (3)	5·19 (7)
C(31)	3088 (3)	−1245 (3)	−556 (3)	4·59 (8)
C(32)	3378 (3)	−2828 (3)	207 (4)	5·33 (9)
C(33)	3660 (4)	−2958 (3)	−1074 (5)	7·13 (11)
C(34)	4316 (4)	−3801 (3)	−1143 (5)	7·43 (12)
C(35)	4483 (6)	−3967 (5)	−2401 (6)	10·06 (16)
C(36)	3407 (5)	−4624 (4)	50 (5)	8·17 (13)
C(37)	3374 (4)	−4465 (3)	1275 (5)	7·20 (11)
C(38)	3294 (3)	−3498 (3)	1262 (4)	5·15 (9)
C(39)	3104 (4)	−3301 (3)	2480 (4)	5·91 (10)
C(310)	3459 (3)	−2301 (3)	2243 (4)	4·87 (8)
C(311)	3741 (3)	−1990 (3)	3174 (4)	5·09 (8)
C(312)	3308 (4)	−2542 (3)	4489 (4)	6·56 (10)
C(313)	3599 (4)	−2207 (3)	5351 (5)	7·50 (12)
C(314)	4232 (4)	−1399 (4)	5011 (5)	7·88 (12)
C(315)	4651 (4)	−878 (3)	3768 (5)	7·07 (11)
C(316)	4402 (4)	−1169 (3)	2889 (4)	6·11 (10)

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

	Molecule (1)	Molecule (2)	Molecule (3)
N(1)–C(1)	1·327 (5)	1·315 (6)	1·330 (6)
O(1)–C(1)	1·234 (5)	1·242 (6)	1·226 (7)
C(1)–N(2)	1·410 (7)	1·406 (7)	1·398 (7)
N(2)–C(2)	1·417 (5)	1·419 (6)	1·407 (6)
N(2)–N(3)	1·388 (6)	1·388 (6)	1·360 (6)
N(3)–C(10)	1·306 (7)	1·297 (7)	1·287 (7)
C(2)–C(3)	1·533 (6)	1·541 (8)	1·488 (8)
C(2)–C(8)	1·320 (6)	1·331 (8)	1·357 (8)
C(3)–C(4)	1·529 (7)	1·580 (9)	1·621 (9)
C(4)–C(5)	1·500 (8)	1·533 (12)	1·507 (10)
C(4)–C(6)	1·539 (8)	1·568 (10)	1·649 (11)
C(6)–C(7)	1·517 (8)	1·504 (9)	1·507 (9)
C(7)–C(8)	1·507 (6)	1·504 (7)	1·498 (8)
C(8)–C(9)	1·479 (7)	1·466 (8)	1·478 (8)
C(9)–C(10)	1·475 (7)	1·476 (7)	1·504 (7)
C(10)–C(11)	1·487 (8)	1·482 (7)	1·450 (8)
C(11)–C(12)	1·345 (8)	1·406 (9)	1·439 (8)
C(11)–C(16)	1·371 (8)	1·371 (8)	1·383 (8)
C(12)–C(13)	1·397 (9)	1·402 (9)	1·401 (9)
C(13)–C(14)	1·263 (9)	1·399 (10)	1·336 (9)
C(14)–C(15)	1·425 (10)	1·358 (9)	1·360 (9)
C(15)–C(16)	1·426 (10)	1·371 (7)	1·355 (9)
N(1)–C(1)–O(1)	122·6 (14)	124·3 (12)	121·9 (15)
O(1)–C(1)–N(2)	121·2 (14)	119·6 (14)	120·5 (16)
N(1)–C(1)–N(2)	116·1 (11)	115·9 (11)	117·6 (11)
C(1)–N(2)–N(3)	111·8 (13)	113·9 (13)	114·3 (14)
C(1)–N(2)–C(2)	126·4 (10)	125·6 (10)	124·4 (10)
C(2)–N(2)–N(3)	121·8 (10)	119·6 (10)	120·9 (12)
N(2)–N(3)–C(10)	117·8 (14)	116·6 (14)	119·2 (16)
N(2)–C(2)–C(3)	118·0 (12)	117·6 (13)	118·7 (12)
N(2)–C(2)–C(8)	118·4 (13)	118·9 (13)	117·5 (12)
C(3)–C(2)–C(8)	123·3 (15)	123·0 (16)	123·5 (14)
C(2)–C(3)–C(4)	112·0 (9)	107·7 (9)	109·1 (11)
C(3)–C(4)–C(5)	111·0 (10)	104·9 (11)	107·2 (13)
C(3)–C(4)–C(6)	109·3 (16)	106·5 (16)	100·0 (13)
C(5)–C(4)–C(6)	111·5 (13)	115·6 (12)	111·0 (13)
C(4)–C(6)–C(7)	111·3 (15)	106·4 (15)	107·8 (13)
C(6)–C(7)–C(8)	113·8 (10)	112·1 (10)	112·1 (10)
C(2)–C(8)–C(7)	122·5 (11)	123·6 (12)	123·0 (10)
C(2)–C(8)–C(9)	122·5 (15)	119·4 (15)	120·7 (14)
C(7)–C(8)–C(9)	114·9 (11)	116·9 (12)	116·3 (12)
C(8)–C(9)–C(10)	111·6 (11)	111·7 (13)	110·4 (9)
C(9)–C(10)–C(11)	121·1 (12)	121·6 (13)	120·3 (11)
N(3)–C(10)–C(9)	124·4 (10)	123·7 (10)	122·5 (12)
N(3)–C(10)–C(11)	114·4 (14)	114·7 (15)	117·2 (14)
C(10)–C(11)–C(12)	121·7 (15)	118·6 (14)	119·9 (15)
C(10)–C(11)–C(16)	120·9 (11)	123·1 (12)	124·0 (10)
C(12)–C(11)–C(16)	117·0 (11)	118·2 (10)	116·1 (11)
C(11)–C(12)–C(13)	121·7 (15)	119·9 (17)	117·6 (13)
C(12)–C(13)–C(14)	122·3 (12)	119·8 (13)	123·1 (10)
C(13)–C(14)–C(15)	120·0 (14)	119·0 (11)	119·9 (16)
C(14)–C(15)–C(16)	116·3 (16)	121·5 (18)	120·0 (14)
C(11)–C(16)–C(15)	121·6 (14)	121·6 (17)	123·6 (11)

The molecules in the crystal are hydrogen bonded through the amide group to form two crystallographically independent dimeric units, as shown in Fig. 1. One dimer is centrosymmetric with the center of symmetry coincident with the crystallographic center at $0,\frac{1}{2},-\frac{1}{2}$ [molecule (1) in the asymmetric unit]; the other is formed by molecules (2) and (3) which have the same enantiomeric configuration and are related by a pseudo binary axis through the center of hydrogen-bond bridges: N(11)···O′(11) = 2·93 (1), N(21)···O′(31) = 2·95 (1), N(31)···O′(21) = 2·89 (1) Å.

The analysis shows that the methyl group is bonded to C(4) in pseudo-equatorial position, as clearly evident in Fig. 1; the formation of one dihydropyridazine derivative in the above-mentioned reactions is therefore a definite indication that they occur with a regioselective attack of semicarbazone to the enamine isomer Δ^6.

Values of bond distances and angles in the three molecules show an overall general agreement, some discrepancies being most likely the consequence of random errors.

Conformational differences in the three independent molecules are present owing to the different orientation of phenyl and dihydropyridazine rings: the angles between pertinent least-squares planes are 9·8 (8), 32·7 (7) and 31·5 (9)° in molecules (1), (2) and (3) respectively; moreover, there are pronounced deviations from planarity in order to reduce the steric hindrance between atoms O(1) and C(3): (i) the planes through the amide groups are rotated by 15 (1), 16 (1) and 18 (1)° in molecules (1), (2) and (3) respectively with respect to those through the pyridazine rings; (ii) the bond angles C(1)–N(2)–C(2) and C(1)–N(2)–N(3) are respectively widened and narrowed with respect to the value of 120° expected for sp^2 hybridization; (iii) the pyridazine rings are folded about the N(2)–C(9) direction, the angles between the N(2)–N(3)–C(10)–C(9) and N(2)–C(2)–C(8)–C(9) least-squares planes being 15 (1), 26 (1) and 25 (1)°; as a consequence of the folding there is also a bending of the N(2)–C(1) bonds. The resulting O(1)···C(3) distances fall in the range 2·73–2·77 Å, which is the lower limit for CH_2–O intramolecular contacts.

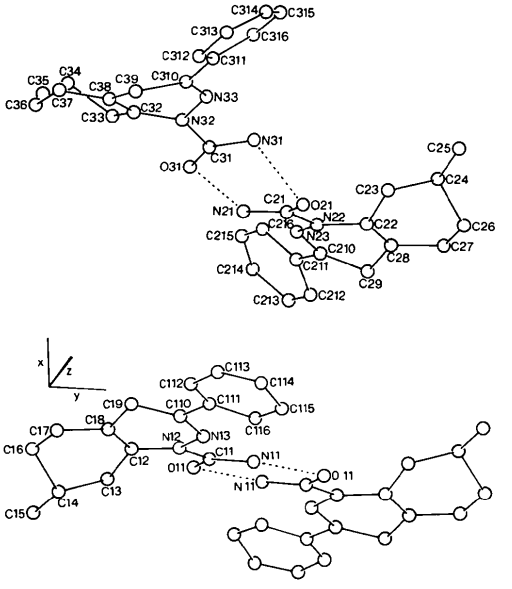


Fig. 1. A projection onto the *ab* plane of the two independent dimers in the crystal: one dimer, lower, is centrosymmetric [molecule (1)]; the other dimer, upper, is formed by molecules (2) and (3) which are related by a pseudo binary axis.

Dimers lie on planes almost parallel to (100) and their packing is regulated by normal van der Waals contacts.

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Structure of [1,4]Benzothiazino[3,2-*i*]phenothiazine, $C_{18}H_{10}N_2S_2$

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Abstract. $M_r = 318{\cdot}2$, monoclinic, $P2_1/c$, $a = 10{\cdot}472\ (2)$, $b = 5{\cdot}430\ (3)$, $c = 12{\cdot}356\ (10)$ Å, $\beta = 107{\cdot}6\ (1)°$, $V = 669{\cdot}7\ (8)$ Å^3, $Z = 2$, $D_x = 1{\cdot}56$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}54178$ Å, $\mu = 33{\cdot}99$ cm^{-1}, $F(000) = 328$, $T = 293$ K, final $R = 0{\cdot}071$ for 669 reflections. The molecule has C_i symmetry and is quasiplanar. The central benzene ring of the molecule has a quinonoid structure with unequal C—C bond lengths. The molecules are arranged in the unit cell in alternately parallel layers, with the planes of neighbouring layers almost perpendicular.

Introduction. Triphenodithiazine ([1,4]benzothiazino-[3,2-*i*]phenothiazine), TPDT, was obtained by reaction of *N,N'*-diphenyl-1,4-phenylenediamine and sulphur (Garbarczyk & Żuk, 1979). In comparison with the analogous phenothiazine, TPDT in the solid phase has exceptional properties, such as paramagnetism detected by EPR, relatively high melting point (594 K) and low solubility in organic solvents. The X-ray structure determination of this compound was undertaken as part of our studies to explain the above properties and particularly to explain the role of TPDT in the polymorphic transition of isotactic polypropylene (Garbarczyk & Paukszta, 1981).

Experimental. Gold-violet thin plate-shaped crystals obtained by sublimation, because crystallization from various solvents did not yield samples suitable for X-ray analysis. Space group and preliminary cell parameters determined on basis of rotation and Weissenberg photographs and refined by least squares from 14 reflections (with $13 < 2\theta < 27°$) measured on a Syntex $P2_1$ diffractometer. Intensities of reflections collected up to $2\theta = 114°$, θ–2θ scan technique, graphite-monochromatized Cu $K\alpha$ radiation. Crystal $0{\cdot}01 \times 0{\cdot}10 \times 0{\cdot}70$ mm. 887 independent reflections, 669 having $I > 1{\cdot}96\sigma(I)$ used in structure analysis. $h -11 \rightarrow 10$, $k\ 0 \rightarrow 5$, $l\ 0 \rightarrow 13$. One standard reflection (112) measured every 50 measurements, rechecked at end of experiment, no significant change in intensity. No absorption correction. Background and integrated intensity for each reflection evaluated by profile analysis procedure (Lehmann & Larsen, 1974), by means of *PRARA* program (Jaskólski, 1979). Structure solved by direct methods using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and refined on F with *SHELX*76 (Sheldrick, 1976). Positional and anisotropic thermal parameters of C, N, and S atoms refined in four cycles up to $R = 0{\cdot}082$. Positions of H atoms attached to C(3*A*), C(4*A*), C(5*A*) and C(6*A*) determined on basis of geometric calculations. Difference Fourier synthesis revealed hydrogen bonded to C(3*B*), simultaneously indicating absence of H atom in vicinity of nitrogen atom. All H atoms allowed to contribute to structure factor calculations, $U_{iso} = 0{\cdot}048$ Å^2 for H's of C(*A*) atoms and $U_{iso} = 0{\cdot}053$ Å^2 for H(C3*B*), with parameters fixed. Final $R(F)$ for observed data and 104 parameters $= 0{\cdot}071$ ($wR = 0{\cdot}071$), $w = 1$. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Largest peak in final difference map 0·4 e Å^{-3}, largest hole −0·4 e Å^{-3}; $S = 1{\cdot}44$; final $\Delta/\sigma = 0{\cdot}02$.* Atomic coordinates and thermal

* Lists of structure factors, anisotropic thermal parameters coordinates of H atoms and least-squares planes have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42073 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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