Table 5. *Hydrogen-bond distances and angles*

Atom A	Atom B	Symmetry code	Distance (Å)	Bond	Angle (°)
O(3')	O(1')	i	2·88	O(3')–H(O3')···O(1')	148
O(5')	O(2')	ii	2·79	O(4')–H(O5')···O(2')	164
O(2')	N(3)	iii	2·81	O(2')–H(O2')···N(3)	151

Symmetry code   i $1+\bar{x}, y+\frac{1}{2}, \bar{z}$;   ii $x, y, z+1$;   iii $\bar{x}, y+\frac{1}{2}, \bar{z}-1$.

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The Crystal and Molecular Structure of 1,2,3-Benzotriazin-4(3H)-one

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The title compound crystallizes in space group $P2_12_12_1$ with $a=3·802$ (2), $b=7·712$ (3), $c=22·213$ (8) Å, $Z=4$. Data were collected on an automatic diffractometer with Cu $K\alpha$ radiation. The structure was solved by the symbolic addition procedure in the $0kl$ projection. Refinement was by full-matrix least-squares methods to an R of 0·036 based on 654 observed reflexions corrected for secondary extinction. The molecules show only small deviations from planarity. The triazine ring has an N(1)–N(2) double bond of 1·274 (3) Å and the hydrogen atom is bonded to N(3). The molecules are bonded together by almost linear N–H···O hydrogen bonds into polymers around screw axes in the x direction. The N···O distance is 2·828 (3) Å and the H···O distance is 1·86 (3) Å.

Introduction

Derivatives of the three possible ring systems 1,3,5-triazine (or s-triazine), 1,2,4-triazine and 1,2,3-triazine (or v-triazine) are known. 1,3,5-Triazine has been extensively studied by both X-ray diffraction (Wheatley, 1955; Coppens, 1967) and neutron diffraction (Coppens, 1967). The parent 1,2,4- and 1,2,3-triazines have never been prepared but 1,2,3-benzotriazine can readily be

obtained as first described by Weddige & Finger (1887). Numerous derivatives of this bicyclic system are known [see reviews by Erickson (1956) or Modest (1961)]. Substituted 1,2,3-benzotriazin-4-ones have potential pharmacological applications (Zaika & Joullié, 1966). The structure of 1,2,3-benzotriazin-4-one is usually drawn as in Fig. 1, but it has a tautomer with the hydrogen atom at N(1) instead of N(3). It was one of the purposes of this investigation to locate this hydrogen. The struc-

ture of the 1,2,3-triazine ring has never been determined by diffraction methods, so that the geometry of the ring itself was also of interest.

Experimental

Crystal data

The crystals are clear colourless needles with a cross-section which is typically a trapezium or a parallelogram. The a axis is parallel to the needle axis. The {010} and {100} forms are well developed.

Crystallographic data:
1,2,3-Benzotriazin-4(3H)-one, $C_7H_5N_3O$.
F.W. 147·04; orthorhombic, $Z=4$;
$\lambda(Cu\ K\alpha)=1\cdot5418$ Å;
$a=3\cdot802$ (2); $b=7\cdot712$ (3); $c=22\cdot213$ (8) Å;
$U=651\cdot24$ Å^3;
$D_x=1\cdot499$ g cm^{-3} for $Z=4$;
$\mu=16\cdot4$ cm^{-1} for Cu $K\alpha$.
Systematic absences: $h00$ when h is odd, $0k0$ when k is odd, $00l$ when l is odd.
Space group: $P2_12_12_1$.

Intensity measurements

Instrument:	Picker FACS-1 automatic diffractometer.
Crystal shape:	Needle, 0·19 mm in the direction of a. Trapezoidal cross section: 0·07 (height) × 0·08 × 0·13 mm.
Radiation:	Cu $K\alpha$, Ni-filter.
Scan-mode:	θ–2θ scan, range $1\cdot4°$ + dispersion correction.
Background:	40 s at each side of the reflexions.
Standards:	035 and 131 measured every 20 reflexions. No significant variations.
Total number of reflexions:	684 (with $2\theta<128°$).
Observed reflexions:	655 (with $\sigma(I)<50\%$).

$\sigma(I)$ is defined as $\sqrt{\sigma_N^2+(0\cdot01\ .\ N)^2}$ where the last term accounts for a 1% instrumental instability and N is the sum of peak and background counts.

The intensities were corrected for Lorentz and polarization effects. The program SCALER (Hjortås, 1970) determined the scale factor and a common temperature factor by a least-squares fit of a straight line to a Wilson-plot. The values obtained were used for the calculation of normalized structure factor amplitudes, $|E_h|$. The values of $\langle|E_h|\rangle=0\cdot862$ and $\langle|E_h^2-1|\rangle=0\cdot744$ compare well with the theoretical values for the non-centric case, 0·886 and 0·736 respectively.

Determination and refinement of the structure

The structure was solved by the symbolic addition method (Karle & Karle, 1963) in the $0kl$ projection (plane group pgg). The 072 and 0,5,17 reflexions were chosen as origin-defining and given a + sign. In addition 0,2,18 was given the symbolic sign A. The computer program SYMBOL (Hjortås, 1969) then generated signs for 42 of the 63 $0kl$ reflexions with $E>1\cdot0$ by using the Σ_2 relations in an iterative process. E maps for both $A=+$ and $A=-$ were calculated. They both contained many maxima to which a six-membered ring could be fitted. A trial and error period followed which eventually gave the correct structure from the map with $A=-$. This map had its two largest maxima

Table 1. Observed and calculated structure factors

The columns are l, $10|F_{obs}|$, $10|F_{calc}|$. Asterisks indicate unobserved reflexions.

in what later proved to be the centre of the two rings. This is a common result of the use of direct methods on molecules with a high degree of internal regularity (Bürgi & Dunitz, 1971).

A preliminary refinement of the y and z coordinates of the C, N and O atoms gave $R_1(0kl) = 0.115$ ($R_1 = \sum ||F_o| - |F_c||/\sum |F_o|$). The approximate orientation of the molecule was found from a 3-dimensional sharpened Patterson map. Approximate x coordinates were determined by systematically moving the molecule in steps in the x direction until a minimum R was found.

The full-matrix least-squares program *CRYLSQ* of the XRAY system (Stewart, Kruger, Kundell & Baldwin, 1971) was used for parameter refinement. It minimizes $\sum w(|F_o| - |F_c|)^2$, and $w = 1$ during this part of the refinement. The scattering factors used are those of Doyle & Turner (1968) for carbon, nitrogen and oxygen and from Stewart, Davidson & Simpson (1965) for hydrogen. Refinement with anisotropic temperature factors converged at $R = 0.080$. A difference map revealed the positions of all hydrogen atoms with a

clear H(3) maximum of 0.35 e Å^{-3} near N(3). Refinement proceeded with isotropic temperature factors for hydrogen and all parameters were allowed to vary. The refinement converged at $R_1 = 0.041$.

Inspection of the observed and calculated structure factors showed that the observed $|F|$'s were systematically too small for the highest $|F|$ values. This is a typical result of secondary extinction. The method given by Zachariasen (1963) was used to correct for this effect. The scale factor and all atomic parameters were refined after the 43 reflexions with $|F_o| > 20.0$ had been removed from the data. The $|F_o|$ and $|F_c|$ for these reflexions were then used to calculate the secondary extinction coefficient c in the expression:

$$|F_{\text{corr}}| = K \cdot |F_o| \, (1 + \beta_{2\theta} c I_o) \, .$$

c was determined to be $3.0 \cdot 10^{-6}$ and all 684 reflexions in the data set were then corrected using this c value in the above expression. Refinement proceeded until all shifts were less than 0.1 standard deviations. The strongest reflexion, 102, was removed from the data. It had $F_{\text{obs}} - F_{\text{calc}}$ of -16.0 and a very uneven background. The final least-squares cycles were calculated with the weight factor $w = 1/\sigma^2(I)$ where $\sigma(I)$ is as defined earlier. The final R_1 is 0.036 and the final weighted reliability index $R_2 = [\sum w(|F_o| - |F_c|)^2/\sum w_o^2]^{1/2}$ is 0.031. All reliability indices given are based on 654 observed reflexions. A final difference map had a largest maximum of 0.13 e Å^{-3} and showed no significant features.

Observed and calculated structure factors are listed in Table 1. Final positional and thermal parameters are given in Tables 2 and 3.

Results and discussion

Planarity of the molecule

Least-squares planes through various parts of the molecule are given in Table 4. Plane *A* through all the ring atoms shows that the whole molecule is nearly planar. The ring system is planar within $+0.019$ to

Table 2. *Final coordinates of* 1,2,3-*benzotriazin*-4(3*H*)-*one*

E.s.d's are given in parentheses.

	x	y	z
N(1)	0·0536 (7)	1·1016 (3)	0·17337 (9)
N(2)	0·0134 (8)	1·2207 (3)	0·13452 (9)
N(3)	0·1344 (8)	1·1939 (3)	0·07690 (9)
C(4)	0·2967 (9)	1·0491 (3)	0·05471 (11)
C(5)	0·4802 (9)	0·7511 (4)	0·08478 (12)
C(6)	0·4991 (10)	0·6256 (4)	0·12864 (14)
C(7)	0·3762 (10)	0·6584 (4)	0·18661 (13)
C(8)	0·2322 (8)	0·8156 (4)	0·20076 (12)
C(9)	0·2085 (8)	0·9446 (3)	0·15654 (10)
C(10)	0·3326 (8)	0·9114 (3)	0·09870 (10)
O	0·3979 (7)	1·0433 (2)	0·00208 (7)
H(3)	0·075 (8)	1·287 (4)	0·0490 (11)
H(5)	0·573 (7)	0·728 (3)	0·0429 (10)
H(6)	0·621 (9)	0·515 (3)	0·1200 (11)
H(7)	0·406 (10)	0·563 (4)	0·2195 (12)
H(8)	0·142 (7)	0·841 (3)	0·2419 (10)

Table 3. *Thermal parameters of* 1,2,3-*benzotriazin*-4(3*H*)-*one*

$U_{ij}(\times 10^4)$ are coefficients in the expression

$$U = \exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})] \, .$$

E.s.d.'s are given in parentheses.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	590 (19)	402 (13)	405 (12)	57 (15)	29 (15)	−39 (12)
N(2)	652 (21)	385 (13)	475 (13)	82 (17)	−8 (15)	−35 (11)
N(3)	622 (19)	310 (12)	365 (12)	46 (16)	−13 (15)	56 (11)
C(4)	476 (21)	310 (14)	395 (14)	−79 (17)	−1 (16)	−14 (13)
C(5)	436 (21)	356 (15)	439 (16)	−23 (18)	33 (16)	−34 (14)
C(6)	480 (23)	302 (15)	715 (21)	61 (19)	−23 (21)	16 (15)
C(7)	511 (21)	439 (19)	555 (18)	−18 (19)	−70 (20)	156 (16)
C(8)	454 (22)	511 (18)	344 (14)	−65 (19)	−27 (16)	46 (14)
C(9)	371 (18)	312 (14)	359 (14)	1 (15)	−11 (14)	2 (12)
C(10)	346 (17)	286 (15)	345 (14)	−51 (16)	−20 (15)	7 (11)
O	882 (17)	433 (10)	333 (9)	−135 (14)	122 (13)	25 (9)
H(3)	$U = 0.081$ (11) Å^2			H(7)	$U = 0.094$ (11) Å^2	
H(5)	0·056 (8)			H(8)	0·053 (8)	
H(6)	0·068 (10)					

−0·024 Å and the carbonyl oxygen deviates 0·037 Å from the ring plane. The largest deviation of −0·132 Å is found at H(3). The benzene ring (plane C in Table 3) is planar with a 75 % probability level. Plane B through the triazine ring shows significant, though small, deviations from planarity. A plane D can be fitted through N(2), N(3), C(9) and C(10) with maximum
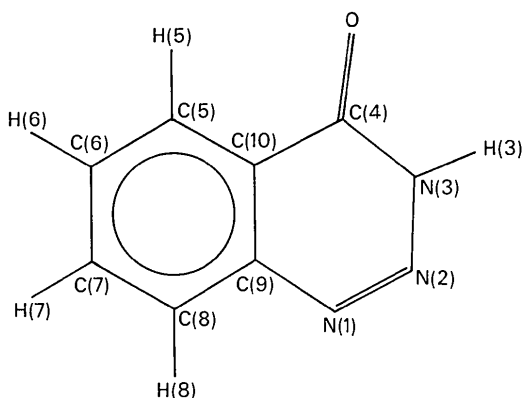

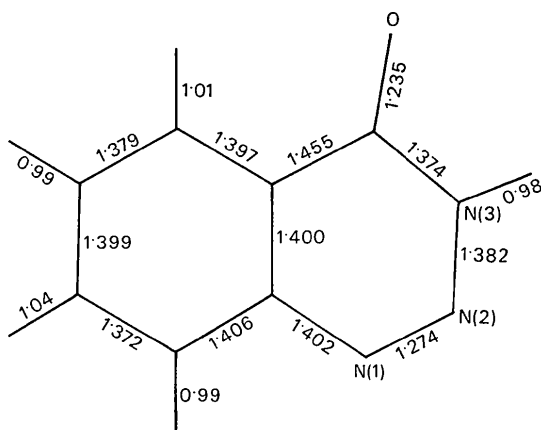Fig. 1. A molecule of 1,2,3-benzotriazin-4(3H)-one with the atomic numbering used in this paper.
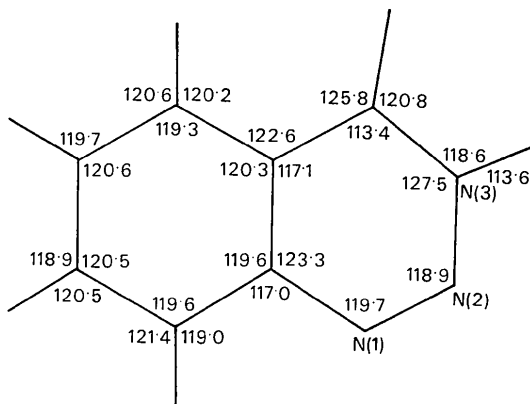

Fig. 2. Bond lengths (Å).

Fig. 3. Bond angles (°).

deviations of ±0·002 Å and N(1) and C(4) then lie 0·019 and 0·015 Å above this plane. Thus the triazine ring has a slight boat conformation. The angle between the two best planes through rings B and C is 1·7°.

Table 4. *Planarity of the molecule*

(a) Equations for best planes

Plane A: N(1), N(2), N(3), C(4), C(5), C(6), C(7), C(8), C(9), C(10)

$$3·415x + 2·721y + 5·808z = 4·173$$

Plane B: N(1), N(2), N(3), C(4), C(9), C(10)

$$3·397x + 2·838y + 5·721z = 4·288$$

Plane C: C(5), C(6), C(7), C(8), C(9), C(10)

$$3·432x + 2·621y + 5·863z = 4·110$$

Plane D: N(2), N(3), C(9), C(10)

$$3·396x + 2·840y + 5·732z = 4·285$$

(b) Deviations (Å) from planes defined above. Deviations for atoms defining the planes are marked with asterisks.

	A	B	C	D
N(1)	0·015*	0·012*	−0·023	0·019
N(2)	−0·024*	−0·009*	−0·076	−0·002*
N(3)	−0·018*	−0·003*	−0·069	0·002*
C(4)	0·014*	0·010*	0·021	0·015
C(5)	0·004*		0·003*	
C(6)	−0·019*		−0·003*	
C(7)	−0·012*		0·001*	
C(8)	0·006*		0·001*	
C(9)	0·019*	−0·004*	−0·001*	0·002*
C(10)	0·017*	−0·007*	−0·001*	−0·002*
O	0·037	0·036	0·002	0·040
H(3)	−0·132	−0·103	−0·195	−0·097
H(5)	0·014		0·016	
H(6)	0·044		0·072	
H(7)	0·020		0·045	
H(8)	0·006		0·000	
Degrees of freedom	9	5	5	3
χ^2	267·24	52·11	2·71	2·48
Probability (%)	<0·1	<0·1	~75	~50

Molecular vibration analysis

The observed thermal parameters are given in Table 3. With programs developed by Evensen (1970) the molecule has been analysed for rigid-body vibration. The program TERMVIB2 uses the method of Schomaker & Trueblood (1968) to determine the rigid-body tensors T, L and S for a rigid-body consisting of all atoms except the hydrogens. Table 5 gives the result of this analysis, which was done in a molecular coordinate system with the origin in the centre of the C(9)–C(10) bond, with the MX axis parallel to this bond and the MZ axis normal to the best plane through the molecule. The difference between the observed U_{ij}'s and those calculated from the rigid-body model was used as a measure of the goodness of the model. The average U_{ij}(obs)−U_{ij}(calc) was 0·0027 Å² which can be compared with an average $\sigma(U_{ij})$ of 0·0016 Å² from the least-squares refinement. The root mean

square translational components along the molecular axes MX, MY and MZ are 0·19, 0·18 and 0·17 Å, respectively. The corresponding r.m.s. angular oscillations are 3·8, 4·5 and 3·2°. Both the translational and angular vibrations are fairly isotropic with the largest oscillations around the long axis of the molecule. The rigid-body tensors are similar to those of naphthalene (Cruickshank, 1957).

Table 5. *Rigid-body tensors*

Standard deviations are given in parentheses.

T (Å²) $\times 10^4$	$\begin{pmatrix} 349\ (12) \\ \\ \end{pmatrix}$	$\begin{matrix} 6\ (10) \\ 334\ (11) \\ \end{matrix}$	$\begin{pmatrix} 19\ (13) \\ 42\ (12) \\ 295\ (22) \end{pmatrix}$
L (deg²)	$\begin{pmatrix} 14·6\ (1·6) \\ \\ \end{pmatrix}$	$\begin{matrix} -3·5\ (1·3) \\ 20·1\ (2·2) \\ \end{matrix}$	$\begin{pmatrix} 0·7\ (1·2) \\ -2·9\ (1·4) \\ 10·5\ (1·0) \end{pmatrix}$
S (Å. rad)	$\begin{pmatrix} 5\ (7) \\ 0\ (8) \\ 9\ (7) \end{pmatrix}$	$\begin{matrix} 8\ (6) \\ 11\ (9) \\ 3\ (9) \end{matrix}$	$\begin{pmatrix} 20\ (12) \\ 9\ (5) \\ -16\ (10) \end{pmatrix}$

Molecular dimensions

The bond lengths are listed in Table 6 and the angles in Table 7. They are also given in Figs. 2 and 3. The bond lengths between heavier atoms have been corrected for rigid-body oscillations with the program *KORREKS* (Evensen, 1970).

Table 6. *Bond lengths*

The bond lengths have been corrected for rigid-body thermal motion (see text). E.s.d.'s are given in parentheses.

	Uncorrected	Corrected
N(1)–N(2)	1·270 (3) Å	1·274 Å
N(2)–N(3)	1·376 (3)	1·382
N(3)–N(4)	1·368 (4)	1·374
N(1)–C(9)	1·397 (4)	1·402
C(4)–C(10)	1·450 (4)	1·455
C(10)–C(5)	1·392 (4)	1·397
C(5)–C(6)	1·375 (4)	1·379
C(6)–C(7)	1·393 (4)	1·399
C(7)–C(8)	1·367 (5)	1·372
C(8)–C(9)	1·401 (4)	1·406
C(9)–C(10)	1·393 (3)	1·400
C(4)–O	1·231 (3)	1·235
N(3)–H(3)	0·98 (3)	
C(5)–H(5)	1·01 (2)	
C(6)–H(6)	0·99 (3)	
C(7)–H(7)	1·04 (3)	
C(8)–H(8)	0·99 (2)	

The C–C bond lengths in the benzenoid ring are very similar to those observed in naphthalene (Cruickshank & Sparks, 1960). A common feature is the shortening of the C(5)–C(6) and C(7)–C(8) type of bond compared with the other benzenoid C–C bonds. In the case of naphthalene this shortening can be explained by using Pauling's method to calculate π-bond orders from the possible Kekulé structures.

In the present structure complete delocalization of the π-electrons through the two rings is absent, since

Table 7. *Bond angles*

E.s.d.'s are given in parentheses.

C(9)–N(1)—N(2)	119·7 (2)°		H(3)–N(3)–N(2)	113·6 (1·8)
N(1)–N(2)—N(3)	118·9 (2)		H(3)–N(3)–C(4)	118·6 (1·7)
N(2)–N(3)—C(4)	127·5 (2)		H(5)–C(5)–C(10)	120·2 (1·5)
N(3)–C(4)—C(10)	113·4 (2)		H(5)–C(5)–C(6)	120·6 (1·5)
N(3)–C(4)—O	120·8 (3)		H(6)–C(6)–C(5)	119·7 (1·6)
O—–C(4)—C(10)	125·8 (3)		H(6)–C(6)–C(7)	119·5 (1·5)
C(6)–C(5)—C(10)	119·3 (3)		H(7)–C(7)–C(6)	118·9 (1·8)
C(5)–C(6)—C(7)	120·6 (3)		H(7)–C(7)–C(8)	120·5 (1·8)
C(6)–C(7)—C(8)	120·5 (3)		H(8)–C(8)–C(7)	121·4 (1·5)
C(7)–C(8)—C(9)	119·6 (3)		H(8)–C(8)–C(9)	119·0 (1·6)
C(8)–C(9)—C(10)	119·6 (3)			
C(8)–C(9)—N(1)	117·0 (2)			
N(1)–C(9)—C(10)	123·3 (2)			
C(4)–C(10)–C(5)	122·6 (2)			
C(4)–C(10)–C(9)	117·1 (3)			
C(9)–C(10)–C(5)	120·3 (2)			

there is a localized N–N double bond (see later). To visualize the bond scheme, approximate π-bond orders were calculated from the linear bond order–bond distance correlation function suggested by Roos & Skancke (1967) and Fischer-Hjalmars & Sundbom (1968): $d = A - p \times 0·180$ (where p is the bond order, d the corresponding bond distance in Å, and A is a constant which has been determined to be 1·517 Å for C–C, 1·458 Å for C–N, 1·453 Å for N–N and 1·368 Å for C–O bonds). These functions have been developed to evaluate bond distances from π-bond orders obtained from MO-calculations of the Pariser–Parr–Pople type on planar molecules. The results are given in Fig. 4. The delocalization of the π-electrons is more complete in the benzenoid ring than in the triazine ring. The N(1)–N(2) bond is clearly a double bond, in agreement with the bond scheme of Fig. 1. Sabcsan & Venkatesan (1971) have carried out MO-calculations by the Hückel method to obtain bond order–bond length relations for the N–N bond. They obtained a length of 1·26 Å for the pure N–N double bond, in good agreement with the length of 1·274 (4) Å in the present study. The N(2)–N(3) bond of 1·382 (3) Å is
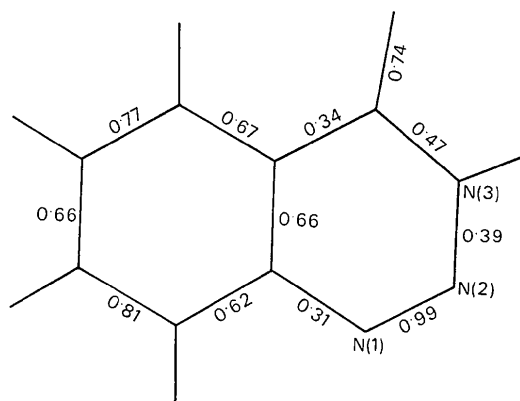

Fig. 4. Estimated π-bond orders obtained from linear bond order–bond distance correlation functions (see text).

appreciably shorter than a normal single bond of 1·46 Å. Its bond order of 0·40 indicates some delocalization of the π-electrons. This delocalization is also evident in the length of the two C–N bonds, N(3)–C(4) at 1·374 (4) Å and N(1)–C(9) at 1·402 (5) Å, both appreciably shorter than the idealized value for sp^2–sp^2 C–N bonds of 1·45 Å (Lide, 1962).

The bond angles around the nitrogen atoms lend support to the statement of Chatar Singh (1965) that a nitrogen in a six-membered ring that has an extraannular hydrogen atom bonded to it gives a ring angle at the nitrogen of $125 \pm 3^\circ$, while a ring nitrogen with no bonded hydrogen has a ring angle of $(116 \pm 3^\circ)$. In the present structure the angle at N(3) is 127·5° and those at N(1) and N(2) are 119·7 and 118·9°, respectively. This confirms the position of the hydrogen at N(3). The angle C(10)–C(4)–O of 125·8 (3)° being significantly larger than the N(3)–C(4)–O angle of 120·8° is probably due to the influence of hydrogen bonding. Other angles are close to expected values.

Hydrogen bonding

The molecules are bonded together in the x direction by N(3)–H(3)$\cdots$O bonds. This bonding is shown in Figs. 5 and 6. A molecule is bonded via an O$\cdots$H–N bond to its neighbour in the $(x-\frac{1}{2}, -y+1\frac{1}{2}, -z)$ position. This molecule is bonded to the molecule at $(x+1,y,z)$ via an N–H$\cdots$O bond. In this way molecules related by screw axes in the x direction are hydrogen bonded together into helices around every second screw axis in this direction. The N(3)$\cdots$O distance is 2·828 (3) Å and the H(3)$\cdots$O distance is 1·86 (3) Å. The H$\cdots$O distance should probably be nearly 0·1 Å shorter due to the normal shortening of N–H and C–H bond lengths in X-ray diffraction work. The N(3)$\cdots$H(3)–O angle is 172·4 (3)° and the C=O$\cdots$H angle is 131·9°. The latter is fairly close to the value of 120° expected when the hydrogen bond lies along an oxygen lone pair. The observed distances and angles for the hydrogen bond agree well with published values for the N–H$\cdots$O bond; see for example Donohue (1968) or more recent high-precision data from neutron diffraction studies on α-amino acids (Koetzle, Lehmann & Hamilton, 1973, and references cited therein).

Intermolecular distances

All short intermolecular distances are listed in Table 8. None of them are shorter than the normal range of van der Waals contacts.
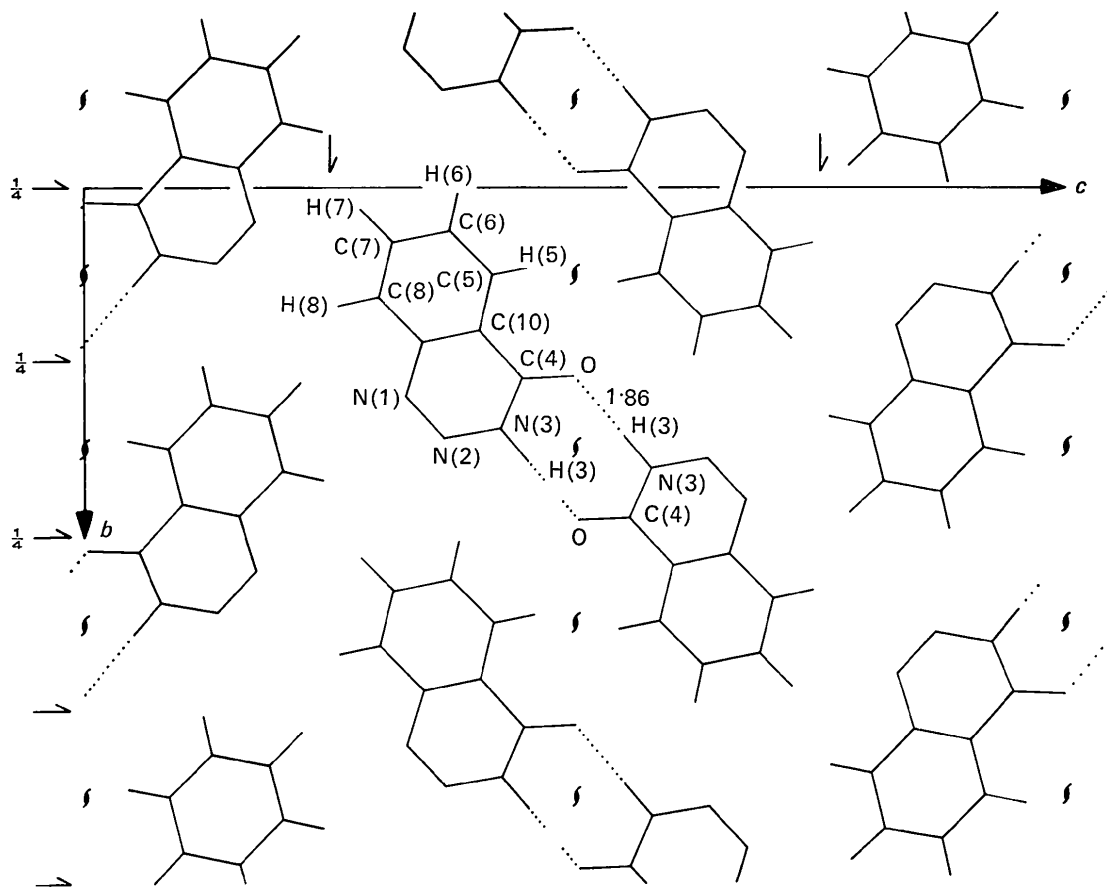

Fig. 5. Molecular packing as seen along the x axis. Dotted lines are hydrogen bonds.
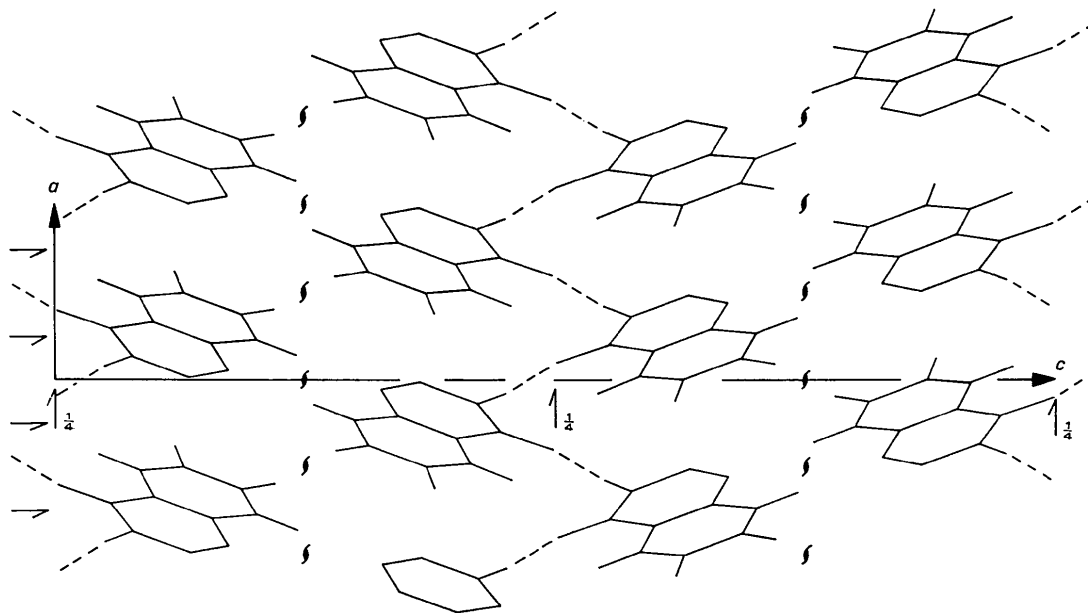
Fig. 6. Molecular packing as seen along the y axis. Dashed lines are hydrogen bonds.

Table 8. *Intermolecular distances*

Distances are included within a limit 0·2 Å greater than the sum of van der Waals radii of the participants. $R_C = 1·80$ Å, $R_N = 1·57$ Å, $R_O = 1·36$ Å, $R_H = 1·17$ Å.

Symmetry operations:

i	$x+1$, y , z;	iv $x+0·5$, $-y+1·5$, $-z$
ii	$x+1$, $y-1$, z;	v $-x+1$, $y+0·5$, $-z+0·5$
iii	$x+0,5$, $-y+2·5$, $-z$;	vi $-x$, $y+0·5$, $-z+0·5$

N(3)–O^{iii}	2·828 (3)	N(2)–C(4^i)	3·510 (4)
H(3)–O^{iii}	1·857 (30)	N(1)–C(10^i)	3·524 (4)
H(5)–O^{iv}	2·627 (27)	N(1)–C(7^{vi})	3·541 (4)
H(6)–N(2^{ii})	2·733 (31)	C(5)–C(10^i)	3·482 (5)
H(8)–N(1^{vi})	2·739 (26)	C(7)–C(8^i)	3·487 (5)
H(3)–C(4^{iii})	2·828 (29)	C(5)–C(9^i)	3·526 (5)
H(7)–C(8^v)	2·949 (33)	C(6)–C(8^i)	3·533 (5)
H(5)–C(4^{iv})	3·161 (26)	C(9)–C(10^i)	3·578 (5)
N(3)–C(4^i)	3·410 (5)	C(6)–C(7^i)	3·583 (6)
N(1)–C(8^{vi})	3·424 (4)	C(6)–C(9^i)	3·702 (5)
N(1)–C(9^i)	3·454 (4)		

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