LIEBAU, F. (1966). *Fortschr. Min.* **42**, 266.
LIEBAU, F. (1970). In Vorbereitung.
LIEBAU, F., BISSERT, G. & KÖPPEN, N. (1968). *Z. anorg. allg. Chem.* **359**, 113.
LIEBAU, F. & HESSE, K. F. (1969). *Naturwissenschaften* **56**, 634.
MIRKIN, J. L. (1964). *Handbook of X-ray Analysis of Polycrystalline Materials*. New York: Consultants Bureau.
PREISINGER, A. (1962). *Naturwissenschaften*, **49**, 345.
RINGWOOD, A. E. (1967). *Earth Planet. Sci. Letters*, **2**, 255.
RINGWOOD, A. E., REID, A. F. & WADSLEY, A. D. (1967) *Acta Cryst.* **23**, 1093.
SMITH, J. V. & BAILEY, S. W. (1963). *Acta Cryst.* **16**, 801.
STISHOV, S. M. & BELOV, N. V. (1962). *Doklady. Akad. Nauk SSSR*, **143**, 951.
STISHOV, S. M. & POPOVA, S. V. (1961). *Geokhimiya*, 837.
VÖLLENKLE, H., WITTMANN, A. & NOWOTNY, H. (1963). *Mh. Chem.* **94**, 956.

Acta Cryst. (1970). B**26**, 240

The Crystal Structure of 1,8,15,22-Tetra-aza-2,7,16,21-tetra-oxocyclo-octacosane, a Cyclic Dimeric Model of Nylon 66*

BY MAURITS G. NORTHOLT
Mellon Institute of Carnegie-Mellon University, Pittsburgh, Pennsylvania 15213, *U.S.A.*

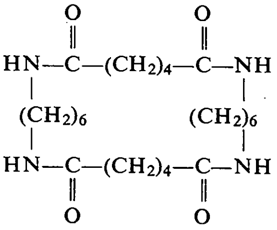
(*Received* 28 *May* 1969)

The crystal structure of 1,8,15,22-tetra-aza-2,7,16,21-tetra-oxocyclo-octacosane has been solved by direct methods using X-ray intensity data and refined by methods of full-matrix least squares. The crystals are monoclinic, space group $P2_1/c$, with cell dimensions $a=9{\cdot}732$ (4), $b=24{\cdot}951$ (8), $c=10{\cdot}845$ (4) Å, $\beta=92°15'$ (2'). The final R value for 2363 observed reflections is 4·5%. All the hydrogen atoms were found and included in the refinement. The four molecules in the unit cell comprise pairs of two conformational isomers. The molecules are 28-membered rings, which are approximately rectangular in shape and lie on symmetry centers. Linked together by N–H---O=C hydrogen bonds, they form sheets parallel to the (010) plane.

Introduction

This investigation is the second in a series of X-ray crystallographic studies of oligomeric models of polyamides. These studies are important because they provide an insight into the conformational aspects of both molecular 'rings' of large size and the related high polymers.

In the description of these oligomers of polyamides, it is convenient to use the symbolism of Zahn, Rahtgeber, Rexroth, Krzikalla, Lauer, Miró, Spoor, Schmidt, Seidel & Hildebrand (1956), who designate the adipic group – $CO(CH_2)_4CO$ – by A and the hexamethylenediamine group – $NH(CH_2)_6NH$ – by B. The crystal-structure determination of the cyclic monomer of nylon 66, c[B–A]$_1$, has been described recently (Northolt & Alexander, 1968). In the present investigation we report the crystallographic study of the cyclic dimer cyclo-bis(hexamethylene-adipamide), c[B–A]$_2$, with the formal configuration



$$\begin{array}{ccccc} & O & & O & \\ & \| & & \| & \\ HN- & C & -(CH_2)_4- & C & -NH \\ | & & & & | \\ (CH_2)_6 & & & & (CH_2)_6 \\ | & & & & | \\ HN- & C & -(CH_2)_4- & C & -NH \\ & \| & & \| & \\ & O & & O & \end{array}$$

The preparation of this oligomer has been described by Zahn & Schmidt (1959).

Experimental

The sample was supplied by H. Zahn of the Technische Hochschule, Aachen and suitable crystals were grown from a water solution. Weissenberg and precession photographs showed the crystals to be monoclinic and gave preliminary unit-cell dimensions that agreed with the values measured by von Dietrich, Zahn & Schmidt (1957). The cell constants were refined by least squares based on diffractometric measurement of the 2θ angles of 16 reflections. The cell constants are listed in Table 1 together with other crystallographic data.

---

* This investigation was supported in part by Public Health Service Grant GM-12396 from the National Institutes of Health.

The crystal selected for intensity measurements had dimensions $0·09\times0·25\times0·68$ mm. The crystal was mounted on a small glass fiber with a drop of glyptal and aligned along [101]. The intensity data were collected with a General Electric automatic single-crystal diffractometer fitted with a scintillation counter. Nickel-filtered Cu $K\alpha$ radiation together with pulse-height discrimination was used in conjunction with the θ–2θ scan technique. The scanning speed was 2° min^{-1} and the scan range was 3°. The background was measured at the beginning and the end of the scan range for a period of 20 sec. The intensities in a quarter of the reflection sphere were measured up to $(\sin\theta)/\lambda=0·5145$ Å^{-1}, yielding a total of 2881 nonequivalent reflections.

Table 1. *Crystal data*

1,8,15,22-Tetra-aza-2,7,16,21-tetra-oxocyclo-octacosane, $C_{24}H_{44}N_4O_4$
M.W. 452·64, m.p. 233 °C
Space group $P2_1/c$
$a=$ 9·732 (4) Å
$b=$24·951 (8)
$c=$10·845 (4)
$\beta=92°15'$ (2′)
$D_m=1·15$ (1) g.cm^{-3}, $D_x=1·15$ g.cm^{-3} for $Z=4$
$F(000)=992$
Absorption coefficient for X-rays ($\lambda=1·5418$ Å): $\mu=6·34$ cm^{-1}
Habit: Colorless, lath-shaped with longest dimension along [101]

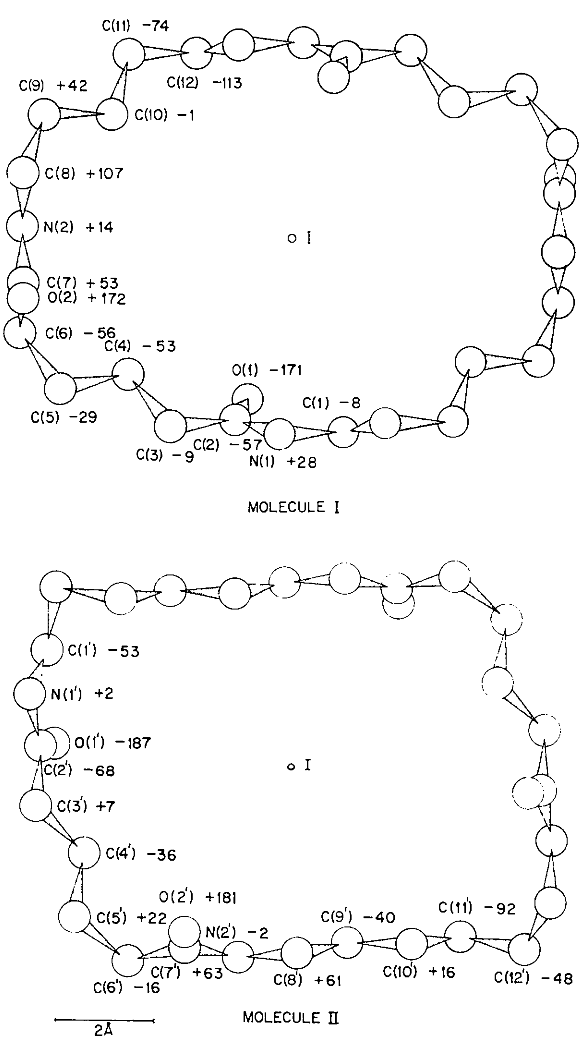


Fig. 1. Projection on the least-squares plane through the atoms in the ring and labeling of the atoms. Numbers indicate perpendicular distances from the plane in Å × 10^2.

Details of the procedure followed for data gathering and processing to observed structure factors have been presented elsewhere (Northolt & Alexander, 1968). A reflection was classed as unobserved when $I<1·5\,\sigma_I$. Standard propagation-of-error methods were used to calculate $\sigma(F_o)$ from $\sigma(I)$. In the least-squares refinement of atomic parameters only observed reflections were used, the function minimized being $\Sigma w(F_o-F_c)^2$.

No corrections were made for absorption, and because of the lack of systematic discrepancies between the observed and calculated structure factors of the strongest reflections, it was decided that no corrections for primary and secondary extinction were necessary. The computations of the Fourier syntheses and the initial least squares were performed on an IBM 7090 computer using the X-ray 63 programs system (Stewart & High, 1965). The final refinements were carried out on an IBM 360 computer.*

Solution by symbolic addition

The structure was solved with the symbolic addition method for centrosymmetric crystals (Hauptman & Karle, 1953) using a program developed by S. R. Hall. The program determines preliminary scale and temperature factors and reduces the structure factors to normalized structure factors (E values). The atomic scattering factors used in the calculations were those of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) for oxygen, nitrogen and carbon, and of Stewart, Davidson & Simpson (1965) for hydrogen. The values calculated for the distribution and statistics of $|E|$ for this structure, together with the corresponding theoretical values (in parentheses) as calculated by Karle, Hauptman, Karle & Wing (1958), are: $\langle|E|\rangle=0·775$ (0·798), $\langle|E|^2\rangle=1·006$ (1·000), $\langle|E^2-1|\rangle=1·034$ (0·968); reflections with $|E|>3$ were 0·9% (0·3%), reflections with $|E|>2$ were 5·1% (5·0%), and reflections with $|E|>1$ were 28·8% (32·0%).

A manual symbolic addition procedure was applied to the 122 reflections with $|E|>2·1$, using the results of a search carried out by the program for sets of reflections that satisfy the Σ_2 relationship. The three origin-defining reflections were selected from among reflections that did not belong to the parity group *ggg* and that were among those with the largest $|E|$'s and with a

---

* For this purpose a program '*SFLS-5*' used in the Department of Chemistry, Massachusetts Institute of Technology, was employed.

high number (NT) of Σ_2 interactions. In addition three reflections were assigned symbols indicative of unknown phases. Together with the origin reflections, they are:

h	k	l	$\|E\|$	NT	Phase or symbol
3	15	6	4·273	18	π
$\bar{8}$	1	2	4·157	15	0
2	17	3	3·613	13	π
0	6	4	4·374	23	p
0	5	2	3·883	24	q
$\bar{6}$	12	5	3·259	11	r

The results of the manual symbolic addition strongly suggested the relation $p=r=\pi$, but q could not be determined. The phase of q was arbitrarily set to zero and eighteen additional reflections, the phases of which had been determined in the manual symbolic addition, were selected as a starting set of phases. This set of phases was extended and refined in ten cycles as described by Oh & Maslen (1968) using the tangent formula (Karle & Hauptman, 1956). New reflections were introduced in the refinement by gradually lowering the minimum E value at the beginning of each cycle. At the end of this process the phases of 426 reflections with $|E| \geq 1{\cdot}40$ had been determined, and an E Fourier synthesis was calculated. It revealed all the heavy atoms as peaks that were well above the noise level. None of the phases was subsequently found to be incorrect when compared with the phases corresponding to the fully refined structure. Structure factors incorporating a uniform isotropic temperature factor were calculated for all reflections with $(\sin\theta)/\lambda < 0{\cdot}38$ Å^{-1}, which yielded an R value of 36% and indicated that the structure deduced from the E map was essentially correct. The molecules are situated on symmetry centers, which requires that the asymmetric unit consist of two half molecules.

Structure refinement

Three cycles of isotropic full-matrix least-squares refinement reduced the agreement index to 16·5%. Next two cycles of refinement with anisotropic temperature factors were performed, causing a further reduction of R to 11%. A difference synthesis at this stage revealed the location of all the hydrogen atoms. Due to limitations of the computer core, it was not possible to refine the parameters of the heavy atoms and the hydrogen atoms of both molecules together. Accordingly it was decided to refine one molecule at a time, using the other molecule as a fixed contribution. After five cycles of full-matrix least squares, each of which consisted of a separate refinement of the two molecules, the shift per error was less than $\frac{1}{3}\sigma$ for the heavy atom parameters and less than $\frac{1}{2}\sigma$ for the hydrogen parameters. At this stage the refinement was halted, and the regular and weighted agreement indices, based on observed reflections only, were found to be

$$R\colon \Sigma|F_o-|F_c||/\Sigma F_o=0{\cdot}045\,,$$

$$wR\colon (\Sigma w\,(F_o-|F_c|)^2/\Sigma wF_o^2)^{1/2}=0{\cdot}030\,.$$

A difference synthesis, calculated on the basis of the parameters at the end of the refinement, showed a few peaks and holes with a maximum value of 0·20 e.Å^{-3} in the neighborhood of the non-hydrogen atoms. Elsewhere the map was rather flat with a background of 0·06 e.Å^{-3}. Tables 2 and 3 give the positional and anisotropic thermal parameters, respectively, of the heavy atoms, Table 4 gives the positional and isotropic thermal parameters of the hydrogen atoms, and Table 5 lists the observed and calculated structure factors. The numerical values in Tables 2, 3 and 4 of the estimated standard deviations (e.s.d.'s) are the values obtained from the least-squares refinement, and they were subsequently used for the calculation of the e.s.d.'s in the bond angles and distances.

Table 2. *Coordinates of non-hydrogen atoms with e.s.d.'s in parentheses*

Molecule I

	x	y	z
O(1)	0·5173 (2)	0·6409 (1)	1·1788 (1)
O(2)	0·6225 (2)	0·6738 (1)	0·6072 (1)
N(1)	0·7405 (3)	0·6196 (1)	1·1872 (2)
N(2)	0·4038 (3)	0·6484 (1)	0·5895 (2)
C(1)	0·7296 (3)	0·5845 (2)	1·2935 (3)
C(2)	0·6334 (3)	0·6464 (1)	1·1379 (2)
C(3)	0·6613 (3)	0·6835 (1)	1·0330 (3)
C(4)	0·5497 (3)	0·6828 (1)	0·9314 (3)
C(5)	0·5619 (3)	0·7276 (1)	0·8386 (3)
C(6)	0·4610 (3)	0·7215 (1)	0·7279 (3)
C(7)	0·5031 (3)	0·6789 (1)	0·6374 (2)
C(8)	0·4276 (3)	0·6072 (1)	0·4973 (3)
C(9)	0·3116 (4)	0·5679 (2)	0·4882 (3)
C(10)	0·2968 (4)	0·5325 (2)	0·6021 (3)
C(11)	0·1733 (4)	0·4954 (2)	0·5915 (3)
C(12)	0·1602 (3)	0·4584 (1)	0·7018 (3)

Molecule II

	x	y	z
O(1′)	0·0112 (2)	0·6374 (1)	0·1006 (1)
O(2′)	0·1236 (2)	0·6650 (1)	0·6640 (1)
N(1′)	0·2375 (2)	0·6230 (1)	0·0932 (2)
N(2′)	−0·0994 (2)	0·6461 (1)	0·6769 (2)
C(1′)	0·2289 (3)	0·5854 (1)	−0·0086 (3)
C(2′)	0·1280 (3)	0·6462 (1)	0·1412 (2)
C(3′)	0·1576 (3)	0·6848 (1)	0·2463 (3)
C(4′)	0·0505 (3)	0·6828 (1)	0·3455 (3)
C(5′)	0·0650 (3)	0·7263 (1)	0·4417 (3)
C(6′)	−0·0374 (3)	0·7184 (1)	0·5432 (3)
C(7′)	0·0036 (3)	0·6744 (1)	0·6316 (2)
C(8′)	−0·0807 (3)	0·6057 (2)	0·7730 (3)
C(9′)	−0·2008 (4)	0·5675 (2)	0·7739 (3)
C(10′)	−0·1965 (3)	0·5279 (1)	0·8789 (3)
C(11′)	−0·3243 (3)	0·4928 (1)	0·8795 (3)
C(12′)	−0·3382 (3)	0·4577 (1)	0·9929 (3)

Discussion

Conformation

The unit cell contains two pairs of conformational isomers. Both molecules are based on a 28-membered alicyclic skeleton, which is rather planar as can be seen from an inspection of Fig. 1. The Figure shows the projections of the atoms on the least-squares planes for

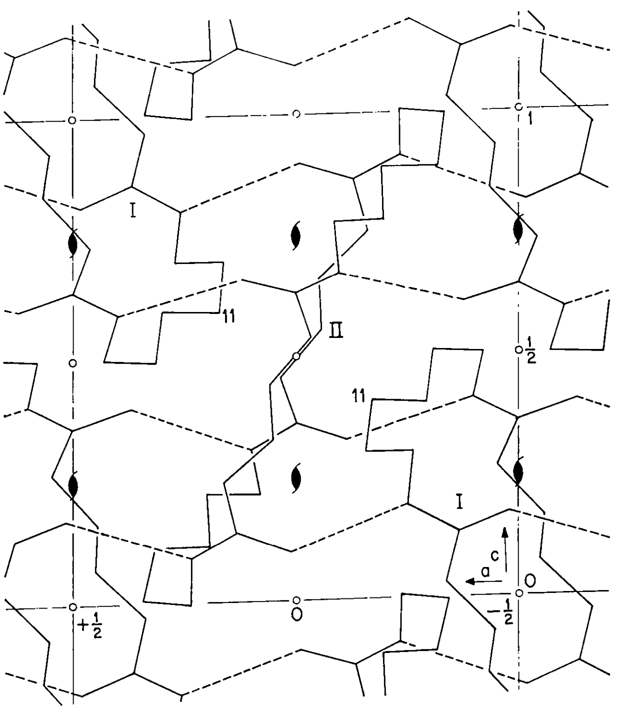


Fig. 2. Hydrogen bonding in a layer of the structure. Projection parallel to [010].

both molecules. The equation of the plane for molecule I is

$$8{\cdot}43x-7{\cdot}01\,y-4{\cdot}85\,z=-4{\cdot}14$$

and for molecule II

$$8{\cdot}53\,x-0{\cdot}21\,y+4{\cdot}85\,z=2{\cdot}32\,,$$

with standard deviations of 0·58 and 0·47 Å respectively. The approximate dimensions of both rings are 12 × 8 Å. The rings resolve themselves into several planar elements, giving them the appearance of open ended boxes. This box-like shape of the rings arises from the fact that the relative orientation of the average planes through the amide groups is nearly perpendicular to the planes of the rings, being 89° 24′ in molecule I and 89° 6′ in molecule II.

Along the chain the following planar elements are found in succession within molecule I: the amide group (*P*) with atoms C(1) C(2) C(3) N(1) O(1), the tetramethylene chain (*Q*) with atoms C(3) C(4) C(5) C(6), the amide group (*R*) with atoms C(6) C(7) C(8) N(2) O(2) and the pentamethylene chain (*S*) with atoms C(8) C(9) C(10) C(11) C(12). In molecule II the same planar elements are found. They are the amide group (*P*′) with atoms C(1′) C(2′) C(3′) N(1′) O(1′), the tetramethylene chain (*Q*′) with atoms C(3′) C(4′) C(5′) C(6′), the amide group (*R*′) with atoms C(6′) C(7′) C(8′) N(2′) O(2′) and

Table 3. *Anisotropic temperature factor coefficients* ($\times 10^5$) *with e.s.d.'s in parentheses*

$T=\exp\,[-(b_{11}h^2+b_{22}k^2+b_{33}l^2+2b_{12}hk+2b_{13}hl+2b_{23}kl)]$.

	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
O(1)	572 (21)	274 (5)	1084 (20)	−1 (8)	162 (16)	43 (7)
O(2)	495 (22)	337 (5)	1313 (23)	53 (8)	192 (17)	56 (8)
N(1)	724 (34)	244 (6)	1151 (32)	12 (12)	249 (27)	70 (11)
N(2)	607 (37)	243 (7)	1287 (34)	58 (13)	237 (29)	−19 (11)
C(1)	1102 (47)	269 (9)	1333 (47)	112 (17)	251 (36)	121 (17)
C(2)	693 (36)	190 (6)	904 (32)	19 (13)	−32 (28)	−94 (11)
C(3)	808 (39)	196 (8)	1001 (36)	−22 (14)	171 (31)	−9 (14)
C(4)	1067 (41)	169 (7)	978 (34)	−38 (14)	73 (31)	25 (14)
C(5)	1082 (46)	213 (8)	1253 (41)	−81 (15)	67 (39)	12 (15)
C(6)	875 (41)	174 (7)	1296 (40)	−2 (13)	211 (34)	87 (14)
C(7)	820 (39)	207 (7)	867 (32)	20 (15)	−22 (29)	132 (12)
C(8)	1445 (51)	268 (9)	945 (41)	27 (18)	258 (38)	1 (17)
C(9)	1877 (62)	260 (9)	1056 (42)	43 (20)	9 (39)	−58 (16)
C(10)	1660 (59)	256 (9)	1136 (46)	30 (19)	−52 (40)	31 (17)
C(11)	1528 (52)	246 (8)	1368 (46)	−40 (17)	−267 (38)	44 (17)
C(12)	1183 (46)	231 (8)	1365 (44)	54 (16)	−104 (35)	−29 (16)
O(1′)	515 (22)	384 (6)	1126 (22)	−31 (9)	14 (18)	−136 (8)
O(2′)	546 (23)	356 (5)	1243 (23)	45 (9)	31 (19)	66 (8)
N(1′)	585 (33)	238 (6)	1109 (31)	3 (11)	−6 (26)	−68 (10)
N(2′)	717 (34)	264 (6)	1141 (32)	40 (12)	8 (27)	102 (11)
C(1′)	1123 (46)	267 (9)	879 (38)	5 (16)	79 (33)	−26 (16)
C(2′)	901 (39)	196 (7)	721 (31)	−1 (14)	163 (28)	46 (11)
C(3′)	612 (35)	217 (8)	1037 (35)	12 (13)	1 (29)	46 (14)
C(4′)	813 (39)	215 (8)	1044 (37)	−21 (14)	67 (32)	28 (15)
C(5′)	1187 (45)	173 (8)	1065 (35)	−58 (14)	118 (32)	−70 (14)
C(6′)	920 (41)	209 (8)	1048 (38)	14 (14)	107 (31)	−65 (15)
C(7′)	754 (37)	230 (7)	825 (32)	−16 (15)	155 (29)	−95 (12)
C(8′)	898 (43)	308 (9)	1303 (46)	25 (17)	118 (35)	122 (17)
C(9′)	1331 (52)	250 (9)	1149 (45)	−1 (17)	86 (36)	−19 (16)
C(10′)	1298 (48)	280 (9)	1080 (41)	10 (17)	112 (34)	51 (16)
C(11′)	1336 (49)	229 (8)	1319 (46)	6 (16)	129 (36)	−98 (16)
C(12′)	1257 (46)	254 (8)	1122 (40)	9 (16)	291 (34)	−88 (16)

the pentamethylene chain (*S′*) with atoms C(8′) C(9′) C(10′) C(11′) C(12′). Although it would appear that the large size of the molecules would permit large differences in conformation between the isomers, it is rather surprising to find good agreement in conformation for the major portions of the rings. In particular, the segment including the amide group (*P*), the tetramethylene chain (*Q*) and the amide group (*R*) is nearly identical in the two molecules.

A major difference, however, is found in the relative orientation of planar elements *R* and *S*; in molecule I the interplanar angle is 77° 23′ and in molecule II, 30° 36′. The conformation of a polymer chain is usually described in terms of internal-rotation angles (Natta, Corradini & Bassi, 1961). The difference in conformation between the two isomers of c[B–A]$_2$ can be described by the internal-rotation angle N(2)C(8)-C(9)$\wedge$C(8)C(9)C(10), the magnitudes of which are 112° 32′ in molecule I and 173° 59′ in molecule II. This difference in the conformation about the bond C(9)–C(8) is matched by a compensating difference in the rotation angles about C(1)–C(12), which, it may be noted, preserves the planarity of the polymethylene and amide elements. The internal rotation angle C(11)C(12)C(1)$\wedge$C(12)C(1)N(1) has magnitude 179° 14′ in molecule I and 116° 57′ in molecule II. A detailed

Table 4. *Hydrogen coordinates and temperature factors* $T=\exp(-B\sin^2\theta/\lambda^2)$ *with e.s.d.'s in parentheses*

The methyl hydrogen atoms are labeled using a three-digit code in which the first two digits identify the carbon atoms to which they are bonded.

	x	*y*	*z*	*B*
		Molecule I		
H(001)	0·807 (2)	0·626 (1)	1·154 (2)	5·5 (9) Å^2
H(002)	0·335 (2)	0·654 (1)	0·602 (2)	2·0 (6)
H(011)	0·743 (3)	0·606 (1)	1·376 (2)	8·6 (1·0)
H(012)	0·649 (3)	0·564 (1)	1·285 (2)	6·9 (9)
H(031)	0·748 (2)	0·677 (1)	1·003 (2)	4·3 (6)
H(032)	0·663 (2)	0·720 (1)	1·064 (2)	3·6 (6)
H(041)	0·549 (2)	0·648 (1)	0·895 (2)	4·2 (7)
H(042)	0·451 (2)	0·685 (1)	0·974 (2)	6·3 (7)
H(051)	0·550 (3)	0·764 (1)	0·889 (2)	8·5 (9)
H(052)	0·646 (2)	0·728 (1)	0·816 (2)	4·2 (7)
H(061)	0·455 (2)	0·758 (1)	0·683 (2)	5·8 (7)
H(062)	0·370 (2)	0·715 (1)	0·756 (2)	3·5 (5)
H(081)	0·436 (2)	0·625 (1)	0·423 (2)	5·4 (8)
H(082)	0·514 (2)	0·584 (1)	0·534 (2)	5·5 (7)
H(091)	0·216 (3)	0·587 (1)	0·477 (2)	8·0 (9)
H(092)	0·327 (3)	0·542 (1)	0·421 (2)	8·2 (1·0)
H(101)	0·386 (2)	0·515 (1)	0·614 (2)	6·3 (8)
H(102)	0·299 (3)	0·555 (1)	0·670 (2)	7·8 (1·0)
H(111)	0·081 (3)	0·520 (1)	0·571 (2)	12·1 (1·1)
H(112)	0·187 (2)	0·468 (1)	0·510 (2)	9·8 (1·0)
H(121)	0·173 (2)	0·481 (1)	0·783 (2)	7·9 (8)
H(122)	0·072 (3)	0·438 (1)	0·681 (2)	10·2 (1·0)
		Molecule II		
H(001′)	0·313 (2)	0·631 (1)	0·121 (2)	2·7 (6)
H(002′)	−0·176 (2)	0·656 (1)	0·645 (2)	5·3 (8)
H(011′)	0·237 (2)	0·606 (1)	−0·082 (2)	4·0 (6)
H(012′)	0·137 (2)	0·566 (1)	−0·011 (2)	3·7 (6)
H(031′)	0·244 (2)	0·679 (1)	0·284 (2)	2·9 (5)
H(032′)	0·159 (2)	0·725 (1)	0·207 (2)	4·9 (6)
H(041′)	−0·031 (2)	0·686 (1)	0·309 (2)	2·2 (5)
H(042′)	0·048 (2)	0·646 (1)	0·391 (2)	4·9 (7)
H(051′)	0·165 (2)	0·728 (1)	0·483 (2)	5·7 (7)
H(052′)	0·052 (2)	0·762 (1)	0·411 (2)	5·2 (7)
H(061′)	−0·134 (2)	0·714 (1)	0·504 (2)	4·1 (6)
H(062′)	−0·041 (2)	0·748 (1)	0·591 (2)	5·1 (8)
H(081′)	−0·057 (3)	0·625 (1)	0·864 (3)	12·8 (1·2)
H(082′)	−0·006 (3)	0·584 (1)	0·758 (2)	7·2 (9)
H(091′)	−0·215 (3)	0·550 (1)	0·690 (2)	8·2 (9)
H(092′)	−0·278 (3)	0·588 (1)	0·783 (2)	8·5 (1·0)
H(101′)	−0·182 (3)	0·551 (1)	0·966 (2)	9·5 (9)
H(102′)	−0·115 (3)	0·506 (1)	0·887 (2)	9·0 (1·0)
H(111′)	−0·331 (2)	0·470 (1)	0·805 (2)	6·2 (8)
H(112′)	−0·411 (3)	0·518 (1)	0·877 (2)	8·9 (9)
H(121′)	−0·443 (3)	0·438 (1)	0·986 (2)	7·6 (8)
H(122′)	−0·335 (2)	0·483 (1)	1·068 (2)	6·8 (8)

Table 5. *Observed and calculated structure factors* (×10)

OBSERVED REFLECTIONS

H	K	FOBS	FCAL
L = 0**			
2	0	142	139
3	0	20	-21
4	0	88	89
6	0	202	210
8	0	210	216
9	0	61	59
10	0	37	-38
2	1	771	766
4	1	66	-70
6	1	103	-95
8	1	194	194
0	2	439	-439
1	2	49	51
2	2	2042	-2145
6	2	108	121
8	2	181	-168
9	2	27	9
2	3	1087	-1127
4	3	78	102
5	3	39	-47
6	3	47	44
7	3	25	10
8	3	47	32
0	4	1164	-1161
1	4	62	-68
2	4	217	-211
4	4	290	-290
5	4	24	12
6	4	360	350
8	4	515	-518
9	4	62	-57
1	5	20	-1
2	5	1113	-1134
3	5	20	14
4	5	569	582
6	5	104	-105
7	5	52	36
8	5	347	-346
0	6	1295	1302
2	6	527	550
3	6	32	1
4	6	647	-629
6	6	453	448
8	6	273	284
1	7	26	9
2	7	225	221
3	7	30	-12
4	7	628	649
6	7	309	-297
7	7	28	-31
8	7	125	146
1	8	80	84
2	8	105	95
3	8	78	-74
4	8	183	190
6	8	280	-285
7	8	30	22
8	8	54	55
9	8	48	52
1	9	104	105
2	9	553	-547
3	9	26	26
4	9	353	359
7	9	49	-54
8	9	57	61
9	9	29	-8
0	10	400	-403
2	10	231	-226
4	10	301	298
6	10	124	-128
7	10	39	-32
8	10	171	-175
9	10	30	-40
1	11	47	-34
2	11	413	-410
3	11	36	-39
4	11	40	-43
5	11	37	37
6	11	79	56
7	11	33	33
8	11	107	-101
0	12	94	97
2	12	49	55
3	12	30	-18
4	12	185	-188
6	12	43	36
8	12	66	52
1	13	46	-35
2	13	247	239
4	13	24	16
6	13	33	-43
0	14	41	57
1	14	43	33
2	14	97	108
3	14	34	-29
4	14	30	-36
5	14	26	-26
1	15	37	46
2	15	126	-134
3	15	33	41
5	15	44	-34
6	15	61	-74
7	15	47	-47
8	15	46	-41
0	16	45	-26
1	16	35	-27
2	16	118	-123
4	16	161	158
5	16	28	22
6	16	118	124
7	16	34	-19
2	17	109	100
3	17	40	-42
4	17	78	81
6	17	93	98
7	17	26	-8
0	18	54	53
2	18	102	88
6	18	64	-63
7	18	32	24
2	19	82	77
3	19	35	44
4	19	48	48
6	19	79	-72
0	20	215	-217
4	20	218	-222
5	20	29	-29
2	21	168	-167
3	21	46	35
4	21	76	-75
5	21	38	-36
0	22	293	290
1	22	31	-34
2	22	158	157
2	23	98	99
4	23	27	20
0	24	151	-150
1	24	41	42
2	24	162	-151
L = 1**			
-9	1	72	-63
-8	1	67	57
-7	1	136	124
-3	1	299	-303
-4	1	388	-384
-5	1	99	-96
-6	1	339	-341
-2	1	46	-28
0	1	113	-108
2	1	737	741
3	1	220	218
4	1	227	-216
5	1	43	-34
6	1	121	129
7	1	204	206
8	1	200	-198
9	1	301	-286
-9	2	230	235
-8	2	117	-128
-7	2	194	-204
-5	2	36	-28
-4	2	464	-453
-3	2	604	-619
-2	2	1150	1203
-1	2	141	-145
0	2	125	-130
1	2	192	193
2	2	125	-120
3	2	346	351
4	2	614	-599
5	2	39	33
6	2	369	-368
7	2	45	54
8	2	92	-85
-9	3	48	66
-8	3	153	135
-7	3	120	116
-6	3	209	215
-5	3	94	-89
-4	3	508	497
-3	3	151	151
-2	3	251	262
-1	3	55	59
0	3	166	-169
1	3	427	-425
2	3	1105	-1193
3	3	500	-509
4	3	307	304
5	3	77	-77
6	3	37	35
7	3	80	70
8	3	161	-137
9	3	107	128
-9	4	33	-12
-8	4	300	-300
-7	4	95	-103
-6	4	35	28
-5	4	157	161
-4	4	69	62
-3	4	146	146
-2	4	450	-476
-1	4	899	892
0	4	315	-318
1	4	295	298
2	4	216	-213
3	4	163	-161
4	4	186	193
5	4	51	44
6	4	120	130
7	4	193	-196
8	4	49	-42
9	4	107	-105
-9	5	196	-188
-8	5	102	93
-7	5	112	-114
-6	5	77	-73
-5	5	68	73
-4	5	305	297
-3	5	40	33
-2	5	460	463
-1	5	727	749
0	5	539	542
1	5	1252	1311
2	5	247	-246
3	5	230	-236
4	5	335	338
5	5	238	238
7	5	80	-88
8	5	315	325
9	5	71	-57
-9	6	100	97
-8	6	239	248
-6	6	124	122
-5	6	55	-40
-4	6	535	520
-3	6	259	267
-2	6	308	-320
-1	6	995	-997
0	6	747	758
1	6	485	-493
2	6	356	356
3	6	345	-352
4	6	753	765
5	6	247	239
8	6	104	98
9	6	34	46
-7	7	80	73
-6	7	63	-49
-5	7	150	150
-4	7	643	-649
-3	7	318	-312
-2	7	263	-257
-1	7	238	-239
0	7	447	-457
1	7	380	-388
2	7	80	-67
3	7	400	-406
4	7	89	-80
5	7	153	151
6	7	290	-290
7	7	31	-23
8	7	76	-80
-9	8	45	-47
-8	8	53	44
-7	8	84	88
-6	8	270	-261
-5	8	161	-164
-3	8	340	339
-2	8	412	-409
-1	8	52	45
0	8	97	-93
1	8	297	297
2	8	364	-367
3	8	61	-71
4	8	151	-150
5	8	97	94
6	8	143	-127
8	8	107	114
9	8	28	32
-9	9	49	53
-8	9	162	-166
-6	9	91	92
-5	9	108	111
-4	9	283	-276
-3	9	383	-387
-2	9	199	197
-1	9	114	113
0	9	192	-187
1	9	32	31
2	9	268	266
3	9	74	67
4	9	141	147
7	9	41	-41
8	9	169	-167
9	9	51	-43
-9	10	52	36
-8	10	255	-249
-7	10	174	178
-6	10	161	-152
-5	10	126	-123
-4	10	86	95
-2	10	155	155
-1	10	27	18
0	10	343	-338
1	10	95	-92
2	10	70	-75
3	10	150	140
4	10	331	-327
6	10	80	-80
7	10	90	-79
8	10	219	-224
9	10	96	-90
-9	11	82	-81
-8	11	196	198
-7	11	103	-96
-6	11	149	148
-5	11	174	167
-4	11	174	161
-3	11	178	-170
-2	11	400	407
-1	11	133	-131
0	11	219	211
1	11	80	69
2	11	139	-134
3	11	71	75
5	11	91	84
6	11	172	172
7	11	136	136
8	11	174	173
-8	12	111	121
-7	12	152	-157
-6	12	191	196
-5	12	154	-158
-4	12	39	40
-3	12	28	26
-1	12	45	-44
0	12	35	-41
1	12	96	-100
2	12	443	439
3	12	121	116
4	12	99	98
6	12	73	60
7	12	37	-23
8	12	141	143
-8	13	54	-52
-7	13	41	-28
-5	13	26	18
-4	13	118	-121
-3	13	153	144
-2	13	178	-161
-1	13	77	64
0	13	253	254
1	13	110	101
2	13	30	-21
3	13	53	-51
4	13	40	34
5	13	34	-34
6	13	100	-94
7	13	79	-65
-8	14	42	42
-7	14	96	85
-6	14	45	-36
-5	14	31	28
-4	14	37	37
-3	14	174	-172
-1	14	34	9
0	14	406	414
1	14	59	50
2	14	115	116
5	14	46	50
8	14	47	49
-8	15	120	-112
-6	15	73	63
-5	15	59	56
-4	15	90	-81
-2	15	288	-287
-1	15	130	-127
0	15	256	-267
3	15	155	-150
4	15	42	-40
5	15	57	-65
6	15	85	-77
7	15	32	-13
8	15	74	-71
-7	16	29	22
-6	16	193	-182
-5	16	175	177
-4	16	28	-28
-1	16	198	201
0	16	237	-234
1	16	61	78
2	16	363	-364
3	16	72	-70
4	16	78	-76
5	16	46	-46
7	16	37	-37
-7	17	104	-101
-6	17	57	48
-4	17	35	43
-3	17	87	-82
-2	17	304	296
0	17	86	67
1	17	200	201
2	17	97	-92
5	17	100	102
6	17	167	166
-7	18	97	-90
-6	18	132	141
-5	18	28	28
-4	18	82	-85
-3	18	119	-115
-1	18	155	-160
0	18	53	-59
1	18	63	-73
2	18	150	141
3	18	47	-54
4	18	61	75
5	18	69	73
6	18	43	48
7	18	81	76
-5	19	64	66
-4	19	107	-102
-2	19	55	44
-1	19	30	29
0	19	155	152
1	19	103	-106
2	19	54	-42
3	19	132	-137
4	19	116	116
5	19	93	96
6	19	50	-44
-6	20	62	64
-5	20	29	29
-1	20	86	86
0	20	152	164
1	20	92	87
2	20	89	87
3	20	63	-87
4	20	56	-39
-5	21	32	26
-4	21	40	-36
-3	21	136	-133
-2	21	136	-131
-1	21	34	37
0	21	104	-110
1	21	37	59
3	21	45	-43
4	21	74	79
5	21	77	69
-5	22	50	-49
-4	22	35	42
-3	22	36	-34
0	22	79	-68
1	22	50	57
2	22	152	-154
3	22	43	37
-4	23	29	-36
-3	23	39	-43
-2	23	152	151
-1	23	125	124
1	23	35	32
2	23	36	-32
4	23	43	46
-3	24	27	-23
-2	24	52	35
1	24	111	-104
2	24	58	57
-2	25	65	71
0	25	35	-27
1	25	104	-102
2	25	93	-93
L = 2**			
-9	0	53	43
-8	0	40	1
-6	0	364	-364
-5	0	284	280
-4	0	582	-574
-3	0	758	773
-2	0	197	196
-1	0	451	439
0	0	91	40
1	0	1416	-1445
2	0	335	-329
3	0	1054	1062
4	0	544	531
5	0	390	381
6	0	379	375
7	0	130	-135
8	0	242	-236
9	0	208	208
-9	1	162	166
-8	1	548	568
-7	1	192	192
-6	1	218	208
-5	1	292	-285
-4	1	191	-190
-3	1	344	344
-2	1	189	183
-1	1	410	-419
0	1	1451	1465
1	1	298	294
2	1	103	96
3	1	19	-9
4	1	45	-45
5	1	316	314
6	1	309	310
7	1	165	-169
8	1	435	438
9	1	74	-73
-9	2	46	40
-8	2	46	34
-7	2	194	197
-6	2	404	397
-5	2	271	-263
-4	2	342	340
-3	2	335	-341
-2	2	110	108
-1	2	406	391
0	2	239	248
1	2	1331	-1394
2	2	255	-259
3	2	131	-128
4	2	422	-419
6	2	215	-208
7	2	87	-75
9	2	110	88
-8	3	120	128
-6	3	93	-86
-5	3	302	-295
-4	3	132	124
-3	3	209	212
-2	3	331	327
-1	3	1608	-1675
0	3	554	545
1	3	1276	1340
2	3	92	76
3	3	60	58
4	3	53	50
5	3	159	153
6	3	169	-159
7	3	101	97
9	3	106	115
-9	4	134	-132
-8	4	99	-92
-6	4	76	-78
-5	4	555	-558
-4	4	245	-245
-3	4	30	35
-2	4	490	-483
-1	4	1166	1193
0	4	401	399
1	4	226	230
2	4	370	375
3	4	145	149
4	4	173	173
5	4	231	-229
6	4	100	89
7	4	258	-265
8	4	161	154
9	4	31	-48
-8	5	385	-390
-7	5	95	-86
-6	5	88	-89
-5	5	157	152
-4	5	119	110
-3	5	393	400
-2	5	278	-278
-1	5	740	-740
0	5	1894	-1988
1	5	515	523
2	5	138	-137
3	5	59	55
4	5	298	296
5	5	474	-472
6	5	104	-98
7	5	100	87
8	5	319	-325
9	5	65	-72
-9	6	29	-40
-8	6	49	50
-7	6	56	65
-6	6	213	-210
-3	6	208	199
-2	6	316	315
-1	6	147	-148
0	6	85	-83
1	6	617	-613
2	6	499	-500
3	6	248	244
4	6	118	111
5	6	211	212
6	6	139	133
7	6	59	-52
8	6	165	-166
9	6	46	57
-9	7	43	50
-8	7	158	156
-7	7	106	-89
-6	7	95	87
-5	7	55	61
-4	7	378	-380
-3	7	386	386
-2	7	345	347
-1	7	266	268
0	7	425	415
1	7	805	-822
2	7	101	101
3	7	202	203
4	7	257	-248
5	7	370	-373
6	7	127	115
7	7	117	108
8	7	153	156
9	7	40	-39
-9	8	94	-88
-7	8	128	136
-6	8	242	237
-5	8	202	198
-4	8	64	54
-3	8	163	-160
-2	8	187	-186
-1	8	788	791
0	8	56	-72
1	8	193	199
2	8	137	133
3	8	259	-259
4	8	80	-74
5	8	328	327
6	8	179	-174
7	8	63	70
8	8	51	-46
9	8	81	-85
-9	9	41	-49
-8	9	132	130
-7	9	34	-31
-6	9	73	-73
-4	9	48	49
-3	9	125	-116
-2	9	104	104
-1	9	130	-131
0	9	825	842
1	9	189	197
2	9	33	-42
3	9	514	513
4	9	72	86
5	9	213	-217
6	9	141	-138
7	9	157	157
8	9	106	119
9	9	116	117
-9	10	54	56
-8	10	118	-127
-6	10	37	36
-4	10	31	36
-3	10	363	-361
-2	10	23	-18
-1	10	81	-87
0	10	157	152
1	10	53	-48
2	10	132	134
3	10	276	-274
4	10	64	-60
5	10	28	11
7	10	73	-64
8	10	159	148
-8	11	104	-99
-7	11	100	120
-5	11	120	-127
-4	11	322	314
-3	11	128	128
-2	11	310	-307
-1	11	22	-7
0	11	316	-314
1	11	155	-152
2	11	256	-258
3	11	195	208
4	11	339	341
5	11	48	-37
6	11	102	-98
7	11	106	-97
8	11	76	-73
-6	12	175	-172
-4	12	30	32
-3	12	98	-108
-2	12	42	48
-1	12	177	-177
1	12	179	-180
2	12	137	-134
3	12	190	-195
4	12	25	25
5	12	60	57
6	12	142	155
7	12	33	-30
-7	13	36	37
-6	13	72	71
-5	13	164	-165
-4	13	168	-172
-3	13	126	121
-1	13	91	89
0	13	216	-209
1	13	301	-298
3	13	47	63
4	13	109	-124
5	13	57	66
6	13	96	95
7	13	31	-7
8	13	32	34
-8	14	99	96
-6	14	64	58
-3	14	71	62
-2	14	142	-145
-1	14	483	473
0	14	53	-50
1	14	374	365
2	14	73	73
5	14	78	81
6	14	67	-60
7	14	75	74
8	14	79	-80
-7	15	41	40
-4	15	212	-211
-3	15	24	7
-2	15	223	224
-1	15	65	-61
0	15	131	136
1	15	160	148
2	15	197	202
3	15	31	12
4	15	188	-188
5	15	70	-75
6	15	28	9
-7	16	68	50
-6	16	74	80
-5	16	72	-87
-3	16	52	-49
-2	16	78	79
-1	16	239	-228
1	16	104	-96
4	16	58	-64
5	16	108	-99
6	16	54	-55
-7	17	33	-17
-6	17	30	25
-5	17	99	-99
-4	17	52	53
-3	17	117	112
0	17	43	41
1	17	63	-54
3	17	96	-89
4	17	37	40
5	17	63	58
7	17	47	-33
-6	18	36	-36
-5	18	51	-51
-4	18	59	-58
-3	18	78	85
-1	18	34	34
1	18	53	64
3	18	39	-48
6	18	69	69
-6	19	30	18
-4	19	105	101
-3	19	96	99
-2	19	110	-113
-1	19	69	56
0	19	56	-50
2	19	80	-75
3	19	55	-50
4	19	129	136
5	19	40	36
6	19	47	46
-6	20	48	31
-4	20	81	88
-1	20	80	-80
1	20	98	-100
2	20	38	-40
3	20	95	-89
4	20	45	-34
5	20	102	97
-4	21	55	-60
-3	21	118	-106
-2	21	41	41
0	21	34	34
3	21	74	77
4	21	99	-107
-4	22	59	-62
-3	22	46	42
-2	22	73	-73
-1	22	51	45
1	22	46	44
3	22	97	87
4	22	70	59
-4	23	64	-72
-3	23	59	-61
-1	23	30	32
1	23	108	-105
3	23	63	57
4	23	32	-25
-3	24	67	-65
-2	24	32	33
-1	24	55	54
1	24	38	-25
2	24	29	-30
3	24	43	-39
-1	25	35	32
0	25	28	34
L = 3**			
-9	1	155	-170
-8	1	43	-41
-7	1	33	-36
-5	1	117	-106
-4	1	171	169
-2	1	203	192
-1	1	422	-421
1	1	233	-231
2	1	54	-64
3	1	101	-91
4	1	182	182
5	1	209	203
6	1	27	-7
8	1	62	-61
9	1	111	101
-9	2	86	-80
-8	2	45	-22
-7	2	171	161
-6	2	50	66
-5	2	276	269
-4	2	205	-201
-3	2	303	-304
-2	2	110	108
-1	2	569	-565
0	2	113	109
1	2	753	-749
2	2	49	-36
3	2	151	-147
5	2	144	-137
6	2	73	-69
7	2	96	85
8	2	83	68
9	2	279	-285
-9	3	222	235
-8	3	27	-20
-7	3	45	-20
4	2	51	-60
-5	3	322	321
-4	3	166	-167
-3	3	154	154
-2	3	91	103
-1	3	401	397
0	3	235	231
1	3	272	274
2	3	102	105
3	3	49	61
4	3	103	-108
5	3	456	-436
6	3	33	-25
7	3	91	-80
9	3	37	-33
-8	4	203	-207
-7	4	76	-61
-6	4	128	129
-5	4	397	-392
-4	4	38	53
-3	4	84	-87
-2	4	345	-348
-1	4	265	269
0	4	338	-339
1	4	78	74
2	4	198	-195
3	4	366	367
4	4	64	65
5	4	86	-82
6	4	158	-149
8	4	94	103
9	4	96	106
-9	5	71	66
-7	5	58	-57
-6	5	215	-207
-5	5	50	-52
-4	5	101	-89
-3	5	548	-550
-2	5	244	-237
-1	5	325	324
0	5	701	-700
1	5	81	92
2	5	373	-373
3	5	415	408
5	5	223	222
6	5	28	-4
7	5	57	48
8	5	200	-200
9	5	37	-33
-9	6	38	-35
-8	6	113	111
-7	6	127	130
-6	6	104	103
-5	6	195	194
-4	6	65	63
-3	6	266	267
-2	6	109	103
-1	6	506	499
0	6	573	586
1	6	470	467
2	6	115	-120
3	6	193	-197
4	6	153	154
7	4	72	66
5	6	27	33
6	6	86	90
7	6	76	66
8	6	56	66
9	6	76	88
-9	7	68	-76
-8	7	207	208
-7	7	84	-80
-6	7	127	126
-5	7	33	27
-4	7	284	283
-3	7	300	297
-2	7	312	-313
-1	7	411	-408
0	7	288	283
1	7	354	-360
2	7	23	23
3	7	367	-363
4	7	215	223
5	7	47	-35
6	7	134	149
7	7	79	-83
8	7	67	66
-9	8	64	-54
-8	8	90	-77
-7	8	35	-24
-6	8	76	-80
-5	8	55	-44
-4	8	57	-69
-3	8	207	-213
-2	8	167	-162
-1	8	267	-270
0	8	556	556
1	8	367	-362
2	8	309	309
3	8	126	-130
4	8	156	-158
5	8	85	84
6	8	79	-60
7	8	70	-76
8	8	59	-65
9	8	65	-81
-8	9	45	40
-6	9	63	-55
-5	9	205	-209
-4	9	96	-105
-3	9	194	189
-2	9	245	252
0	9	1094	1100
1	9	321	319
2	9	192	189
5	9	129	126
6	9	31	-22
7	9	75	77
-8	10	145	-147
-7	10	48	46
-6	10	26	-32
-4	10	45	-42
-3	10	74	-80
-2	10	761	-759
-1	10	324	316
0	10	463	-468
1	10	70	-72
2	10	191	189
3	10	82	86
4	10	84	-72
5	10	85	-86
6	10	36	41
7	10	85	-90
8	10	81	-88
-8	11	137	-143
-7	11	198	199
-6	11	28	-34
-4	11	308	-306
-2	11	218	210
-1	11	198	194

analysis of the molecules in terms of least-squares planes and interplanar angles is presented in Table 6 and in terms of internal-rotation angles in Table 7.

The existence of conformational isomers in large rings has been observed previously in the structure of cyclo(hexaglycyl) (Karle & Karle, 1963) and in such

Table 5 (*cont.*)

H	K	FOBS	FCAL
**L =		3****	
0	11	-681	-693
1	11	151	-145
2	11	690	-697
4	11	199	-208
5	11	85	-95
6	11	73	-60
7	11	73	-70
8	11	143	-136
-8	12	91	99
-7	12	37	-52
-6	12	93	105
-5	12	52	46
-4	12	323	325
-3	12	211	-212
-2	12	503	495
-1	12	93	85
0	12	395	399
1	12	48	38
2	12	406	-399
3	12	26	-9
4	12	123	-119
5	12	55	66
6	12	112	115
7	12	118	121
-8	13	61	-61
-7	13	163	-157
-6	13	361	361
-5	13	46	-50
-4	13	320	-313
-3	13	80	81
-2	13	133	124
-1	13	80	-83
0	13	237	244
1	13	236	-237
2	13	187	179
3	13	181	183
4	13	173	171
5	13	36	-11
6	13	117	112
8	13	36	-45
-6	14	57	-51
-5	14	82	88
-4	14	37	-35
-3	14	155	158
-2	14	93	-86
0	14	78	80
1	14	74	-63
2	14	93	-92
4	14	196	193
5	14	115	124
6	14	41	-36
7	14	28	-30
-8	14	30	30
-7	15	29	21
-6	15	236	239
-5	15	145	-144
-4	15	141	-133
-3	15	125	128
-2	15	35	-24
0	15	245	242
1	15	24	-27
2	15	136	-133
4	15	199	212
5	15	28	-6
6	15	33	53
7	15	26	-26
-7	16	30	-19
-6	16	35	-28
-5	16	64	-68
-4	16	163	-170
-3	16	26	-32
-2	16	108	-106
-1	16	85	-81
0	16	128	-124
2	16	90	88
4	16	152	166
5	16	30	-82
6	16	231	-229
7	16	85	-81
-7	17	140	136
-6	17	177	-182
-5	17	105	-102
-3	17	42	-48
-2	17	27	15
-1	17	26	-32
0	17	50	-46
1	17	64	67
2	17	395	-394
3	17	96	93
4	17	90	87
5	17	44	53
6	17	139	-138
-5	18	54	46
-4	18	122	-118
-3	18	29	-19
-2	18	318	307
-1	18	55	-53
0	18	48	-34
2	18	66	-68
3	18	40	-45
4	18	41	50
5	18	99	-110
6	18	34	42
-5	19	73	81
-3	19	117	121
-2	19	40	35
-1	19	27	29
0	19	91	79
1	19	58	-57
2	19	29	24
3	19	51	46
4	19	65	59
5	19	96	-93
6	19	31	-33
-5	20	26	-9
-3	20	123	132
-2	20	171	174
-1	20	69	80
0	20	119	-113
1	20	58	46
2	20	30	-42
3	20	99	104
5	20	41	42
-4	21	50	-51
-2	21	66	61
0	21	59	-58
1	21	125	-127
2	21	103	106
3	21	50	-44
-3	22	75	-69
-2	22	40	-34
-1	22	130	-124
0	22	81	-74
2	22	70	68
3	22	47	-38
4	22	26	18
-3	23	39	-39
-2	23	65	65
-1	23	33	-32
0	23	143	-136
1	23	105	114
3	23	71	67
-2	24	37	30
-1	24	29	-14
1	24	34	34
2	24	29	29
**L =		4****	
-9	0	39	27
-8	0	348	-341
-7	0	119	-115
-6	0	116	-113
-5	0	87	84
-4	0	185	-186
-3	0	507	-498
-2	0	650	-660
-1	0	249	-244
0	0	672	-674
1	0	71	56
2	0	265	-262
3	0	35	-12
4	0	169	170
5	0	366	-358
6	0	99	-90
7	0	34	33
8	0	215	-214
-6	1	44	40
-5	1	510	496
-4	1	398	392
-3	1	545	532
-2	1	332	321
-1	1	34	18
0	1	150	-144
1	1	171	164
2	1	605	-613
3	1	694	699
4	1	343	-338
5	1	305	296
6	1	25	-15
7	1	53	41
8	1	135	-129
-9	2	34	48
-8	2	135	137
-7	2	32	28
-6	2	40	-36
-5	2	56	57
-4	2	106	102
-3	2	352	343
-2	2	352	344
-1	2	108	109
0	2	280	280
1	2	218	-218
2	2	238	231
3	2	84	-82
4	2	72	-72
5	2	63	60
6	2	87	-100
7	2	93	-90
8	2	124	117
-6	3	127	-126
-5	3	126	114
-4	3	86	-87
-2	3	165	160
-1	3	224	210
0	3	43	68
1	3	70	78
2	3	176	-176
3	3	121	-121
4	3	104	101
5	3	38	-33
6	3	63	59
8	3	69	-60
-9	4	66	-70
-8	4	287	295
-6	4	79	72
-5	4	285	-274
-3	4	112	-109
-2	4	463	457
-1	4	98	-93
0	4	332	317
1	4	381	395
2	4	182	186
3	4	295	298
4	4	44	-29
5	4	390	382
6	4	134	126
7	4	35	29
8	4	222	219
-8	5	107	110
-7	5	37	30
-6	5	154	146
-5	5	428	-425
-4	5	50	-55
-3	5	532	-527
-2	5	58	-61
-1	5	234	-230
0	5	435	437
1	5	123	134
2	5	159	165
3	5	351	-350
5	5	194	-195
6	5	29	-21
7	5	79	80
8	5	42	39
-9	6	69	-68
-8	6	133	-134
-7	6	158	169
-5	6	278	277
-4	6	38	-27
-3	6	44	65
-2	6	135	-128
-1	6	361	355
0	6	1372	-1415
1	6	360	-357
2	6	113	-118
3	6	261	-262
4	6	52	63
5	6	373	-375
6	6	92	-88
7	6	66	-62
8	6	104	-102
-9	7	121	-133
-6	7	110	-114
-5	7	181	187
-3	7	293	282
-2	7	192	-184
-1	7	54	-54
1	7	24	46
2	7	118	-112
3	7	168	175
4	7	63	-56
5	7	45	-44
6	7	163	169
7	7	90	-94
8	7	62	-54
-8	8	44	32
-7	8	126	-129
-6	8	122	-125
-5	8	125	-130
-4	8	29	32
-3	8	237	-226
-2	8	515	506
-1	8	402	417
0	8	646	-638
1	8	517	-522
2	8	459	464
3	8	200	195
4	8	61	57
5	8	59	65
6	8	136	-132
7	8	33	32
8	8	54	26
-8	9	67	63
-7	9	50	57
-6	9	88	-88
-5	9	198	203
-4	9	37	-53
-1	9	63	60
0	9	234	-232
1	9	233	-225
3	9	79	80
4	9	79	67
5	9	179	190
6	9	109	112
7	9	170	179
8	9	129	-126
-8	10	162	152
-7	10	101	98
-6	10	146	-144
-5	10	35	-36
-4	10	196	-196
-3	10	147	-141
-2	10	381	377
-1	10	28	25
0	10	405	401
1	10	83	70
2	10	34	22
3	10	66	63
5	10	134	136
6	10	63	-55
8	10	41	35
-6	11	92	97
-5	11	132	-139
-4	11	146	138
-3	11	101	-102
-2	11	37	-48
-1	11	220	225
0	11	107	98
1	11	171	163
2	11	230	232
3	11	43	41
4	11	291	-290
5	11	139	-149
8	11	51	57
-7	12	135	137
-6	12	73	-71
-4	12	146	146
-3	12	141	146
-2	12	200	-183
-1	12	118	-125
0	12	127	-128
1	12	262	259
2	12	303	-303
3	12	207	-216
4	12	242	255
5	12	43	62
-7	13	40	-45
-6	13	123	-127
-5	13	170	-175
-4	13	193	201
-3	13	87	87
-2	13	113	-97
-1	13	162	-164
1	13	44	-47
2	13	60	71
4	13	207	-211
5	13	144	-146
6	13	91	73
7	13	130	-119
-7	14	106	-114
-6	14	27	10
-5	14	170	-162
-4	14	238	231
-3	14	86	84
-1	14	28	27
0	14	29	-26
3	14	90	-97
4	14	293	297
5	14	158	162
-7	15	110	114
-6	15	135	-132
-4	15	126	127
-3	15	137	141
-2	15	28	-33
-1	15	137	-145
0	15	62	-59
1	15	129	-127
4	15	114	112
5	15	165	170
7	15	110	124
-7	16	76	67
-5	16	183	183
-4	16	192	-197
-2	16	33	-38
-1	16	91	87
0	16	42	-29
1	16	143	-142
2	16	235	-239
3	16	43	-44
4	16	110	-111
5	16	145	-144
6	16	41	39
-5	17	50	40
-3	17	72	75
-2	17	193	-208
-1	17	146	145
1	17	81	77
2	17	102	115
3	17	44	44
4	17	29	12
5	17	51	-54
6	17	52	-51
-5	18	60	-63
-3	18	201	-205
-2	18	90	95
-1	18	56	-47
0	18	60	75
1	18	52	53
2	18	106	106
3	18	201	198
5	18	35	36
6	18	26	-18
-4	19	46	40
-3	19	109	-103
-2	19	69	63
-1	19	31	-23
1	19	55	-54
2	19	33	23
3	19	37	55
4	19	53	-52
-4	20	76	79
-3	20	122	127
-1	20	46	38
1	20	29	-28
2	20	72	76
3	20	107	-107
4	20	64	63
5	20	29	37
-4	21	57	-54
-2	21	79	84
0	21	46	-36
1	21	47	-63
2	21	40	53
3	21	77	-71
4	21	75	74
-2	22	65	-69
0	22	33	-33
1	22	46	40
2	22	84	-66
3	22	49	-41
0	23	31	-45
1	23	46	37
2	23	38	-34
**L =		5****	
-9	1	53	46
-7	1	140	149
-5	1	59	-62
-4	1	53	47
-3	1	25	-5
-2	1	41	41
-1	1	215	213
1	1	263	260
2	1	38	35
5	1	34	47
7	1	102	110
-9	2	170	-196
-7	2	86	-93
-6	2	98	-105
-5	2	91	-93
-4	2	109	113
-3	2	65	49
-2	2	161	159
-1	2	291	-293
0	2	74	70
1	2	48	40
2	2	56	58
3	2	58	-57
4	2	88	105
5	2	176	176
6	2	77	-80
7	2	60	-80
-9	3	102	-104
-8	3	45	64
-7	3	63	-72
-5	3	44	52
-4	3	162	-168
-3	3	23	-16
-2	3	135	137
-1	3	257	-252
0	3	26	33
1	3	541	-542
2	3	134	-132
3	3	64	53
4	3	62	67
5	3	55	55
6	3	65	65
7	3	143	-140
-8	4	74	62
-6	4	118	114
-5	4	140	-143
-4	4	69	-64
-3	4	218	-210
-2	4	164	-160
-1	4	481	478
0	4	218	215
1	4	100	-91
3	4	47	-45
4	4	82	-75
5	4	50	52
6	4	81	80
-8	5	162	-168
-7	5	42	-31
-5	5	73	-73
-4	5	78	80
-3	5	260	-256
-2	5	261	-261
-1	5	312	310
0	5	169	-171
1	5	51	-64
2	5	251	249
3	5	168	-172
5	5	119	-119
6	5	98	-105
7	5	101	-96
-8	6	40	-51
-7	6	82	78
-6	6	126	-126
-5	6	191	193
-4	6	113	105
-3	6	136	-126
-2	6	254	243
-1	6	471	480
0	6	353	-342
1	6	212	-195
2	6	36	-20
3	6	176	177
4	6	91	85
5	6	94	-86
6	6	60	-66
-8	7	87	89
-7	7	42	-31
-6	7	68	76
-5	7	50	49
-4	7	98	102
-3	7	138	136
-2	7	276	275
-1	7	475	472
1	7	208	220
2	7	361	-353
3	7	57	60
4	7	141	-142
5	7	120	113
6	7	59	-63
7	7	72	-69
-8	8	28	-40
-7	8	39	34
-6	8	91	-84
-4	8	163	-172
-3	8	193	194
-2	8	113	-121
-1	8	26	-31
0	8	178	-169
1	8	420	-434
2	8	116	120
3	8	91	-80
-6	9	99	-91
-5	9	33	29
-4	9	202	-203
-3	9	129	125
-2	9	57	-60
-1	9	217	-205
0	9	127	147
1	9	343	-340
2	9	192	199
3	9	179	175
4	9	267	274
5	9	209	218
6	9	168	177
7	9	89	-88
-8	10	191	189
-7	10	76	83
-6	10	307	312
-5	10	403	-406
-4	10	125	123
-3	10	149	148
-2	10	26	26
-1	10	27	-20
0	10	182	177
1	10	60	-66
2	10	54	59
3	10	46	-39
4	10	103	-89
5	10	163	170
6	10	113	115
-8	11	116	-109
-7	11	88	90
-6	11	132	135
-5	11	140	-144
-4	11	264	261
-3	11	39	-39
-2	11	118	-112
-1	11	278	-275
0	11	115	-117
1	11	326	-323
2	11	111	110
3	11	125	127
4	11	223	-217
5	11	196	-190
6	11	275	-291
7	11	36	-26
-7	12	162	163
-6	12	316	-324
-5	12	32	-29
-4	12	59	-54
-3	12	44	-39
-2	12	101	100
-1	12	58	55
0	12	139	-134
1	12	191	194
3	12	239	239
4	12	102	104
5	12	136	-131
6	12	129	-140
7	12	103	-99
-7	13	32	-26
-6	13	114	-119
-5	13	204	-210
-4	13	165	-171
-3	13	288	286
-2	13	83	-83
-1	13	91	88
1	13	27	-33
2	13	27	-21
3	13	273	266
4	13	108	99
5	13	217	-226
6	13	189	182
7	13	51	36
-7	14	104	-95
-6	14	104	91
-5	14	137	139
-3	14	128	-127
-2	14	40	-38
-1	14	72	66
0	14	76	-84
1	14	212	-216
2	14	61	-70
3	14	173	168
4	14	57	-58
5	14	133	-137
-5	15	98	-100
-4	15	160	158
-3	15	327	323
-2	15	102	112
0	15	85	84
2	15	89	-99
3	15	166	175
4	15	95	-113
5	15	29	-22
-6	16	125	130
-5	16	92	85
-4	16	65	-64
-3	16	45	38
-1	16	28	20
0	16	181	180
1	16	103	-112
2	16	96	112
3	16	50	-43
5	16	43	-54
6	16	62	61
-6	17	25	14
-5	17	38	-39
-4	17	97	95
-3	17	37	34
-2	17	154	-163
-1	17	153	-161
0	17	49	-68
1	17	40	-56
2	17	141	139
4	17	31	-21
5	17	29	-16
-5	18	57	54
-3	18	55	58
-1	18	213	-208
0	18	108	-116
1	18	250	252
2	18	64	-70
3	18	54	-58
4	18	68	69
5	18	42	-41
-5	19	51	-50
-4	19	98	-96
-1	19	70	-64
1	19	52	-47
2	19	27	22
3	19	39	33
4	19	55	57
-3	20	50	49
-1	20	146	-147
0	20	42	28
1	20	160	162
2	20	52	-51
3	20	40	-22
-3	21	35	27
-2	21	59	60
-1	21	99	93
2	21	49	-54
-2	22	27	-24
-1	22	37	-28
0	22	54	62
**L =		6****	
-8	0	96	79
-7	0	84	-87
-6	0	73	60
-5	0	415	-419
-4	0	210	-209
-3	0	37	-43
-2	0	70	-68
-1	0	310	-315
0	0	195	184
1	0	123	120
2	0	140	124
3	0	206	-214
4	0	106	101
5	0	225	-229
6	0	51	-59
-8	1	134	-133
-6	1	34	-25
-3	1	117	-113
-2	1	107	-100
-1	1	43	30
0	1	312	-318
1	1	160	-156
2	1	48	41
3	1	40	-35
4	1	94	85
5	1	172	-172
6	1	30	-26
-8	2	36	34
-6	2	27	21
-5	2	106	104
-4	2	80	98
-3	2	174	178
-2	2	176	180
-1	2	177	-178
1	2	74	-63
2	2	186	-174
3	2	48	52
4	2	84	-85
6	2	45	-31
-8	3	63	75
-7	3	126	-137
-5	3	26	7
-4	3	48	55
-3	3	180	-183
-2	3	105	113
-1	3	202	-197
0	3	353	-360
1	3	45	36
2	3	53	68
3	3	45	41
4	3	63	-61
5	3	53	-52
6	3	38	-45
-8	4	30	-34
-7	4	29	-28
-6	4	173	-173
-5	4	299	294
-4	4	103	-112
-3	4	156	164
-2	4	77	70
-1	4	74	-71
0	4	274	-265
1	4	31	34
2	4	33	-42
3	4	245	247
4	4	147	158
5	4	155	167
6	4	91	94
-8	5	167	160
-7	5	35	27
-6	5	45	-43
-5	5	172	172
-4	5	31	-47
-3	5	239	237
-2	5	348	350
-1	5	259	-241
0	5	155	155
1	5	175	169
2	5	144	141
3	5	83	-93
5	5	167	168
6	5	156	158
-8	6	90	94
-7	6	159	-164
-6	6	164	164
-5	6	214	-213
-2	6	96	92
-1	6	119	126
0	6	77	-87
1	6	444	427
2	6	261	257
3	6	152	-146
5	6	252	-263
6	6	96	-112
-8	7	66	-71
-7	7	83	-76
-6	7	85	-87
-5	7	108	-109
-4	7	104	-97
-2	7	111	-100
-1	7	66	60
0	7	116	-121
1	7	257	259
2	7	144	-136
3	7	83	91
4	7	31	-23
5	7	69	73
6	7	70	-70
-8	8	48	-41
-7	8	58	51
-6	8	33	-23
-5	8	93	-88
-3	8	199	-208
-2	8	24	-5
-1	8	444	-441
0	8	110	-119
1	8	37	17
2	8	98	91
3	8	156	-157
4	8	154	-154
5	8	60	51
6	8	38	-36
-7	9	72	-65
-5	9	228	225
-4	9	185	190
-3	9	71	-62
-2	9	107	-119
-1	9	153	142
0	9	49	48
1	9	332	-328
2	9	70	77
3	9	220	-220
4	9	134	142
5	9	208	-213
6	9	90	-97
-6	10	217	-223
-5	10	300	306
-4	10	134	142
-3	10	236	243
-2	10	112	123
-1	10	136	-131
0	10	136	-144
2	10	68	-73
3	10	90	88
4	10	129	132
5	10	60	59
-7	11	28	-28
-5	11	71	63
-4	11	52	41
-3	11	159	-152
-1	11	188	192
0	11	193	199
1	11	187	-188
2	11	110	-109
3	11	159	164
5	11	111	103
6	11	91	88
-7	12	51	-50
-5	12	95	92
-4	12	126	172
-3	12	37	-43
-1	12	177	174
0	12	34	22
1	12	70	62
2	12	33	2
3	12	60	50
4	12	52	56
5	12	140	-132
6	12	85	-86
-5	13	81	-84
-4	13	63	-58
-3	13	195	-199
-2	13	135	-133
0	13	90	-87
1	13	185	184
2	13	118	-110
3	13	143	149
4	13	168	-180
5	13	152	152
-5	14	117	-117
6	13	31	35
-4	14	118	-117
-3	14	250	-261
-2	14	144	-138
-1	14	67	-60
2	14	54	59
3	14	88	93
5	14	112	-96
6	14	43	-42
-6	15	46	33
-5	15	101	103
-4	15	112	124
-3	15	125	119
0	15	35	22
1	15	31	21
2	15	300	315
3	15	344	-337
4	15	61	65
5	15	43	-27
-4	16	29	21
-3	16	203	206
-2	16	170	184
-1	16	70	-78
0	16	47	-48
2	16	30	-51
3	16	67	55
4	16	68	58
5	16	120	-114
-5	17	85	-86
-4	17	37	-30
-1	17	63	64
0	17	35	-32
2	17	33	-31
3	17	29	-39
4	17	76	-81
5	17	55	47
-4	18	78	-79
-3	18	64	65
-2	18	26	6
0	18	31	-19
3	18	36	43
4	18	64	63
-3	19	71	-69
-2	19	32	-37
1	19	51	18
2	19	47	-41
3	19	40	31
-3	20	46	-49
0	20	40	41
1	20	56	-42
2	20	47	-16
1	21	36	52
**L =		7****	
-8	1	55	-51
-7	1	26	17
-6	1	32	-25
-4	1	63	63
-3	1	104	-104
-2	1	249	254
-1	1	204	214
0	1	64	-60
1	1	123	-121
2	1	114	100
3	1	70	70
4	1	184	183
5	1	56	-51
-8	2	53	-57
-7	2	77	76
-6	2	57	-63
-5	2	42	45
-4	2	111	-109
-3	2	48	-49
-2	2	69	71
-1	2	333	339
0	2	143	-150
1	2	342	344
2	2	47	-53
3	2	65	-61
4	2	35	20

molecules as cyclononylamine hydrobromide (Bryan & Dunitz, 1960). In the cyclic monomer and dimer of nylon 66 it would appear that the conformation of minimum potential energy is one that is formed of a relatively small number of planar elements each of which consists of an inherently planar amide group, a

Table 5 (*cont.*)

H	K	FOBS	FCAL
**L =		7****	
1	3	86	76
2	3	111	-117
4	3	163	-160
5	3	42	-54
-7	4	109	-119
-6	4	165	174
-5	4	36	5
-4	4	133	134
-3	4	100	104
-2	4	210	210
-1	4	220	-210
0	4	96	-87
1	4	223	-220
3	4	138	136
4	4	51	-50
5	4	70	63
-6	5	49	51
-5	5	296	-303
-4	5	55	41
-3	5	28	28
-1	5	43	-32
0	5	76	-77
1	5	55	48
2	5	148	149
3	5	48	-53
4	5	76	75
5	5	220	222
-7	6	63	70
-6	6	50	-44
-3	6	130	-131
-2	6	94	-93
-1	6	154	-152
0	6	138	-143
1	6	143	-148
2	6	225	226
3	6	125	-118
4	6	38	39
5	6	65	-72
-7	7	125	123
-6	7	105	-110
-5	7	120	117
-4	7	243	237
-1	7	120	116
2	7	144	139
3	7	29	-38
4	7	121	126
5	7	143	-152
-6	8	146	-154
-5	8	106	-109
-4	8	79	-77
-2	8	158	-159
-1	8	191	177
0	8	83	-82
1	8	229	229
2	8	131	135
4	8	63	-60
5	8	65	-92
-7	9	74	-83
-6	9	94	-109
-5	9	95	88
-4	9	43	-41
-3	9	135	-139
-2	9	208	-206
-1	9	66	-66
0	9	117	-118
2	9	91	-92
3	9	179	190
4	9	218	-220
5	9	53	-54
-5	10	86	86
-4	10	245	250
-2	10	108	107
-1	10	37	40
0	10	53	54
1	10	26	32
2	10	61	61
3	10	141	144
4	10	175	-178
5	10	117	115
-6	11	55	55
-5	11	90	-87
-2	11	172	187
-1	11	82	84
0	11	268	268
1	11	192	-203
2	11	314	324
3	11	149	-151
4	11	143	-147
5	11	41	36
-5	12	46	-38
-4	12	63	64
-3	12	214	-217
-2	12	111	-123
-1	12	158	-170
0	12	101	-98
1	12	95	-86
2	12	85	93
3	12	128	-128
4	12	50	-34
-6	13	97	94
-4	13	29	17
-3	13	30	-22
-2	13	122	-126
-1	13	73	-70
0	13	199	-212
1	13	194	200
2	13	36	-48
3	13	73	77
4	13	70	-60
-2	14	28	20
0	14	32	-8
2	14	42	-47
4	14	55	-56
5	14	57	-60
-5	15	87	75
-4	15	69	66
-2	15	147	-140
-1	15	37	3
1	15	28	-16
-4	16	104	-97
-3	16	109	111
-2	16	78	74
-1	16	83	82
0	16	71	82
1	16	62	61
2	16	48	-47
3	16	63	65
4	16	74	67
-4	17	81	84
-3	17	27	-25
-2	17	50	-56
-1	17	66	68
0	17	190	204
1	17	109	-108
2	17	43	43
-3	18	66	-56
-2	18	30	-33
-1	18	48	-46
3	18	66	-66
-2	19	56	-56
-1	19	41	-32
0	19	40	-48
1	19	74	76
**L =		8****	
-7	0	121	-123
-6	0	78	78
-4	0	129	-137
-3	0	143	135
-2	0	92	-88
-1	0	356	-355
0	0	222	220
1	0	268	264
2	0	95	-99
3	0	75	69
-7	1	116	-109
-6	1	221	227
-5	1	265	-264
-3	1	81	-87
-2	1	55	-39
-1	1	48	-49
0	1	33	33
1	1	200	192
3	1	75	-70
4	1	127	-124
-3	2	147	151
-2	2	88	-82
-1	2	127	-134
0	2	154	153
1	2	112	114
4	2	56	-57
-7	3	30	32
-6	3	37	31
-5	3	95	-105
-3	3	87	-93
-2	3	67	63
-1	3	182	-181
0	3	80	76
1	3	125	130
2	3	30	20
3	3	160	-157
-7	4	78	-71
-6	4	80	70
-3	4	59	-52
-2	4	212	-215
-1	4	48	-52
1	4	147	-144
3	4	74	-69
4	4	48	46
-6	5	94	-93
-5	5	310	322
-4	5	37	21
-3	5	148	153
-2	5	143	150
-1	5	38	29
0	5	29	-43
1	5	98	101
2	5	189	-200
3	5	50	42
4	5	122	114
-6	6	57	66
-5	6	32	28
-3	6	48	54
-2	6	91	92
-1	6	108	110
0	6	52	62
2	6	95	-88
3	6	142	149
-6	7	117	112
-5	7	81	79
-4	7	52	-47
-3	7	159	-169
-2	7	87	-88
0	7	77	80
1	7	58	-57
3	7	48	-41
4	7	69	75
-6	8	67	-66
-5	8	30	20
-4	8	31	-53
0	8	106	-119
1	8	27	0
2	8	37	37
4	8	97	-98
-6	9	82	81
-4	9	181	-183
-3	9	113	-128
-1	9	67	82
0	9	63	-46
2	9	36	51
4	9	51	-53
-5	10	42	-31
-4	10	37	-38
-3	10	114	-121
-2	10	34	-25
-1	10	42	-40
0	10	53	42
1	10	44	48
2	10	118	136
3	10	73	-73
-3	11	45	45
-2	11	128	135
-1	11	52	-59
0	11	51	-65
3	11	64	67
4	11	46	-35
-5	12	27	30
-4	12	67	68
-3	12	49	53
-2	12	39	39
-1	12	27	32
0	12	91	98
2	12	28	-37
3	12	36	-49
4	12	48	42
-4	13	89	91
-3	13	35	31
-2	13	65	52
4	13	27	18
0	13	32	25
3	13	37	-30
-4	14	30	-10
1	13	38	-30
-2	14	58	-61
-1	14	49	-47
0	14	68	-69
1	14	28	19
2	14	128	-131
3	14	39	34
4	14	84	-72
-4	15	33	-35
-3	15	27	9
-2	15	60	-58
-1	15	127	132
1	15	64	70
-3	16	39	36
0	16	29	23
1	16	94	105
2	16	55	60
-2	17	53	-29
-1	17	137	-136
1	17	101	-93
**L =		9****	
-6	1	36	48
-3	1	33	16
-1	1	310	-308
0	1	44	-54
1	1	54	-54
2	1	80	83
-4	2	303	306
-3	2	88	-82
-1	2	117	112
0	2	36	21
1	2	32	-10
2	2	40	43
-6	3	84	-99
-4	3	39	-42
-3	3	61	54
-2	3	87	84
-1	3	188	185
0	3	31	-31
1	3	337	333
2	3	76	-81
-6	4	69	-63
-5	4	30	30
-4	4	134	-127
-3	4	148	-153
-2	4	113	-121
-1	4	48	-53
0	4	93	90
1	4	88	94
2	4	112	-113
3	4	32	32
-5	5	84	73
-4	5	41	52
-3	5	27	-32
-2	5	100	-104
-1	5	59	-55
2	5	91	92
3	5	52	-40
-4	6	73	-69
-3	6	111	109
-2	6	57	48
-1	6	26	22
2	6	70	74
3	6	183	-183
-5	7	47	58
-4	7	95	101
-3	7	50	-42
3	7	33	-45
-4	8	102	96
-3	8	42	42
1	8	43	58
2	8	65	65
3	8	130	-133
-4	9	66	-66
-3	9	115	-118
-1	9	56	-71
0	8	106	-107
1	9	40	-31
2	9	30	-43
3	9	87	-87
-3	10	72	-70
-2	10	41	-52
0	10	87	87
1	10	29	34
2	10	27	-29
3	10	41	31
-4	11	48	-39
-3	11	108	111
-2	11	36	-15
-1	11	58	66
1	11	59	62
2	11	54	61
3	11	54	61
-3	12	26	-29
-2	12	38	-46
-1	12	31	31
1	12	39	-36
-2	13	50	45
-1	13	55	-45
1	13	44	-45
2	13	29	-22
-2	14	47	50
-1	14	27	30
-1	15	45	35
**L =		10****	
-4	0	106	107
-3	0	45	50
-2	0	55	-52
-1	0	54	-65
0	0	91	89
1	0	120	-108
2	0	280	-274
-4	1	39	30
-3	1	83	90
-2	1	229	228
-1	1	45	-37
0	1	32	53
1	1	43	-43
2	1	35	-27
-2	2	70	-66
-1	2	114	106
0	2	239	235
1	2	45	-45
2	2	29	35
-4	3	82	-82
-3	3	30	22
-2	3	48	40
-1	3	65	-63
0	3	201	-192
1	3	74	66
2	3	42	-40
-4	4	133	-134
-3	4	54	-63
-2	4	134	-129
-1	4	53	51
0	4	71	-68
2	4	33	19
-4	5	51	-44
-3	5	31	-37
-2	5	33	34
-1	5	56	-63
2	5	74	75
-3	6	29	8
-2	6	65	66
0	6	68	-79
2	6	31	10
-3	7	127	126
-2	7	105	111
0	7	104	109
1	7	76	-82
2	7	60	-60
-3	8	28	14
-2	8	28	20
-1	8	88	83
0	8	89	85
2	8	78	76
-3	9	32	35
0	9	47	-48
1	9	48	44
2	9	128	-126
-2	10	83	-81
0	10	29	-25

UNOBSERVED REFLECTIONS

H	K	FOBS	FCAL
**L =		0****	
1	0	-12	-7
5	0	21	28
7	0	25	-9
1	1	20	-4
3	1	18	16
5	1	21	-10
7	1	24	-8
9	1	27	-11
3	2	18	-1
4	2	19	19
5	2	21	-10
7	2	25	-12
1	3	14	-1
3	3	28	37
9	3	27	20
3	4	18	7
7	4	25	-9
5	5	23	-9
9	5	26	22
1	6	18	3
5	6	22	21
7	6	26	28
9	6	26	-13
5	7	22	0
9	7	26	-9
0	8	30	-14
5	8	22	-2
5	9	22	2
6	9	25	-14
1	10	19	-0
3	10	21	12
5	10	24	33
9	11	25	9
1	12	21	-14
5	12	24	2
7	12	26	5
3	13	22	6
5	13	24	6
7	13	26	28
8	13	26	29
6	14	26	-14
7	14	26	-5
8	14	26	26
4	15	24	-27
3	16	24	18
1	17	24	-21
5	17	26	-16
1	18	25	20
3	18	25	13
4	18	26	-47
5	18	25	8
1	19	26	-10
5	19	26	14
1	20	26	10
2	20	26	-19
3	20	26	-19
6	20	26	4
1	21	26	7
3	22	26	-8
4	22	26	24
5	22	25	-19
1	23	26	-5
3	23	26	-16
3	24	25	25
1	25	25	6
2	25	26	-29
**L =		1****	
-1	1	13	23
1	1	13	36
-6	2	23	8
9	2	27	18
6	5	23	0
-7	6	25	-22
6	6	24	-1
7	6	25	14
-9	7	26	20
-8	7	27	-14
9	7	26	6
-4	8	22	-8
7	8	26	31
-7	9	26	-3
5	9	23	-34
6	9	24	-12
-3	10	21	3
5	10	23	-6
4	11	22	0
-2	12	22	-6
5	12	24	-15
-6	13	26	-7
8	13	26	-24
-2	14	23	35
3	14	23	20
4	14	24	-5
6	14	26	-18
7	14	26	35
-7	15	26	-28
-3	15	24	36
1	15	23	17
2	15	23	-12
-3	16	24	5
-2	16	24	-12
6	16	26	-7
-5	17	26	14
-1	17	24	-2
3	17	25	15
4	17	26	-31
7	17	25	-6
-2	18	26	20
-6	19	26	2
-3	19	26	-20
-4	20	26	-12
-3	20	26	-11
-2	20	26	8
5	20	26	5
6	20	25	16
2	21	26	-13
-2	22	27	15
-1	22	26	8
4	22	25	-3
5	22	25	22
0	23	26	9
3	23	26	-27
-1	24	26	-3
0	24	25	-5
3	24	25	19
-1	25	33	24
**L =		2****	
-7	0	25	3
5	2	21	23
8	2	28	3
-9	3	27	-20
-7	3	25	-13
8	3	27	27
-7	4	25	11
-9	5	26	-5
-5	6	22	17
-4	6	21	-19
-8	8	27	15
-5	9	23	-29
-7	10	26	16
-5	10	23	8
6	10	25	-2
-6	11	25	-2
-8	12	26	16
-7	12	26	-9
-5	12	24	27
0	12	22	9
8	12	26	-18
-6	13	25	3
-2	13	22	-12
2	13	22	-6
-7	14	26	13
-5	14	25	-5
-4	14	24	-16
3	14	23	3
4	14	25	-1
-6	15	26	-8
-5	15	26	-18
7	15	26	10
-4	16	26	-27
0	16	24	7
2	16	25	4
3	16	25	-2
7	16	26	0
-2	17	25	8
-1	17	25	-24
2	17	25	-10
6	17	26	10
-2	18	41	45
0	18	25	25
2	18	26	23
4	18	27	18
5	18	26	19
-5	19	25	8
1	19	26	-9
-5	20	25	8
-3	20	27	8
-2	20	26	9
0	20	26	-13
-5	21	25	-5
-1	21	26	-6
1	21	26	15
2	21	26	-32
5	21	25	-1
0	22	26	8
2	22	26	7
-2	23	26	-7
0	23	26	-9
2	23	26	28
0	24	26	15
1	25	25	7
**L =		3****	
-6	1	23	31
-3	1	19	18
0	1	18	0
7	1	25	7
-6	3	23	14
8	3	27	14
-9	4	26	2
-8	5	27	20
4	5	21	-18
9	7	25	-2
-9	9	25	2
-7	9	26	2
-1	9	21	-14
3	9	22	-2
4	9	23	12
8	9	26	17
-5	10	24	20
-5	11	24	17
-3	11	22	-1
3	11	23	21
8	12	25	-5
7	13	27	22
-7	14	26	28
-1	14	23	-8
3	14	25	14
-1	15	24	1
3	15	25	-16
1	16	24	-4
3	16	26	6
-4	17	26	-5
-6	18	26	-10
1	18	25	-2
-6	19	24	4
-4	19	26	-8
-4	20	25	-6
4	20	26	-8
-5	21	24	-12
-3	21	26	-31
-1	21	27	14
4	21	26	-9
-4	22	25	-1
1	22	26	-3
2	23	26	-4
0	24	26	-9
**L =		4****	
-9	1	28	-51
-8	1	27	2
-7	1	25	-29
-9	3	25	-2
-8	3	27	-14
-7	3	26	-13
-3	3	21	-4
7	3	26	28
-7	4	26	-10
-4	4	22	-9
-9	5	25	15
4	5	22	-7
-6	6	25	-44
-8	7	26	-2
-7	7	27	-19
-4	7	22	-3
0	7	24	55
-3	9	22	14
-2	9	23	11
2	9	31	-23
4	10	25	-1
7	10	27	9
-8	11	26	-25
-7	11	27	-46
6	11	27	-21
7	11	27	-6
-8	12	26	10
-5	12	27	-7
0	13	24	42
3	13	25	-9
-2	14	24	27
1	14	24	-16
2	14	25	-7
6	14	27	-22
7	14	26	0
-5	15	27	-12
2	15	25	4
3	15	26	5
6	15	27	41
-6	16	26	-4
-3	16	27	-10
-6	17	25	-2
-4	17	27	-1
0	17	26	-26
-6	18	25	-14
-4	18	33	-32
4	18	26	6
-5	19	25	-24
0	19	26	-20
5	19	25	1
-5	20	24	16
-2	20	26	32
0	20	26	-16
-3	21	25	-10
-1	21	26	-2
-3	22	25	1
-1	22	25	-26
-2	23	25	-25
-1	23	25	2
**L =		5****	
-8	1	25	-19
-6	1	24	17
0	1	20	-6
3	1	21	10
4	1	22	-8
6	1	25	-15
-8	2	25	6
-6	3	25	5
-7	4	26	1
2	4	22	-17
7	4	26	6
-6	5	26	-14
4	5	23	14
7	6	26	-24
0	7	22	-1
-5	8	25	-12
4	8	25	-29
5	8	26	17
6	8	26	-2
7	8	26	-36
-8	9	26	-9
-7	9	26	1
7	10	26	22
2	12	24	4
0	13	24	8
-4	14	27	4
6	14	27	-13
-6	15	25	0
-1	15	25	4
1	15	26	-9
6	15	26	34
-2	16	26	17
4	16	27	-11
3	17	27	4
-4	18	26	-12
-2	18	27	44
-3	19	25	-17
-2	19	26	4
0	19	27	26
-4	20	25	19
-2	20	26	-32
4	20	24	-10
0	21	26	-14
1	21	26	9
3	21	25	5
1	22	25	6
2	22	25	13
**L =		6****	
-7	1	25	2
-5	1	25	0
-4	1	27	-4
-7	2	26	-14
0	2	22	-13
5	2	26	26
-6	3	25	0
4	5	25	-19
-4	6	24	-24
-3	6	24	9
4	6	25	-5
-3	7	24	-19
-4	8	25	2
-6	9	29	-15
-7	10	25	6
1	10	25	5
6	10	26	23
-6	11	27	-2
-2	11	25	-7
4	11	27	-15
-6	12	27	18
-2	12	25	-32
-6	13	25	-8
-1	13	25	0
-6	14	25	8
0	14	25	-3
1	14	26	-6
4	14	27	-8
-2	15	27	32
-1	15	26	-25
-5	16	25	-4
1	16	27	-29
-3	17	27	-3
-2	17	26	-14
1	17	26	12
-1	18	26	5
1	18	26	9
2	18	26	-17
-4	19	25	-28
-1	19	26	-5
0	19	26	4
-2	20	25	-2
-1	20	25	7
3	20	25	0
-2	21	24	7
-1	21	25	-14
0	21	25	11
**L =		7****	
-5	1	26	13
5	2	26	2
-2	3	24	-23
3	3	25	-8
2	4	24	26
-7	5	25	17
-2	5	24	-10
-5	6	27	-10
-4	6	26	-3
-3	7	25	32
0	7	24	-17
1	7	25	22
-7	8	29	12
-3	8	25	3
3	8	27	-8
1	9	25	-17
-6	10	26	-26
-4	11	27	-2
-6	12	25	-2
5	12	26	-4
-5	13	25	-10
5	13	26	12
-5	14	25	-11
-4	14	25	-8
-3	14	26	16
-1	14	26	-10
1	14	27	1
3	14	27	19
-3	15	26	-14
0	15	27	10
2	15	27	-9
3	15	27	9
4	15	26	15
3	17	26	-15
0	18	26	-6
1	18	26	-8
2	18	26	-23
2	19	25	-34
**L =		8****	
-5	0	27	-12
4	0	27	-6
2	1	25	1
-7	2	25	6
-6	2	26	2
-5	2	26	14
2	2	26	9
3	2	26	-8
4	3	26	-17
-5	4	26	-12
0	4	25	-27
2	4	26	4
-4	6	26	-11
1	6	25	6
4	6	26	-21
-1	7	26	0
2	7	27	36
-3	8	26	-9
-2	8	27	29
-1	8	26	-13
3	8	27	35
-5	9	25	-6
-2	9	26	-5
1	9	26	21
3	9	27	-43
-6	10	24	15
4	10	26	28
-5	11	25	19
-4	11	25	-17
1	11	26	1
2	11	27	-30
1	12	26	-14
-5	13	24	-27
-1	13	26	12
2	13	26	-10
-3	14	25	-6
0	15	26	-10
2	15	26	0
3	15	25	-11
-2	16	25	5
-1	16	26	20
0	17	25	0
**L =		9****	
-5	1	26	-10
-4	1	27	22
-2	1	27	0
3	1	26	-4
-6	2	25	17
-5	2	25	14
-2	2	27	5
3	2	27	-22
-5	3	25	-2
3	3	26	-8
0	5	27	28
1	5	26	-5
-5	6	25	-4
0	6	26	-8
1	6	26	23
-2	7	26	0
-1	7	26	6
0	7	26	-15
1	7	26	15
2	7	26	7
-5	8	25	-7
-2	8	26	11
-1	8	26	0
-5	9	24	-7
-2	9	26	24
0	9	26	-12
-4	10	25	18
-1	10	26	-29
0	11	26	28
0	12	26	15
2	12	25	-26
3	12	25	4
-3	13	24	-17
0	13	25	-20
0	14	25	20
1	14	25	16
0	15	25	-19
**L =		10****	
-4	2	25	2
-3	2	26	0
1	4	26	1
0	5	26	-11
1	5	27	41
-4	6	25	6
-1	6	27	-39
1	6	26	10
-1	7	26	-9
1	8	26	-21
-2	9	25	-15
-1	9	25	12
-1	10	25	-10
1	10	25	11

planar sequence of methylene groups, or both. Thus within the constraints imposed by its cyclic configuration and the hydrogen bonds binding it to its neighbors the molecule strives to assume the pure planar zigzag conformation that characterizes the linear polymer (Bunn & Garner, 1947; Natta & Corradini, 1960).

Bond distances and angles

The bond distances and angles are listed in Tables 8 and 9. The equivalent bond dimensions in the four amide groups are in general agreement with the idealized values of Corey & Pauling (1953). The spread in the values, however, is rather large, being 0·015 Å for

Table 6. *Analysis of the planar elements in the molecules*

(*a*) Deviations (Å) from the least-squares plane

Plane										
					Molecule I					
P	C(1)	0·020	C(2)	−0·010	C(3)	0·017	N(1)	−0·025	O(1)	−0·002
Q	C(3)	0·049	C(4)	−0·050	C(5)	−0·047	C(6)	0·048		
R	C(6)	−0·014	C(7)	0·014	C(8)	−0·015	N(2)	0·015	O(2)	−0·001
S	C(8)	−0·016	C(9)	0·026	C(10)	0·006	C(11)	−0·025	C(12)	0·009
Plane					Molecule II					
P′	C(1′)	−0·002	C(2′)	0·008	C(3′)	−0·004	N(1′)	0·001	O(1′)	−0·002
Q′	C(3′)	0·032	C(4′)	−0·034	C(5′)	−0·029	C(6′)	0·031		
R′	C(6′)	0·032	C(7′)	−0·019	C(8′)	0·039	N(2′)	−0·049	O(2′)	−0·004
S′	C(8′)	0·042	C(9′)	0·022	C(10′)	−0·101	C(11′)	−0·029	C(12′)	0·066

(*b*) Interplanar angles.
The least-squares plane through the atoms of the ring is indicated by *T*.

	P	*Q*	*R*	*S*	*T*
P	–	49°18′	89°24′	45°58′	69°43′
Q		–	86°28′	10°7′	20°55′
R			–	77°23′	89°7′
S				–	28°11′
T					–

	P′	*Q′*	*R′*	*S′*	*T′*
P′	–	44°	89°6′	81°24′	76°31′
Q′		–	88°18′	62°18′	36°7′
R′			–	30°36′	73°29′
S′				–	75°54′
T′					–

Table 7. *Internal-rotation angles*

	Molecule I	Molecule II
N(1)C(2)C(3)–C(2)C(3)C(4)	140°35′	143°30′
C(2)C(3)C(4)–C(3)C(4)C(5)	168°17′	171°21′
C(3)C(4)C(5)–C(4)C(5)C(6)	172°0′	174°53′
C(4)C(5)C(6)–C(5)C(6)C(7)	104°12′	104°6′
C(5)C(6)C(7)–C(6)C(7)N(2)	139°45′	145°38′
C(7)N(2)C(8)——N(2)C(8)C(9)	162°4′	159°43′
N(2)C(8)C(9)——C(8)C(9)C(10)	112°32′	173°59′
C(8)C(9)C(10)——C(9)C(10)C(11)	176°53′	176°28′
C(9)C(10)C(11)—C(10)C(11)C(12)	177°43′	171°8′
C(10)C(11)C(12)–C(11)C(12)C(1)	109°13′	114°34′
C(11)C(12)C(1)—C(12)C(1)N(1)	179°14′	116°57′
C(12)C(1)N(1)—C(1)N(1)C(2)	154°53′	144°5′

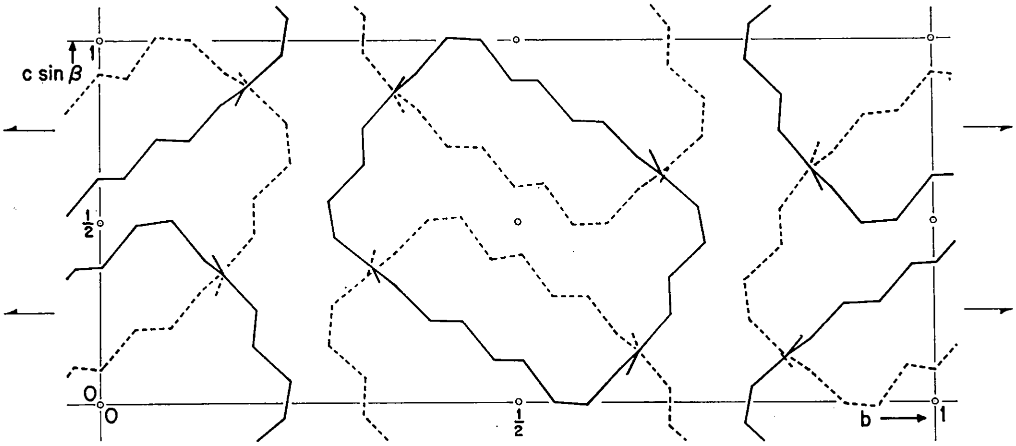


Fig. 3. Projection of the structure parallel to [100]. Dashed lines indicate molecules of type I; full lines indicate molecules of type II.

the bond distances and 1° for the bond angles. A systematically smaller value is found for the O–C–N angle as compared with the O–C–αC angle.

Table 8. *Bond distances* (in Å) *with e.s.d.'s in parentheses*

	Molecule I	Molecule II
C(1)—N(1)	1·454 (5)	1·448 (4)
N(1)—C(2)	1·335 (4)	1·336 (4)
C(2)—O(1)	1·238 (3)	1·224 (3)
C(2)—C(3)	1·500 (4)	1·511 (4)
C(3)—C(4)	1·517 (4)	1·528 (4)
C(4)—C(5)	1·511 (5)	1·508 (5)
C(5)—C(6)	1·529 (4)	1·527 (4)
C(6)—C(7)	1·514 (4)	1·501 (4)
C(7)—O(2)	1·225 (3)	1·230 (3)
C(7)—N(2)	1·320 (4)	1·335 (4)
N(2)—C(8)	1·458 (4)	1·457 (5)
C(8)—C(9)	1·494 (5)	1·508 (5)
C(9)—C(10)	1·532 (5)	1·507 (5)
C(10)-C(11)	1·517 (5)	1·521 (5)
C(11)-C(12)	1·521 (5)	1·519 (5)
C(12)-C(1)	1·515 (5)	1·517 (5)

Table 9. *Bond angles*

The e.s.d.'s given in parentheses refer to the last decimal position.

	Molecule I	Molecule II
C(1)—N(1)—C(2)	122·5 (3)°	123·7 (2)°
N(1)—C(2)—O(1)	120·8 (2)	121·7 (2)
N(1)—C(2)—C(3)	116·8 (2)	116·0 (2)
O(1)—C(2)—C(3)	122·4 (2)	122·2 (2)
C(2)—C(3)—C(4)	113·5 (2)	113·3 (2)
C(3)—C(4)—C(5)	113·7 (3)	114·5 (3)
C(4)—C(5)—C(6)	112·6 (3)	111·0 (3)
C(5)—C(6)—C(7)	113·4 (2)	113·0 (3)
C(6)—C(7)—O(2)	122·0 (3)	123·2 (3)
C(6)—C(7)—N(2)	116·6 (3)	115·9 (3)
N(2)—C(7)—O(2)	121·4 (3)	120·9 (3)
C(7)—N(2)—C(8)	122·9 (3)	123·6 (3)
N(2)—C(8)—C(9)	111·6 (3)	111·5 (3)
C(8)—C(9)—C(10)	114·8 (3)	114·9 (3)
C(9)—C(10)-C(11)	113·0 (3)	112·5 (3)
C(10)-C(11)-C(12)	113·7 (3)	115·7 (3)
C(11)-C(12)-C(1)	112·0 (3)	114·5 (3)
C(12)-C(1)—N(1)	112·1 (3)	110·8 (3)

Nearly all the bond lengths between sp^3 hybridized carbon atoms are smaller than the accepted value of 1·526 Å (Lide, 1962) for this kind of bond. For both molecules the average value is 1·517 Å with a standard deviation of the mean amounting to 0·004 Å. The αC–C bond distances are close to the accepted value of 1·501 Å (Lide, 1962) for sp^3–sp^2 hybridized carbon–carbon bonds. The bond distances found in the tetramethylene groups are, for molecule I: 1·514, 1·529, 1·511, 1·517, 1·500 Å and for molecule II: 1·511, 1·528, 1·508, 1·527, 1·501 Å, which might be interpreted as evidence for alternation in bond character.

The average bond angle between adjoining carbon–carbon bonds of sp^3 hybridization is 113° 20′ in molecule I and 113° 48′ in molecule II, both being considerably larger than the tetrahedral angle. Similar results concerning the bond distances and angles between sp^3 hybridized carbon atoms were observed in the study of the corresponding monomer (Northolt & Alexander, 1968).

For either molecule taken alone the average value ($\bar{d}$) of the C–H bond length is 1·004 Å with a $\sigma(\bar{d})$ of 0·016 Å in molecule I and 1·005 with a $\sigma(\bar{d})$ of 0·017 Å in molecule II. With a few exceptions most of the hydrogen temperature factors are larger than the isotropic temperature factors of the corresponding carbon atoms to which they are bonded.

Packing and hydrogen bonding

In addition to the planar character of the amide group and of the zigzag methylene chain segments, van der Waals forces are also assumed to be factors in establishing the shape of the skeleton of the molecules as observed. For instance, as can be seen in Fig. 2, the methylene group C(11) of molecule I centered on $(\frac{1}{2}, \frac{1}{2}, 1)$ contacts the equivalent methylene group of molecule I centered at $(-\frac{1}{2}, \frac{1}{2}, 0)$ inside the ring of molecule II with position $(0, \frac{1}{2}, \frac{1}{2})$; the contact distance C(11)... C(11) is 3·853 Å. On the other hand, inside the ring of molecule I two close methyl–methyl contacts occur between molecules of type II, with the dis-

Table 10. *Intermolecular methyl–methyl distances shorter than* 4 Å

Code of symmetry operating on the second atom of the pair.

a	$-x$	$1-y$	$-z$	*e*	x	$\frac{1}{2}-y$	$\frac{1}{2}+z$
b	$1-x$	$1-y$	$-z$	*f*	x	$\frac{3}{2}-y$	$\frac{1}{2}+z$
c	$-x$	$1-y$	$1-z$	*g*	$-x$	$\frac{1}{2}+y$	$\frac{1}{2}-z$
d	$1-x$	$1-y$	$1-z$	*h*	$1-x$	$\frac{1}{2}+y$	$\frac{3}{2}-z$

Inside a layer

C(8′)----C(1′)	*a*	3·794 Å
C(12′)---C(11′)	*b*	3·819
C(12′)---C(12′)	*b*	3·800
C(4′)----C(1)	*c*	3·994
C(11) ---C(11)	*c*	3·853
C(8) ----C(1)	*d*	3·789

Between layers

C(3) ---C(6′)	*e*	3·818 Å
C(6) ---C(3′)	*f*	3·777
C(5′)---C(2′)	*f*	3·882
C(2′)---C(6′)	*g*	3·874
C(3′)---C(6′)	*g*	3·737
C(3′)---C(7′)	*g*	3·999
C(5) ---C(2)	*h*	3·902
C(6) ---C(2)	*h*	3·842
C(6) ---C(3)	*h*	3·769
C(7) ---C(3)	*h*	3·947

tances C(12′)...C(12′), 3·800 Å and C(12′)–C(11′), 3·819 Å.

Each molecule is connected by eight hydrogen bonds to four molecules of the other type, as shown in Fig. 2, thereby forming a layer parallel to (010). There are two of these layers per unit cell length *b*, related by the two-fold screw axis, as can be seen in Fig. 3. The intermolecular methyl–methyl distances inside a layer and between layers that are shorter than the accepted sum of the van der Waals radii, 4·0 Å, are listed in Table 10.

Angles and distances involved in the hydrogen bonding between the molecules are listed in Table 11. The N...O distances range from 2·865 to 2·904 Å and the angles N–H...O lie between 166 and 173°. Both results agree well with the values found in the monomer (Northolt & Alexander, 1968).

Table 11. *Dimensions of the hydrogen bonds*

The hydrogen bonds are labeled as follows: (*a*) C(2)O(1)---H(001′)N(1′), (*b*) C(7)O(2)---H(002′)N(2′), (*c*) C(7′)O(2′)---H(002)N(2) and (*d*) C(2′)O(1′)---H(001)N(1).

Distances	(*a*)	(*b*)	(*c*)	(*d*)
N---O	2·876	2·865	2·904	2·866 Å
N–H	0·803	0·842	0·701	0·767
O---H	2·080	2·039	2·208	2·113
Angles				
N–H---O	171°	166°	173°	168°
C–O---H	141	152	145	143
C–O---N	140	148	147	140

The author wishes to thank Professor Helmut Zahn for supplying the compound and Dr Leroy E. Alexander for reading the manuscript and for many helpful discussions. Thanks are also due to Dr Robert F. Stewart and Dr E. N. Maslen who respectively adapted the *X-ray* 67 programs system and S. Hall's symbolic addition program for use on the CDC 1604 computer at Mellon Institute.

References

BERGHUIS, J., HAANAPPEL, IJ. M., POTTERS, M., LOOPSTRA, B. O., MACGILLAVRY, C. H. & VEENENDAAL, A. L. (1955). *Acta Cryst.* **8**, 478.

BRYAN, R. F. & DUNITZ, J. D. (1960). *Helv. Chim. Acta*, **43**, 3.

BUNN, C. W. & GARNER, E. V. (1947). *Proc. Roy. Soc.* A**189**, 39.

COREY, R. B. & PAULING, L. (1953). *Proc. Roy. Soc.* B**141**, 10.

DIETRICH, H. VON, ZAHN, H. & SCHMIDT, F. (1957). *Acta Cryst.* **10**, 477.

HAUPTMAN, H. & KARLE, J. (1953). *Solution of the Phase Problem.* I. *The Centrosymmetric Crystal.* A.C.A. Monograph No. 3.

KARLE, I. L., HAUPTMAN, H., KARLE, J. & WING, A. B. (1958). *Acta Cryst.* **11**, 257.

KARLE, I. L. & KARLE, J. (1963). *Acta Cryst.* **16**, 969.

KARLE, J. & HAUPTMAN, H. (1956). *Acta Cryst.* **9**, 635.

LIDE, D. R. JR (1962). *Tetrahedron*, **17**, 125.

NATTA, G. & CORRADINI, P. (1960). *Nuovo Cim.* **15**, Suppl. No. 1, 9.

NATTA, G., CORRADINI, P. & BASSI, I. W. (1961). *J. Polymer Sci.* **51**, 505.

NORTHOLT, M. G. & ALEXANDER, L. E. (1968). *J. Phys. Chem.* **72**, 2838.

OH, Y. L. & MASLEN, E. N. (1968). *Acta Cryst.* B**24**, 883.

STEWART, J. M. & HIGH, D. (1965). *X-ray* 63 *Programs System.* Univ. of Maryland, College Park, and Univ. of Washington, Seattle.

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175.

ZAHN, H. RATHGEBER, P., REXROTH, E., KRZIKALLA, R., LAUER, W., MIRÓ, P., SPOOR, H., SCHMIDT, F., SEIDEL, B. & HILDEBRAND, D. (1956). *Angew. Chem.* **68**, 229.

ZAHN, H. & SCHMIDT, F. (1959). *Chem. Ber.* **92**, 1381.