Tableau 7. *Isomère syn–cis: distances intermoléculaires les plus intéressantes*

$\sigma=0{,}006$ Å.

Atome Mol. située à *xyz*	Atome	Molécule			Distance ($\sigma=$ 0,006 Å)
C(2)	C(12)	x	$y-1$	z	3,626 Å
C(7)	C(10)		–		3,637
	C(11)		–		3,657
C(18)	O(20)		–		3,680
C(3)	C(16)		–		4,031
N(4)	C(14)		–		4,042
	C(15)		–		4,156
C(17)	C(16)		–		4,063
C(10)	C(10)	$2-x$	$y-\frac{1}{2}$	$\frac{3}{2}-z$	3,758
C(12)	C(14)	x	$\frac{3}{2}-y$	$\frac{1}{2}+z$	3,740
C(15)	O(20)	x	$\frac{1}{2}-y$	$z-\frac{1}{2}$	3,469
C(18)	O(20)	$1-x$	$1-y$	$1-z$	3,511

Les calculs ont été effectués au C.I.R.C.E. à Orsay, sur les ordinateurs IBM 360/75 et CDC 3600, en utilisant les programmes suivants:

- pour les calculs préliminaires, *PHOTO* (Riche, 1969),
- pour les calculs d'affinement: une modification de *ORFLS* (Busing, Martin & Levy, 1962),
- pour les calculs de distances et angles, la série de programmes NRC (Ahmed, Hall, Pippy & Huber, 1966),
- pour le tracé des figures: *ORTEP* (Johnson, 1965),
- pour le calcul de la fonction des phases, et la sélection des valeurs numériques les plus probables des symboles: le programme *DEVIN* (Riche, 1972).

Les auteurs sont reconnaissants à MM P. Potier, H.-P. Husson et C. Thal de leur constant intérêt au cours de ce travail, et remercient M T. Imbert pour leur avoir préparé de beaux cristaux.

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Crystal Structures of Analogues of Purine Nucleoside.

II.* 2-(4-*O*-Acetyl-2,3-dideoxy-β-L-*glycero*-pent-2-enopyranosyl)-5,6-dichlorobenzotriazole (*trans*-CLBA)

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Trans-CLBA was synthesized as a potential antimetabolite. The crystal structure was determined by Patterson and Fourier methods and refined to an R of 5·0% by full-matrix least-squares methods. The unit cell is orthorhombic, with $a=16{\cdot}286$ (2), $b=9{\cdot}976$ (2), $c=8{\cdot}792$ (2) Å, and there are 4 molecules per unit cell. The space group is $P2_12_12_1$. The intensity data were collected on a Philips PW 1100 four-circle diffractometer. All hydrogen atoms were directly located.

Introduction

This work is part of a systematic study of several compounds synthesized by García-Muñoz, Iglesias, Lora-Tamayo, Madroñero & Stud (1969) for the investigation of the activities of purine nucleosides as potential antimetabolitites. The crystal structure of the first compound of this series, *cis*-ATD, has recently been reported by Fayos & García-Blanco (1972). In the present paper we report the crystal structure of *trans*-

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* Part I. *Acta Cryst.* B**28**, 2863.

CLBA, another member of the series, based on single-crystal X-ray diffraction data collected at room temperature.

Experimental

A crystalline sample of *trans*-CLBA was kindly provided by Dr García Muñoz. The sample was recrystallized by slow evaporation, at room temperature, from a xylene/ethyl acetate mixture. Prismatic colourless crystals showing predominantly the {001} habit were obtained. The crystals were mostly twinned.

A single crystal of ~0·3 × 0·4 × 0·2 mm was selected for the X-ray investigation. The crystals belong to the orthorhombic system. The lattice constants were obtained from a least-squares analysis of the settings of 25 reflexions measured on a four-circle diffractometer with Mo $K\alpha$ radiation. The crystal data are listed in Table 1.

Table 1. *Crystal data for trans-CLBA*

Standard deviations, given in parentheses, refer to the least significant digits.

Molecular formula	$C_{13}H_{11}N_3O_3Cl_2$
Molecular weight	328·145
Melting point	184–185°C
Space group	$P2_12_12_1$
a = 16·286 (2) Å	ϱ_x = 1·49 g cm^{-3}
b = 9·976 (2)	$Z=4$
c = 8·792 (2)	μ_{Mo} = 4·49 cm^{-1}
V = 1457·7 Å^3	$F_{000}=672$

The θ–2θ scan mode of the Philips PW 1100 diffractometer, monochromated with a graphite crystal, was used for the recording of intensity data. Three reflexions were monitored after every 47 measurements and showed good stability, as indicated by a root-mean-square deviation of less than 1% in intensity and a maximum deviation of 3%. A total of 1785 independent reflexions were collected in the range $6° < \theta < 80°$. Of this total, 1143 were directly observed, 167 had C_b (background counts) larger that C_p (peak counts), and 485 were considered as unobserved according to the criterion $I < 2\sigma(I)$, where $I = C_p - C_{b1} - C_{b2}$ and $\sigma^2(I) = C_p + C_{b1} + C_{b2} + (0{\cdot}04 \times I)^2$, I being the integrated intensity and $\sigma(I)$ its estimated standard deviation.

The structure amplitudes were obtained after the usual Lorentz and polarization reduction. No correction for absorption was applied, because of the adequate size of crystal used. The extinction effect did not appear to be appreciable, and consequently no correction was made. The absolute scale of F_o was determined during the refinement.

Solution and refinement of the structure

First, location of the positions of the two chlorine atoms, determined from the three Harker sections $u=\frac{1}{2}, v=\frac{1}{2}\, w=\frac{1}{2}$ was performed. A three-dimensional Fourier synthesis was calculated by using the two chlorine phases. However, the rest of atoms could not be located by this procedure. The three-dimensional Patterson function was further studied, and all vectors joining chlorine and non-hydrogen atoms were examined for different orientations of the molecule, by comparison with conventional bond lengths and angles. In this way the location of the plane containing the vectors joining the benzotriazole and the chlorine atoms was achieved and four atoms of the ring were unequivocally positioned. A three-dimensional Fourier synthesis with phases based upon the established positions of these six atoms revealed the location of nine new non-hydrogen atoms. The remaining atoms of the structure appeared in the electron-density map, calculated from the phases of the previous 15 atoms. After two steps of conventional structure-factor (with all non-hydrogen atoms) and electron-density calculations, the conventional reliability index R was 0·246. The refinement was carried out by a full-matrix least-squares program (Busing, Martin & Levy, 1962) from three-dimensional data. Individual isotropic temperature factors were assigned to all non-hydrogen atoms. Three refinement cycles with unit weights for all the observed reflexions reduced the reliability index to $R=0{\cdot}113$. The hydrogen atoms were located from a difference map which was evaluated at this stage. Their peaks heights varied between 0·45 and 0·70 e Å^{-3}. These positions for the hydrogen atoms, with an isotropic temperature factor (the same as that of the neighbouring heavy atom), were included in subsequent structure-factor calculations, giving a residual of $R=0{\cdot}104$. The interatomic distances for hydrogen and non-hydrogen atoms were likewise correct.

At this stage of the refinement the least-squares treatment for non-hydrogen atoms with anisotropic temperature factors was begun by means of the full-matrix method. The hydrogen atoms were fixed, and the weighting factor was $w=1{\cdot}0$. After two cycles the R value dropped to 0·057. An additional least-squares refinement, in which only the coordinates of the hydrogen atoms were varied, reduced the R index to 0·054. Finally, two cycles of a full-matrix least-squares refinement were computed with fixed isotropic temperature factors for the hydrogen atoms and varying anisotropic temperature factors for the rest. An individual weight, $w=1/\sigma^2$, for each reflexion was used for the last cycles. The final discrepancy for the observed reflexions was

$R_{\text{obs}}=0{\cdot}050$. Other values computed in this stage were:
R $=0{\cdot}089$ (for all reflexions observed and unobserved);
R_w $=0{\cdot}045$ (observed), $R_w=0{\cdot}052$ (all reflexions);
R_1 $=0{\cdot}7152$ (where $R_1=[\sum w(F_o-F_c)^2/(N_o-N_v)]^{1/2}$;
N_o $=1785$ reflexions and $N_v=190$ variables);
R_w $=[\sum w(F_o-F_c)^2]^{1/2}/(\sum wF_o^2)^{1/2}$.

Each sequence of the refinement was ended when all parameter shifts were less than one fifth of the corresponding standard deviations. All reflexions were included.

Table 2. *The positional and thermal parameters for non-hydrogen atoms*

Standard deviations given in parentheses refer to the least significant digits. Thermal factors are those in the expression $\exp[-2\pi^2 \sum U_{ij} a_i^X a_j^X h_i h_j]$.

	10^4x	10^4y	10^4z	10^3U_{11}	10^3U_{22}	10^3U_{33}	10^3U_{12}	10^3U_{13}	10^3U_{23}
1 Cl(5)	5369 (1)	2300 (1)	1461 (2)	43 (1)	64 (1)	56 (1)	16 (1)	11 (1)	9 (1)
2 Cl(6)	3933 (1)	741 (2)	−111 (2)	74 (1)	70 (1)	67 (1)	20 (1)	3 (1)	−31 (1)
3 O(1′)	912 (2)	2787 (3)	3148 (4)	41 (2)	33 (2)	55 (2)	−5 (2)	8 (2)	−6 (2)
4 O(4′)	−820 (2)	3377 (3)	4071 (4)	34 (2)	40 (2)	60 (2)	−1 (2)	2 (2)	−5 (2)
5 O(6′)	−1599 (2)	5013 (4)	5010 (7)	49 (2)	82 (3)	155 (5)	12 (2)	5 (3)	−47 (3)
6 N(1)	2075 (2)	4153 (4)	2726 (5)	33 (2)	41 (2)	41 (2)	−2 (2)	−3 (2)	−9 (2)
7 N(2)	2269 (2)	5152 (4)	3713 (5)	33 (2)	48 (3)	49 (3)	−5 (2)	−2 (2)	−13 (2)
8 N(3)	3063 (2)	5187 (4)	3884 (5)	36 (2)	46 (3)	60 (3)	−1 (2)	−7 (2)	−15 (2)
9 C(4)	4224 (3)	3833 (5)	2759 (6)	36 (2)	37 (3)	50 (3)	−4 (2)	2 (2)	0 (3)
10 C(5)	4362 (2)	2782 (5)	1811 (5)	35 (2)	46 (3)	39 (3)	8 (2)	4 (2)	14 (3)
11 C(6)	3710 (3)	2077 (5)	1081 (5)	63 (3)	38 (3)	36 (3)	8 (3)	4 (3)	−0 (2)
12 C(7)	2906 (3)	2427 (5)	1295 (5)	41 (2)	43 (3)	45 (3)	2 (2)	1 (2)	−2 (3)
13 C(8)	2766 (3)	3512 (4)	2258 (5)	35 (2)	36 (3)	31 (3)	−0 (2)	3 (2)	−0 (2)
14 C(9)	3398 (2)	4184 (5)	2985 (5)	35 (2)	35 (3)	37 (3)	−1 (2)	2 (2)	−2 (3)
15 C(1′)	1212 (3)	3874 (5)	2323 (5)	35 (2)	47 (3)	36 (3)	−12 (2)	2 (2)	−4 (3)
16 C(2′)	709 (3)	5116 (5)	2465 (6)	41 (3)	44 (3)	55 (4)	−7 (2)	−13 (3)	14 (3)
17 C(3′)	93 (3)	5217 (5)	3429 (6)	40 (2)	31 (3)	66 (4)	−0 (2)	−11 (3)	−3 (3)
18 C(4′)	−89 (3)	4131 (5)	4523 (6)	33 (2)	45 (3)	49 (3)	1 (2)	1 (2)	7 (3)
19 C(5′)	623 (3)	3156 (5)	4617 (6)	41 (3)	46 (3)	41 (3)	9 (2)	5 (2)	12 (3)
20 C(6′)	−1542 (3)	3970 (6)	4350 (7)	44 (3)	52 (4)	78 (4)	1 (3)	1 (3)	2 (3)
21 C(7′)	−2252 (3)	3156 (6)	3789 (8)	49 (3)	84 (5)	−104 (6)	−10 (3)	−11 (4)	8 (4)

Atomic scattering factors used throughout the refinement were those given by Hanson, Herman, Lea & Skillman (1964) for neutral C,N,O and Cl atoms, and those of Stewart, Davidson & Simpson (1965) for H atoms. No correction for anomalous dispersion was made at any stage of the refinement.

As a final check of the correctness of the structure a difference Fourier synthesis with the structure factors calculated in the last cycle of the refinement was made. The resulting electron density map showed no peak exceeding $\pm 0{\cdot}3$ e Å^{-3}.

The positional and thermal parameters, with estimated least-squares standard deviations (e.s.d'.s) are given in Tables 2 and 3. Copies of observed and calculated structure factors are available from the authors on request.

Table 3. *Positional and thermal parameters for hydrogen atoms*

Standard deviations, given in parentheses, refer to the least significant digits. Thermal factors are $U=B/8\pi^2$.

	10^3x	10^3y	10^3z	U	ϱ (e Å^{-3})
22 H(7)	240 (3)	201 (5)	79 (6)	42 (2)	0·59
23 H(1′)	124 (3)	361 (5)	136 (5)	37 (2)	0·66
24 H(5′*a*)	105 (3)	349 (5)	549 (6)	38 (2)	0·65
25 H(5′*b*)	44 (3)	230 (5)	522 (6)	38 (2)	0·65
26 H(4′)	−19 (3)	434 (5)	560 (6)	38 (2)	0·63
27 H(3′)	−28 (3)	598 (5)	351 (5)	38 (2)	0·62
28 H(2′)	84 (3)	584 (5)	177 (6)	42 (2)	0·63
29 H(7′*a*)	−230 (3)	347 (6)	273 (6)	70 (3)	0·70
30 H(7′*b*)	−224 (3)	241 (6)	428 (7)	70 (3)	0·61
31 H(7′*c*)	−280 (3)	361 (6)	374 (6)	70 (3)	0·61
32 H(4)	469 (3)	444 (5)	337 (5)	38 (2)	0·63

Description of the structure and discussion

Intramolecular bond distances and angles, with their associated e.s.d.'s from the least-squares refinement, are listed in Table 4. Distances and angles are uncorrected for thermal motion. The principal intermolecular contact distances are listed in Table 5.

Table 4. *Intramolecular bond distances and angles with their associated standard deviations given in parentheses*

Cl(6)—C(6)	1·734 (5) Å	Cl(6)—C(6)—C(7)	118·6 (4)°
C(6)—C(7)	1·370 (7)	C(6)—C(7)—C(8)	115·9 (4)
C(7)—C(8)	1·393 (7)	C(7)—C(8)—C(9)	122·4 (4)
C(8)—C(9)	1·385 (6)	C(8)—C(9)—C(4)	121·7 (4)
C(9)—C(4)	1·405 (6)	C(9)—C(4)—C(5)	115·9 (4)
C(4)—C(5)	1·358 (7)	C(4)—C(5)—C(6)	122·4 (4)
C(5)—C(6)	1·425 (7)	C(4)—C(5)—Cl(5)	188·6 (4)
C(5)—Cl(5)	1·736 (4)	Cl(5)—C(5)—C(6)	119·1 (3)
Cl(5)—Cl(6)	3·130 (2)	C(7)—C(8)—N(1)	133·3 (4)
C(8)—N(1)	1·359 (6)	C(8)—N(1)—N(2)	110·3 (4)
N(1)—N(2)	1·358 (6)	C(9)—C(8)—N(1)	104·3 (4)
N(2)—N(3)	1·303 (5)	N(1)—N(2)—N(3)	108·9 (4)
N(3)—C(9)	1·386 (6)	N(2)—N(3)—C(9)	107·8 (4)
N(1)—C(1′)	1·475 (5)	N(3)—C(9)—C(4)	129·6 (4)
C(1′)—C(2′)	1·491 (7)	N(3)—C(9)—C(8)	108·7 (4)
C(1′)—O(1′)	1·393 (6)	N(2)—N(1′)-C(1′)	120·9 (4)
C(2′)—C(3′)	1·318 (7)	N(1)—C(1′)-C(2′)	110·2 (4)
C(3′)—C(4′)	1·477 (7)	N(1)—C(1′)-O(1′)	110·9 (4)
C(4′)—C(5′)	1·516 (6)	O(1′)—C(1′)-C(2′)	114·2 (4)
C(5′)—O(1′)	1·423 (6)	C(1′)—C(2′)-C(3′)	122·4 (4)
C(4′)—O(4′)	1·462 (5)	C(2′)—C(3′)-C(4′)	121·0 (4)
O(4′)—C(6′)	1·340 (6)	C(3′)—C(4′)-C(5′)	110·6 (4)
C(6′)—C(7′)	1·496 (8)	C(4′)—C(5′)-O(1′)	111·7 (4)
C(6′)—O(6′)	1·195 (8)	C(5′)—O(1′)-C(1′)	112·8 (3)
H(7)—C(7)	1·03 (5)	H(7)—C(7)—C(6)	127 (3)
H(1′)—C(1′)	0·89 (5)	H(1′)—C(1′)-N(1)	103 (3)
H(5′*a*)-C(5′)	1·09 (5)	H(5′*a*)-C(5′)-C(4′)	109 (3)
H(5′*b*)-C(5′)	1·05 (5)	H(5′*b*)-C(5′)-C(4′)	109 (3)
H(4′)—C(4′)	0·98 (5)	H(4′)—C(4′)-C(3′)	120 (3)
H(3′)—C(3′)	0·98 (5)	H(3′)—C(3′)-C(2′)	125 (3)
H(2′)—C(2′)	0·97 (5)	H(2′)—C(2′)-C(1′)	116 (3)
H(7′*a*)-C(7′)	0·99 (6)	H(7′*a*)-C(7′)-C(6′)	101 (3)
H(7′*b*)-C(7′)	0·86 (6)	H(7′*b*)-C(7′)-C(6′)	106 (4)
H(7′*c*)-C(7′)	1·00 (5)	H(7′*c*)-C(7′)-C(6′)	116 (3)
H(4)—C(4)	1·11 (4)	H(4)—C(4)—C(9)	117 (2)

Table 5. *Main intermolecular contact distances less than* 3·5 Å *for non-hydrogen to non-hydrogen distances*

Less than 3·0 Å for non-hydrogen to hydrogen distances. The symmetry relationship of the atoms concerned is denoted by

I	x	y	z
II	$\frac{1}{2}-x$	$1-y$	$-\frac{1}{2}+z$
III	$-x$	$-\frac{1}{2}+y$	$\frac{1}{2}-z$
IV	$\frac{1}{2}-x$	$1-y$	$\frac{1}{2}+z$
V	$-x$	$\frac{1}{2}+y$	$\frac{1}{2}-z$
VI	$1-x$	$-\frac{1}{2}+y$	$\frac{1}{2}-z$
VII	$\frac{1}{2}+x$	$\frac{1}{2}-y$	$-z$

N(1) (I)	N(3) (II)	3·450 (6) Å
N(2) (I)	C(7) (IV)	3·327 (6)
N(2) (I)	C(8) (IV)	3·390 (6)
N(3) (I)	C(1) (IV)	3·379 (6)
O(1′) (I)	C(3′) (III)	3·343 (7)
O(6′) (I)	C(7) (V)	3·412 (6)
Cl(5) (I)	N(3) (VI)	3·325 (4)
N(3) (I)	H(1′) (IV)	2·72 (5)
O(1′) (I)	H(3′) (III)	2·48 (5)
O(4′) (I)	H(2′) (III)	2·61 (5)
O(6′) (I)	H(7) (V)	2·39 (5)
Cl(5) (I)	H(1′) (VII)	2·99 (5)
Cl(5) (I)	H(4) (VI)	2·90 (5)
Cl(6) (I)	H(4) (VI)	3·00 (4)

The equations for the best least-squares planes calculated by the method of Schomaker, Waser, Marsh & Bergman (1959) are:

(i) for the benzotriazole

$$-0{\cdot}0616X-0{\cdot}6317Y+0{\cdot}7728Z+0{\cdot}9532=0;$$

(ii) for the *O*-acetyl group

$$-0{\cdot}0303X-0{\cdot}4792Y+0{\cdot}8772Z-1{\cdot}5378=0;$$

(iii) for the enopyranosyl

$$0{\cdot}6888X+0{\cdot}4127Y+0{\cdot}5959Z-4{\cdot}1037=0;$$

(iv) for the C(1), C(2), C(3) and C(4) atoms

$$0{\cdot}6425X+0{\cdot}3836Y+0{\cdot}6634Z-4{\cdot}1153=0\,.$$

The deviations of the atoms from these planes are given in Table 6.

The deviations of the atoms forming the benzotriazole group (i) show that this group lies almost on a plane and that as expected N(1) and C(4) have opposite deviations from N(3) and C(7) of nearly the same order. The chlorine atoms are deviated from the plane of the benzotriazole in opposite directions, giving the correct distance Cl(5)–Cl(6) of 3·130 Å. The hydrogen atoms H(7) and H(4) are slightly deviated from the plane.

The atoms belonging to the acetyl group (ii) are nearly planar.

The deviations of the atoms belonging to the enopyranosyl (iii) show that C(5) and O(1) are out the plane in opposite directions.

The deviations of the atoms C(1′), C(2′), C(3′) and C(4′) from plane (iv) are negligible in comparison with the deviations of the same atoms from plane (iii), the C(5′) atom being twice as far from the plane than the O(1′).

Such deviations yield the half-chair conformation of the enopyranosyl. In this chair the atoms C(2′) and C(3′) are joined by a double bond.

The angle between the benzotriazole and the enopyranosyl, is 80·2°, that between the benzotriazole plane and the acetyl is 9·9° and that between the enopyranosyl and the acetyl is 72·7°.

In the benzene ring the distance between C(4) and C(7) indicates that this ring is slightly elongated. A similar feature was recently reported in the crystal structure of *cis*-ATD (Fayos & García-Blanco (1972)). The resonance structure of the benzotriazole group is indicated by some double-bond character for the C(4)–C(5), C(6)–C(7), C(8)–C(9) and N(2)–N(3) bonds. This is in good agreement with the above-mentioned crystal structure of *cis*-ATD.

The N–N distances have a resonance value between 1·26 and 1·46 Å, corresponding to a double–single bond.

Fig. 1 illustrates a molecule with all the hydrogen atoms and the torsion angles shown. These are $\chi=86{\cdot}6$, $\psi=102{\cdot}1$ and $\varphi=177{\cdot}7°$. χ is the angle between the O(1′), C(1′), N(1) and C(1′), N(1), C(8) planes. ψ is the angle between the C(3′), C(4′), O(4′) and C(4′), O(4′), C(6′) planes and φ the angle between the C(4′), O(4′), C(6′) and O(4′), C(6′), C(7′) planes.

A projection of the structure along [001] is presented in Fig. 2. Intermolecular distances lower than 4·0 Å

Table 6. *Deviations of the atoms from some least-squares planes in the molecule, with their dihedral angles*

Benzotriazole (i)	Δ (Å)	*O*-Acetyl (ii)	Δ (Å)	Enopyranosyl (iii)	Δ (Å)	C(1)C(2)C(3)C(4) (iv)	Δ (Å)
N1()	−20	C(4′)	−20	C(1′)	68	C(1′)	−10
N(2)	2	O(4′)	28	C(2′)	90	C(2′)	22
N(3)	16	C(6′)	− 5	C(3′)	−54	C(3′)	−22
C(4)	−11	O(6′)	9	C(4′)	−133	C(4′)	10
C(5)	− 7	C(7′)	−13	C(5′)	313		
C(6)	6			O(1′)	−284	C(5′)	436
C(7)	12					O(1′)	−259
C(8)	− 3						
C(9)	4						
Cl(5)	−42						
Cl(6)	17			∠(i) (iii)	80·2°		
H(7)	41			∠(iii) (ii)	72·7		
H(4)	34			∠(i) (ii)	9·9		

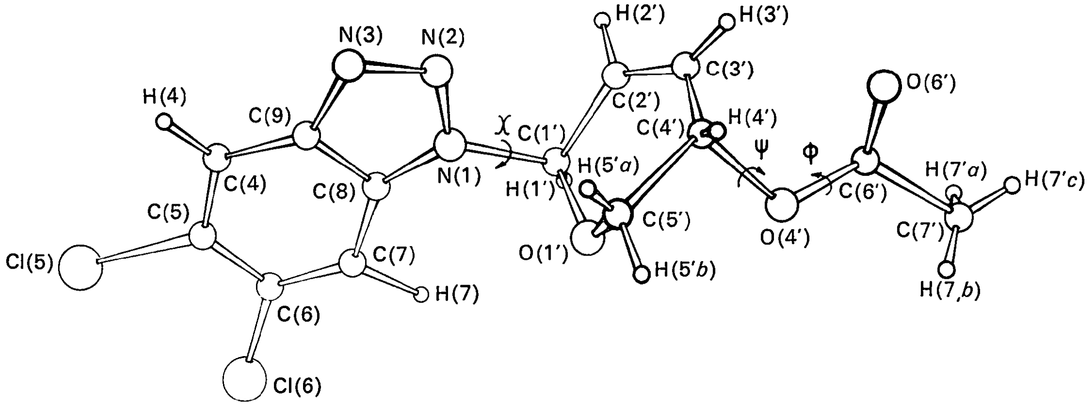

Fig. 1. Conformation of the *trans*-CLBA molecule showing the torsional angles and hydrogen atoms.

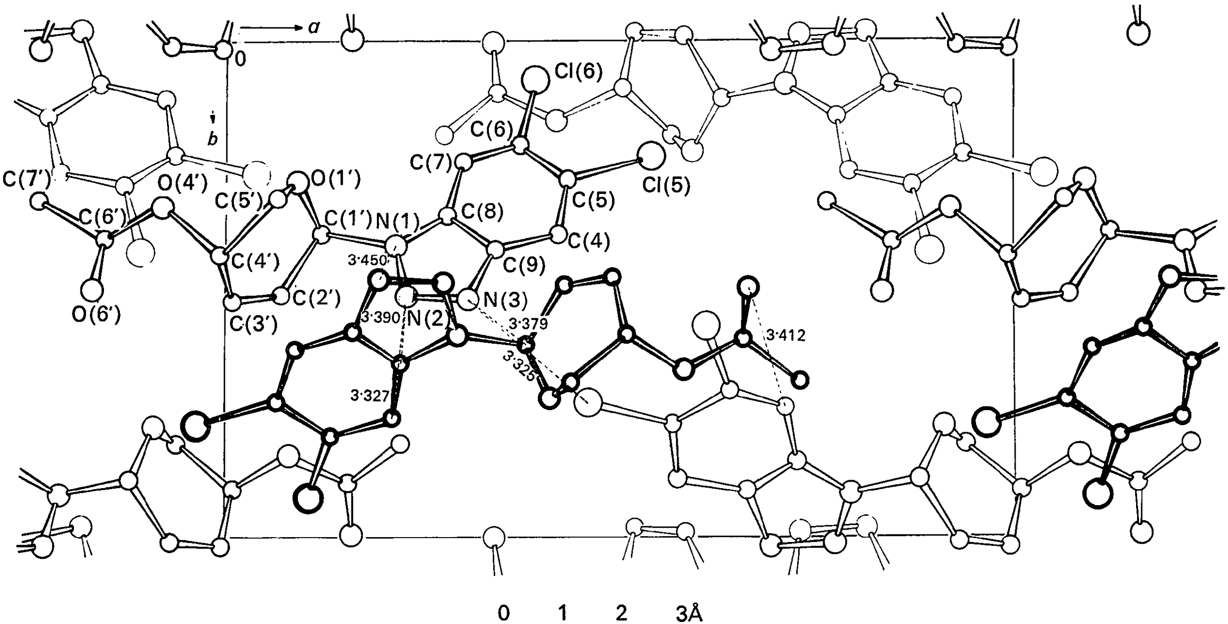

Fig. 2. *trans*-CLBA structure. Projection along the *c* axis. Hydrogen atoms are omitted.

are also drawn. The packing of the molecules is entirely due to van der Waals forces. The distances between all non-hydrogen atoms are normal. The distances O(1')–H(3'), O(6')–H(7), Cl(5)–H(1') and Cl(5)–H(4) are smaller than the sum of the van der Waals radii.

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