clearly $2/m$ even though the value of β is very near $90°$. The fraction of reflections having $I > 3\sigma(I)$ (2377/7618 = 0.31) was low, even though reflection intensities were measured with 100 s scans (scan width $0.8°$ ω plus allowance for $K\alpha_1 - K\alpha_2$ split), with an additional 10 s at each end of the scan for a background measurement. Only 299 reflections had $2\sigma(I) < I < 3\sigma(I)$. Even though one of the axes was 50 Å long, there were no obvious problems with reflection overlap.

The structure proved difficult to solve even though the cell dimensions put clear limits on the possible positions and orientations of the three independent molecules. The solution was eventually found with the 1983 version of the program package *DIRDIF* (Beurskens *et al.*, 1983) after numerous possible orientations and shift vectors had been examined. Later experiments, however, showed that the newest version of *DIRDIF* finds the solution nearly automatically (Beurskens, 1992). In each case the structure solution started from a 21-atom fragment [C(01)-C(20), C(30)] of a similar molecule found by searching the CSD. The absolute configuration was chosen to correspond with that expected from the synthetic pathway. After isotropic refinement, coordinates for all H atoms connected to C atoms were calculated on the basis of the expected stereochemistry ($R_{C-H} = 1.00$ Å) and the H atoms were included in the refinement as fixed contributions ($B = 1$ Å^2 larger than that of the attached C atom). The H atoms of the hydroxyl groups could not be located in difference Fourier syntheses with sufficient certainty to justify their inclusion. The relatively low number of reflections with measurable intensity precluded anisotropic refinement. Before the final cycles, coordinates for all H atoms were re-idealized. After refinement was complete, $(I_{obs} - I_{calc})/\sigma(I)$ was calculated for the 5241 reflections having $I < 3\sigma(I)$, which therefore were omitted from the refinement. The average value of -0.4 suggests a minor overlap problem; for the 55 reflections that had $|(I_{obs} - I_{calc})/\sigma(I)| > 3$, all had $I_{obs} < I_{calc}$. Only 3 reflections had $|(I_{obs} - I_{calc})/\sigma(I)| > 5$; an additional 11 had $|(I_{obs} - I_{calc})/\sigma(I)| > 4$.

Data collection: *CAD-4-VAX* (Enraf-Nonius, 1988). Cell refinement: *CAD-4-VAX*. Data reduction: local program (Brock). Program(s) used to solve structure: *DIRDIF*. Program(s) used to refine structure: local program [based on Ibers' least-squares program, which is in turn based on *ORFLS* (Busing, Martin & Levy, 1962)]. Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *ORFFE* (Busing, Martin & Levy, 1964); local program (Brock).

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meso- and (±)-1,2-Dicyano-1,2-diphenylethane

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Abstract

Of the title compounds, (I) *meso*- and (II) (±)-2,3-diphenylbutanedinitrile, $C_{16}H_{12}N_2$, (I) adopts the *trans* conformation with disorder in the inner part of the molecule, whereas in (II), the two CN groups are *gauche* and the phenyl groups *trans*.

Comment

We have reported previously the crystal structures of *meso*- and (±)-2,3-dicyano-2,3-diphenylbutane and *meso*- and (±)-3,4-dicyano-3,4-diphenylhexane (Lam, Koh & Huang, 1991). This paper is concerned with the structures of *meso*-1,2-dicyano-1,2-diphenylethane, (I), and its (±) isomer, (II).

The crystal structure of (I) is partly disordered over two sites, each with a site occupancy factor of 0.5. The atomic numbering and thermal ellipsoid diagrams of the two sets of atoms are shown in Fig. 1. The atoms which are not disordered are the 'outer' atoms, *i.e.* N(1), C(1N), H(1) and C(14). The 'inner' atoms C(1), C(11), C(12), C(13), C(15) and C(16) are disordered. The relative positions of the atoms are shown in Fig. 2. This is similar to the case of 1,2-dinitro-1,2-diphenylethane where the central C atom is disordered (Koh, Lam, Sim & Huang, 1993). The molecule of (I) is situated at the centre of symmetry and the conformation is therefore *trans*, which is the same as for its butane and hexane analogues. Selected bond lengths and bond angles of the disordered pair are given in Table 2. Most of the equivalent bonds and angles have similar values. The only exception is the central C—C bond which is 1.585 (12) Å in one and 1.518 (12) Å in the other, the

average being 1.55 (3) Å, which is, as expected, shorter than the corresponding values of 1.595 (4) and 1.607 (4) Å of its butane and hexane analogues, respectively (Lam, Koh & Huang, 1991). Some of the angles around the central C atoms, particularly those involving the H atom, deviate appreciably from the tetrahedral value of 109.5°. This probably results from the disorder, as well as the relatively inaccurate positioning of the H atoms. In each of the disordered structures, the phenyl ring is planar (mean deviation from plane = 0.01 Å) and is oriented at about 111° to the C_{sp}—C—C plane. The H atom H(1) is slightly out of the plane of the phenyl ring with the torsion angle H(1)—C(1)—C(11)—C(12) equal to 8.0 (2.2)°.

There is no disorder in the structure of (II). The atomic numbering and thermal ellipsoid diagram are given in Fig. 3. Selected bond lengths and angles are given in Table 3. The molecule of (II) is situated on the twofold rotation axis. The two CN groups are *gauche* and the two phenyl groups *trans* [structure (6) in Fig. 5]. The phenyl ring is almost perfectly planar (mean deviation from plane = 0.002 Å), and oriented at 64.0 (2)° from the plane of C_{sp}—C—C. In contrast with (I), the CN group of (II) is almost coplanar with the phenyl ring, with the C(1N)—C(1)—C(11)—C(12) torsion angle equal to 2.6 (2)°. The central C—C bond length is 1.569 (2) Å which is close to that of (I). Other bond lengths are comparable to those of (I) and to those of the butane and hexane analogues.
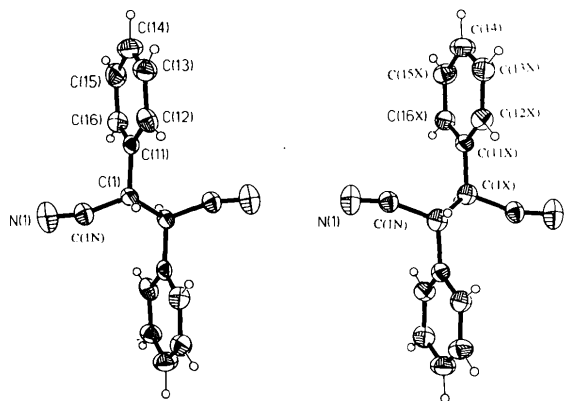

Fig. 1. Atomic numbering and thermal ellipsoid diagram of *meso*-1,2-dicyano-1,2-diphenylethane (I) showing disorder.

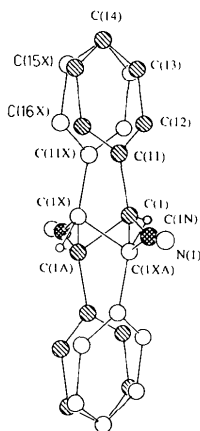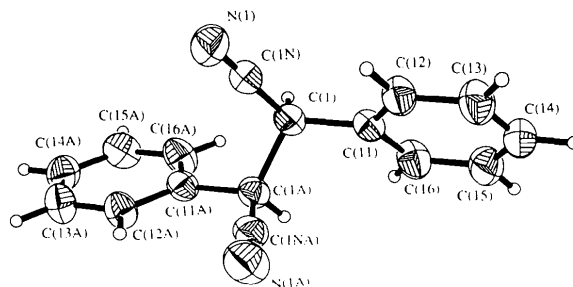Fig. 2. Diagram showing relative positions of the disordered atoms of *meso*-1,2-dicyano-1,2-diphenylethane (I).

Fig. 3. Atomic numbering and thermal ellipsoid diagram of (±)-1,2-dicyano-1,2-diphenylethane (II).

(1) *gauche*   (2) *trans*   (3) *gauche*
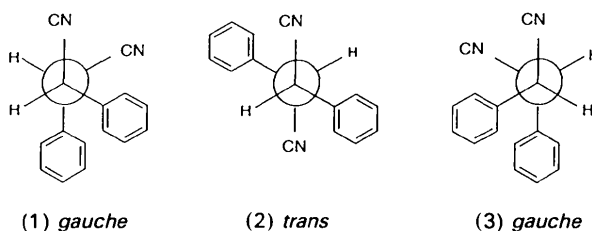
Fig. 4. Stable conformations of (I).

(4) *gauche*   **(5)** *trans*

(6) *gauche*

Fig. 5. Stable conformations of (II).

Fig. 7. Energy of ($\pm$)-1,2-dicyano-1,2-diphenylethane as a function of the NC—C—C—CN torsion angle calculated using AM1 parameterization.
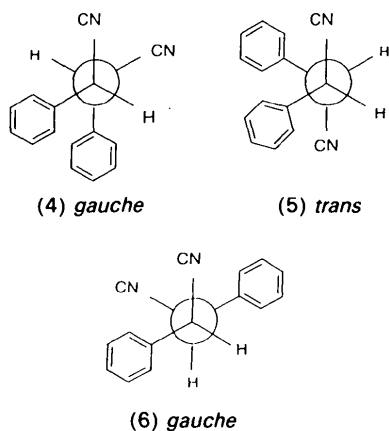
(I) and (II) have almost the same calculated density. In most other *meso*/($\pm$) pairs, the *meso* form usually has higher density (Lam, Koh & Huang, 1991; Lam, Chong, Koh & Huang, 1991). This suggests that the inability of (I) to pack well has led to its disorder.

AM1 calculations with full geometry optimization predict that molecule (I) should exist almost exclusively in the *trans* configuration (92%) in the gas phase (Fig. 4). This is consistent with the solid-state X-ray results. The energy profile of (I) as a function of the $\equiv$C—C—C—C$\equiv$ dihedral angle is shown in Fig. 6. In the case of (II), AM1 calculations predict that the most stable conformation is (4), followed by (6), both of which are *gauche* and occupy 57 and 40%, respectively, of the total population (Figs. 5 and 7). Again, this is qualitatively consistent with the solid-state structure determined by the present X-ray diffraction study. In the solid state, it appears that packing efficiency is greater for a conformation with the phenyl groups *trans*.
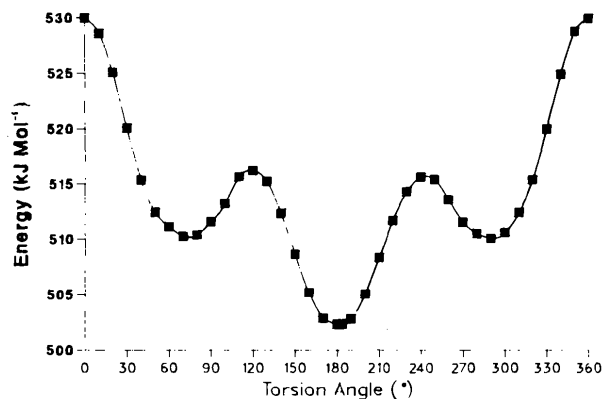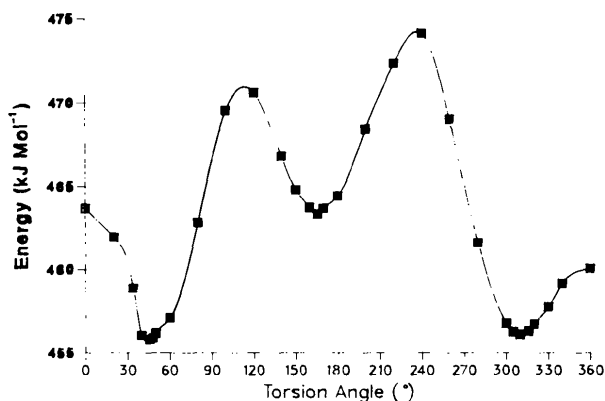
Experimental

Compounds (I) and (II) were prepared as described previously (Huang & Lim, 1967). Compound (I) was recrystallized from xylene (colourless needles, m.p. 508–510 K). Samples of (II) were chromatographed over silica gel (230–400 mesh) and after slow recrystallization from acetone without heating, had m.p. 435–441 K.

Compound (I)

Crystal data

$C_{16}H_{12}N_2$
$M_r = 232.3$
Monoclinic
$C2/c$
$a = 19.044\ (5)$ Å
$b = 5.794\ (2)$ Å
$c = 12.494\ (3)$ Å
$\beta = 115.28\ (2)°$
$V = 1246.6\ (6)$ Å^3
$Z = 4$
$D_x = 1.238$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 20
   reflections
$\theta = 7.5–14.0°$
$\mu = 0.074$ mm^{-1}
Needle
$0.40 \times 0.20 \times 0.20$ mm
Colourless

Data collection

Siemens $R3m/V$ diffractometer
ω scans (speed 2.5–26°
   min^{-1}, width 1.20°)
Absorption correction:
   none
1136 measured reflections
1102 independent reflections
710 observed reflections
   $[I > 2\sigma(I)]$

$R_{int} = 0.025$
$\theta_{max} = 25°$
$h = 0 \rightarrow 21$
$k = 0 \rightarrow 6$
$l = -14 \rightarrow 13$
3 standard reflections
   monitored every 97
   reflections
   intensity variation: $\pm1.5\%$

Refinement

Refinement on F
$R = 0.046$
$wR = 0.043$
$S = 1.74$
710 reflections

Extinction correction:
$F^* = F[1 + (0.002\chi$
   $\times F^2/\sin2\theta)]^{-1/4}$
Extinction coefficient:
   $\chi = 0.0011$

Fig. 6. Energy of *meso*-1,2-dicyano-1,2-diphenylethane as a function of the NC—C—C—CN torsion angle calculated using AM1 parameterization.

140 parameters
$w = 1/[\sigma^2(F) + 0.0001F^2]$
$(\Delta/\sigma)_{max} = 0.33$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.11$ e Å^{-3}

Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Compound (II)

Crystal data

$C_{16}H_{12}N_2$
$M_r = 232.3$
Monoclinic
$C2/c$
$a = 17.702$ (6) Å
$b = 5.720$ (2) Å
$c = 12.725$ (4) Å
$\beta = 104.58$ (3)°
$V = 1247.0$ (7) Å^3
$Z = 4$
$D_x = 1.237$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 18 reflections
$\theta = 4-13°$
$\mu = 0.074$ mm^{-1}
$T = 298$ K
Prism
$0.55 \times 0.40 \times 0.35$ mm
Colourless

Data collection

Siemens $R3m/V$ diffractometer
ω scans (speed 2.5–26° min^{-1}, width 1.20°)
Absorption correction: none
842 measured reflections
811 independent reflections
724 observed reflections
$[I > 2\sigma(I)]$

$R_{int} = 0.0065$
$\theta_{max} = 22.5°$
$h = 0 \rightarrow 18$
$k = 0 \rightarrow 6$
$l = -13 \rightarrow 12$
3 standard reflections monitored every 97 reflections
intensity variation: $\pm1.5\%$

Refinement

Refinement on F
$R = 0.031$
$wR = 0.048$
$S = 1.55$
724 reflections
86 parameters
$w = 1/[\sigma^2(F) + 0.0007F^2]$
$(\Delta/\sigma)_{max} = 0.016$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.10$ e Å^{-3}

Extinction correction:
$F^* = F[1 + (0.002\chi \times F^2/\sin2\theta)]^{-1/4}$
Extinction coefficient:
$\chi = 0.0031$
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for compounds* (I) *and* (II)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	Occupancy	x	y	z	U_{eq}
(I)					
C(1)	0.5	0.0035 (3)	0.0177 (9)	0.4395 (4)	0.043 (2)
C(1X)	0.5	−0.0418 (3)	−0.0125 (9)	0.4911 (5)	0.054 (3)
C(11)	0.5	−0.0728 (3)	0.0158 (10)	0.3303 (4)	0.042 (2)
C(11X)	0.5	−0.0989 (3)	0.0037 (9)	0.3604 (4)	0.045 (2)
C(12)	0.5	−0.0904 (8)	−0.1660 (18)	0.2518 (10)	0.056 (4)
C(12X)	0.5	−0.1041 (8)	−0.1644 (18)	0.2789 (10)	0.054 (4)
C(13)	0.5	−0.1577 (9)	−0.1528 (26)	0.1493 (12)	0.060 (6)
C(13X)	0.5	−0.1604 (10)	−0.1609 (25)	0.1635 (11)	0.064 (6)
C(14)	1.0	−0.2090 (2)	0.0256 (4)	0.1278 (2)	0.072 (1)
C(15)	0.5	−0.1928 (7)	0.2049 (26)	0.2067 (15)	0.065 (7)
C(15X)	0.5	−0.2033 (7)	0.1958 (28)	0.2071 (14)	0.062 (6)
C(16)	0.5	−0.1253 (7)	0.1948 (19)	0.3093 (14)	0.055 (4)
C(16X)	0.5	−0.1483 (7)	0.1907 (19)	0.3222 (14)	0.055 (4)
C(1N)	1.0	0.0477 (1)	0.2349 (4)	0.4519 (2)	0.055 (1)
N(1)	1.0	0.0671 (1)	0.4087 (4)	0.4369 (1)	0.086 (1)
(II)					
N(1)		0.5808 (1)	0.3973 (2)	0.3871 (1)	0.063 (1)
C(1N)		0.5497 (1)	0.2261 (3)	0.3574 (1)	0.044 (1)
C(1)		0.5058 (1)	0.0156 (2)	0.3132 (1)	0.039 (1)
C(11)		0.4288 (1)	−0.0030 (2)	0.3462 (1)	0.038 (1)
C(12)		0.4040 (1)	0.1667 (2)	0.4067 (1)	0.047 (1)
C(13)		0.3342 (1)	0.1418 (3)	0.4354 (1)	0.055 (1)
C(14)		0.2881 (1)	−0.0500 (3)	0.4040 (1)	0.053 (1)
C(15)		0.3120 (1)	−0.2205 (3)	0.3437 (1)	0.056 (1)
C(16)		0.3821 (1)	−0.1980 (2)	0.3151 (1)	0.052 (1)

Table 2. *Geometric parameters* (Å, °) *for compound* (I)

C(1)—C(1A)	1.585 (12)	C(1X)—C(1XA)	1.518 (12)
C(1)—C(11)	1.510 (6)	C(1X)—C(11X)	1.530 (7)
C(1)—C(1N)	1.486 (6)	C(1X)—C(1NA)	1.500 (6)
C(1)—H(1)	1.027 (26)	C(1X)—H(1A)	1.039 (27)
C(1N)—N(1)	1.115 (4)		
C(11)—C(1)—C(1N)	112.6 (4)	C(11X)—C(1X)—C(1NA)	113.3 (4)
C(11)—C(1)—H(1)	118.7 (13)	C(11X)—C(1X)—H(1A)	120.5 (12)
C(11)—C(1)—C(1A)	114.9 (6)	C(11X)—C(1X)—C(1XA)	111.9 (7)
C(1N)—C(1)—C(1A)	106.5 (4)	C(1NA)—C(1X)—C(1XA)	107.4 (5)
H(1)—C(1)—C(1A)	100.2 (16)	H(1A)—C(1X)—C(1XA)	101.5 (15)
C(1N)—C(1)—H(1)	102.2 (15)	C(1NA)—C(1X)—H(1A)	100.7 (15)

Table 3. *Geometric parameters* (Å, °) *for compound* (II)

C(1)—C(1A)	1.569 (2)	C(1)—C(11)	1.527 (2)
C(1)—C(1N)	1.466 (2)	C(1N)—N(1)	1.140 (2)
C(11)—C(1)—C(1N)	112.1 (1)	C(1N)—C(1)—C(1A)	108.2 (2)
C(11)—C(1)—C(1A)	112.7 (2)		

Both structures were solved by direct methods using the *SHELXTL-Plus* programs (Sheldrick, 1989). Structure solution and refinement for (II) was straightforward. For (I), the initial structure obtained by direct methods could only be refined to $R = 0.10$ giving very large anisotropic displacement parameters for the inner C atoms, particularly C(1) and C(11). Final results with $R = 0.046$ were obtained with a disordered model in which the central C and the five inner C atoms of the phenyl ring were disordered over two sets of positions with occupancy factors of 0.5 each, while the CN group and the outermost C atom of the phenyl ring and the H atom attached to C(1) were ordered. This disordered model also resulted in far more reasonable displacement parameters.

All H atoms were assigned fixed displacement parameters with U equal to 1.3 times that of the C atom to which the H atom was bonded. Coordinates of H(1) were refined for both compounds. Other H atoms were placed at calculated positions. The plots of the molecular structures were produced using XP (Sheldrick, 1989).

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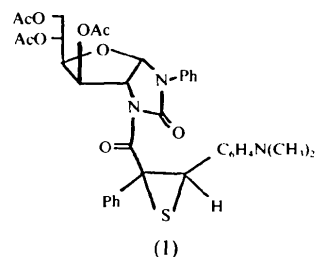
(1)

3-[(2R,3R)-3-(4-Dimethylaminophenyl)-2-phenyl-2,3-epithiopropanoyl]-1-phenyl-(3,5,6-tri-O-acetyl-1,2-dideoxy-α-D-glucofuranoso)[1,2-d]imidazolidin-2-one

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Abstract

This work unambiguously establishes the overall conformation of the title molecule, $C_{36}H_{37}N_3O_9S$, which includes a thiirane ring. The configuration is α-D-glucofuranose with the furanosyl ring T_4^3; the imidazolidine-2-one group assumes a form in which the fused C2′ atom deviates by 0.14 Å from the best plane.

Comment

3-[(2R,3R)-3-(4-Dimethylaminophenyl)-2-phenyl-2,3-epithiopropanoyl]-1-phenyl-(3,5,6-tri-O-acetyl-1,2-dideoxy-α-D-glucofuranoso)[1,2-d]imidazolidine-2-one (1) was synthesized (Areces, Avalos, Babiano, González, Jiménez & Palacios, 1992) by the reaction of 2,5-diphenyl-(3,5,6-tri-O-acetyl-1,2-dideoxy-α-D-glucofuranoso)[1,2:4,5]-4aH,4bH-imidazo[2,1-b]thiazolium-3-olate (Areces, Avalos, Babiano, González, Jiménez, Palacios & Pilo, 1991) with 4-(N,N-dimethylamino)benzaldehyde. Compound (1) and related compounds are of interest as intermediates in the synthesis of chiral synthons and also because of the molecular overcrowding and the effect it has on geometrical parameters.

In order to elucidate the molecular conformation and the orientations of the substituents at the bond-forming sites, the structure of the product was determined by a single-crystal X-ray analysis.

An *ORTEP* drawing (Johnson, 1976) of the molecule is shown in Fig. 1. In the thiirane ring, the C—C distance of 1.510 (5) Å is longer than that found (1.468 Å) for the analogous bond in (2S,3S)-1-cyano-2-hydroxy-3,4-epithiobutane-α-naphthylurethane (Bates, Grady & Sneath, 1972). In thiirane itself (Cunningham, Boyd, Myers & Gwinn, 1951), the corresponding bond length is 1.492 Å. The C—S bonds have more normal lengths of 1.832 (5) and 1.804 (4) Å. In the above 3,4-epithiobutane-α-naphthylurethane (Bates *et al.*, 1972), the two C—S distances are 1.802 and 1.815 Å. In 1,3,5,7-tetrathiocane (Frank & Degen, 1973), the average C—S length is 1.817 Å, and in thiirane the experimental (Cunningham *et al.*, 1951) and calculated value (Rohmer & Roos, 1975) is 1.819 Å. However, C—S distances as long as 1.84–1.85 Å have been found, *e.g.* in dibenzyl disulfide (Lee & Bryant, 1969) and in L-α-(p-chlorobenzenesulphonamido)-β-propionothiolactone (Milinovic & Bezjak, 1973).

Bond lengths and angles in the furanosyl ring agree with the mean values reported for these compounds. The asymmetry of the endocyclic bonds [O—C1′ = 1.415 (5) and O—C4′ = 1.442 (5) Å] clearly shows the anomeric effect. The furanosyl ring is not planar and in terms of ring-puckering coordinates (Cremer & Pople, 1975) the amplitude–phase magnitudes are $Q = 0.38$ (1) Å and $\varphi = -59.4$ (6)° for the sequence O—C1′—C2′—C3′—C4′, and the resulting conformation is twist T_4^3 with C_2 symmetry through the C1′ atom [Nardelli (1983) asymmetry parameter $\Delta C_2(C1') = 0.018$ (1)].

Bond lengths and angles in the imidazolidine ring are normal. The bond lengths N1—C1′ 1.454 (5) and N3—C2′ 1.455 (4) Å, and the O2—C2 length of 1.203 (5) Å clearly indicate double-bond character as found in analogous compounds (Conde, Bernier & Márquez, 1980). This partial double-bond character reflects the resonance of the urea system. The remaining bond lengths and angles have expected values within the limits of experimental error. The imidazolidine-2-one group is corrugated (maximum deviation from the best plane is 0.140 Å). The imidazolidine substituents C71 and C1″ are at deviations of 0.123 and −0.067 Å, respectively.

Evidence for steric hindrance is seen in the short intramolecular contacts (Table 3). These may be