[1·342 (6) Å] bond indicate lack of delocalization. The glycosidic link has torsion angles of C(8)—C(7)—O(1′)—C(1′) = −166·3 (4), C(7)—O(1′)—C(1′)—O(5′) = −85·2 (5), O(1′)—C(1′)—O(5′)—C(5′) = −179·2 (4)°. A search of the conformations of all aromatic β-glucopyranosides in the Cambridge Crystallographic Database (Allen *et al.*, 1979) indicates that this conformation and the one related by an 180° rotation about the C(7)—O(1′) bond are the most commonly observed (14 out of 17 observations). All three exceptions have at least one large *ortho* substituent. The crystal packing, illustrated in Fig. 2, shows two different intermolecular interactions that are completely separated: alternating layers of stacked hydrophobic areas and hydrophilic carbohydrate and solvent regions. The molecules stacked along the *b* axis are related to one another by the transformation 1·5−*x*, 0·5±*y*, 2·0−*z*. The shortest stacking distance is 3·423 (9) Å for C(4)—C(8). The superposition of the molecules along the stacking direction is not perfectly perpendicular. Based on the coordinates of the C(9) and C(10) atoms, the atomic centers are offset by 0·33 and −0·33 Å in the **a** and **c** directions respectively. Table 2 shows the intermolecular hydrogen-bonding distances. Since not all H atoms were located it is not possible to assign a complete image of the bonding pattern. Assignment of donors and acceptors for those bonds for which the H atoms were not located is based on the pattern observed in the structure of 7-β-D-glucopyranoside-8-hydroxycoumarin dihydrate (Ueno, Sato & Saito, 1983) which is similar.

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Table 2. *Hydrogen bonding*

Donor		Acceptor	$D\cdots A$ (Å)	$\mathrm{H}\cdots A$ (Å)	D—$\mathrm{H}\cdots A$ (°)
O(2′)	O(6′)	(−0·5+*x*, −0·5+*y*, *z*)	2·679 (5)	1·83 (4)	163 (3)
O(6′)	O(2)	(1·5−*x*, 0·5+*y*, 2·0−*z*)	2·691 (5)	1·88 (5)	156 (4)
O(3′)	O(1*S*)	(*x*, *y*, *z*)	2·690 (6)		
O(4′)	O(3′)	(1·5−*x*, 0·5+*y*, 1·0−*z*)	2·691 (7)	1·68 (6)	167 (4)
O(2*S*)	O(4′)	(*x*, *y*, *z*)	2·832 (7)		
O(1*S*)	O(2*S*)	(−0·5+*x*, 0·5+*y*, *z*)	2·815 (9)	2·23 (5)	109 (3)
O(2*S*)	O(2′)	(0·5+*x*, 0·5+*y*, *z*)	2·947 (8)		

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Structure of 2,5-Bis(ethylenedithio)-7-(2-methoxy-3-methylphenyl)bicyclo[4.2.0]octane

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Abstract. 14-(2-Methoxy-3-methylphenyl)dithiolane-2-spiro-1′-bicyclo[4.2.0]octane-4′-spiro-2″-dithiolane, $C_{20}H_{26}OS_4$, $M_r = 410·69$, monoclinic, $P2_1/c$, $a = 13·850$ (3), $b = 7·453$ (1), $c = 20·161$ (4) Å, $\beta = 104·16$ (2)°, $V = 2017·8$ (6) Å^3, $Z = 4$, $D_x = 1·35$ g cm^{-3}, Mo $K\alpha$ radiation, $\lambda = 0·71069$ Å, $\mu = 4·21$ cm^{-1}, $F(000) = 872·0$, room temperature, $R = 0·062$ and $S = 1·42$ for 3875 independent reflections. The six-membered ring is *cis* fused to the four-membered ring, adopting a flattened chair conformation. The four-membered ring adopts the usual puckered conformation (puckering angle 30·3°) and displays the usual geometrical parameters. The dihedral angle between the best least-squares planes (b.l.s.p.'s) of the six-membered ring and the four-membered ring is 58°. The dihedral angle between the b.l.s.p.'s of the two

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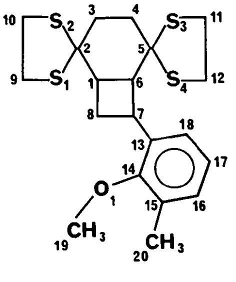
dithiolane groups is 42°. The phenyl ring is nearly perpendicular to the general plane of the rest of the molecule.

Introduction. The title compound (1) occurred in one of the intermediate steps in the process of synthesis of diisocyanoadociane (Baker, Wells, Oberhänsli & Hawes, 1976). The overall structure and the conformation of this synthetic intermediate could not be determined unambiguously by conventional physical methods. Hence an X-ray structural analysis was undertaken.



Experimental. Crystallized from Et_2O/hexane solution; colorless sharp single crystals, 0·5 × 0·4 × 0·3 mm; Nicolet $R3m$ diffractometer, Mo radiation, graphite monochromator; lattice parameters were determined by least-squares fit of 48 reflections (24 Friedel pairs) in the range $16 < 2\theta < 25°$, space group $P2_1/c$. Intensity data were collected in the $\theta/2\theta$ scan mode, $3 \leq 2\theta \leq 60°$, $00\bar{l} \rightarrow hkl$, in 5 shells; 3 intensity check reflections (006; 040; 0,0,10) measured every 60 reflections, intensity of check reflections varied on average by 1·5% and decayed during data collection by about 4%. Intensity data were reduced, corrected for Lorentz and polarization effects, radiation damage and absorption (North, Phillips & Mathews, 1968). Min., max. transmission coefficients 0·91, 0·99. 6790 reflections were measured, of which 5821 were unique ($R_{\rm int}=0{\cdot}02$), and 3947 reflections were $>2{\cdot}0\sigma(F_o)$. For the Patterson function, direct methods and the refinement, only those reflections for which $F_o \geq 3{\cdot}0\sigma(F_o)$ were included (3875 reflections, 67% of the unique data).

The structure was solved by direct methods (*MULTAN*78; Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) in the noncentrosymmetric space group Pc, since neither systematic absences nor intensity statistics suggested a space group with higher symmetry. A fragment of the molecule with about half of the non-H atoms could be recognized in the electron density map. All the other atoms (except 4 H atoms) were located by successive cycles of least-squares refinements on F and difference electron density maps. High correlation factors during refinement suggested a higher internal symmetry. The molecule was then transferred to the centrosymmetric space group $P2_1/c$ resulting in a better R factor and a smoother convergence of the refinement. Conventional blocked full-matrix least-squares techniques were used for refinement of atomic parameters (Sheldrick, 1975; Cruickshank, 1970). All non-H atoms were refined anisotropically (9 parameters per atom), and 22 out of the 26 H atoms were refined isotropically (4 parameters per atom). The 4 H atoms on C(9) and C(10) were positioned at an idealized distance of 1·08 Å from the corresponding C atom, and only their isotropic temperature factors were refined independently. A weighting scheme based on $w = a/[\sigma^2(F) + bF^2]$ was introduced and optimized in the final stages of refinement. The overall scale factor was refined as well. Altogether, 319 parameters (P) in two blocks were refined using 3875 observations (O), $O/P = 12{\cdot}2$. Final $R = 0{\cdot}062$, $wR = 0{\cdot}057$. Final $S = 1{\cdot}42$. In the final cycle of refinement the maximum ratio of shift/e.s.d. was 0·05 where the average ratio was 0·004. In the final difference map, max. and min. electron densities were 0·42 and $-0{\cdot}44$ e Å^{-3}, respectively. Atomic scattering factors were taken from *SHELX*.

Discussion. Final results are presented in Tables 1 and 2* and in Figs. 1 and 2. In the central bicyclo[4.2.0]octane unit, the six-membered ring and the four-membered ring are *cis* fused. As can be seen in a stereodrawing of the molecule (Fig. 1), as well as from the values of the relevant torsion angles (Table 2), the six-membered ring adopts a flattened chair conformation and the four-membered ring adopts a puckered conformation. The conventional parameter used to describe the twist in cyclobutane rings is the dihedral angle between the two opposite planes in the ring (Benedetti, Corradini & Pedone, 1970). In the structure of (1), the dihedral angle between the planes specified by C(8), C(1), C(6) and C(6), C(7), C(8) is 149·7 (1)° (puckering angle 30·3°). Puckering angles in the range 0 (planar) to 35° were reported for free and fused cyclobutanes (Cotton & Frenz, 1974). As has been pointed out before (Barnett & Davis, 1970), it seems that the ring strain in this bicyclo[4.2.0]octane system is mainly accommodated by the more flexible six-membered ring. There is considerable flattening of the ideal chair conformation (torsion angles of 60°), leaving the cyclobutane ring practically undistorted. As a result the substituents on C(1) and C(6) are significantly out of the axial and equatorial orientations, which are ideal for cyclohexane, while the cyclobutane

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* A table of anisotropic thermal parameters, lists of observed and calculated structure factors, a table of coordinates and temperature factors for H atoms and a complete list of structural parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44619 (29 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional atomic coordinates and temperature factors for non-*H *atoms*

	x	y	z	$U_{\rm eq}$*(Å^2)
S(1)	0·0634 (1)	0·1617 (1)	0·0894 (1)	0·0525 (4)
S(2)	−0·0474 (4)	0·3029 (1)	0·1857 (1)	0·0516 (3)
S(3)	0·3338 (1)	0·4607 (1)	0·3060 (1)	0·0461 (3)
S(4)	0·4159 (1)	0·3789 (1)	0·1889 (1)	0·0406 (3)
O(1)	0·3066 (1)	0·4007 (2)	−0·0047 (1)	0·0443 (11)
C(1)	0·1124 (1)	0·4895 (3)	0·1660 (1)	0·0320 (13)
C(2)	0·0772 (1)	0·2937 (4)	0·1696 (1)	0·0353 (13)
C(3)	0·1505 (2)	0·1945 (4)	0·2261 (1)	0·0418 (16)
C(4)	0·2549 (2)	0·1937 (4)	0·2135 (1)	0·0377 (15)
C(5)	0·2994 (1)	0·3823 (3)	0·2178 (1)	0·0288 (12)
C(6)	0·2267 (1)	0·5157 (3)	0·1748 (1)	0·0269 (12)
C(7)	0·2062 (2)	0·5223 (3)	0·0953 (1)	0·0293 (12)
C(8)	0·0972 (2)	0·5720 (4)	0·0944 (1)	0·0392 (16)
C(9)	−0·0635 (3)	0·1035 (9)	0·0742 (3)	0·1107 (39)
C(10)	−0·1011 (3)	0·1142 (6)	0·1344 (2)	0·0839 (30)
C(11)	0·4502 (2)	0·3378 (6)	0·3271 (1)	0·0553 (22)
C(12)	0·5037 (2)	0·3760 (5)	0·2723 (1)	0·0462 (18)
C(13)	0·2652 (1)	0·6447 (3)	0·0608 (1)	0·0287 (12)
C(14)	0·3113 (2)	0·5828 (3)	0·0109 (1)	0·0326 (13)
C(15)	0·3644 (2)	0·6962 (4)	−0·0224 (1)	0·0452 (16)
C(16)	0·3683 (2)	0·8774 (4)	−0·0055 (1)	0·0461 (17)
C(17)	0·3241 (2)	0·9419 (4)	0·0435 (1)	0·0440 (17)
C(18)	0·2735 (2)	0·8271 (4)	0·0766 (1)	0·0379 (15)
C(19)	0·2248 (4)	0·3535 (6)	−0·0601 (2)	0·0672 (28)
C(20)	0·4159 (4)	0·6264 (8)	−0·0751 (2)	0·0788 (32)

* $U_{\rm eq} = \frac{1}{3}$(trace of the orthogonalized U_{ij} matrix).

Table 2. *Important molecular structural parameters*

Selected bond lengths (Å)

C(2)–S(1)	1·862 (3)	C(9)–S(1)	1·763 (5)
C(2)–S(2)	1·833 (3)	C(10)–S(2)	1·796 (5)
C(5)–S(3)	1·821 (3)	C(11)–S(3)	1·812 (4)
C(5)–S(4)	1·846 (3)	C(12)–S(4)	1·818 (3)
C(14)–O(1)	1·392 (3)	C(19)–O(1)	1·426 (5)
C(2)–C(1)	1·546 (4)	C(6)–C(1)	1·562 (4)
C(8)–C(1)	1·536 (4)	C(3)–C(2)	1·520 (4)
C(4)–C(3)	1·528 (5)	C(5)–C(4)	1·529 (4)
C(6)–C(5)	1·526 (3)	C(7)–C(6)	1·559 (4)
C(8)–C(7)	1·551 (4)	C(13)–C(7)	1·503 (4)
C(10)–C(9)	1·435 (8)	C(12)–C(11)	1·500 (6)

Selected bond angles (°)

C(9)–S(1)–C(2)	99·6 (2)	C(10)–S(2)–C(2)	98·3 (2)
C(11)–S(3)–C(5)	94·1 (2)	C(12)–S(4)–C(5)	98·4 (1)
C(19)–O(1)–C(14)	113·7 (3)	C(6)–C(1)–C(2)	115·8 (2)
C(8)–C(1)–C(2)	116·7 (2)	C(8)–C(1)–C(6)	87·6 (2)
S(2)–C(2)–S(1)	105·8 (1)	C(1)–C(2)–S(1)	115·2 (2)
C(1)–C(2)–S(2)	107·1 (2)	C(3)–C(2)–S(1)	107·6 (2)
C(3)–C(2)–S(2)	111·7 (2)	C(3)–C(2)–C(1)	109·5 (2)
C(4)–C(3)–C(2)	111·3 (3)	C(5)–C(4)–C(3)	111·8 (3)
S(4)–C(5)–S(3)	105·8 (1)	C(4)–C(5)–S(3)	110·9 (2)
C(4)–C(5)–S(4)	109·9 (2)	C(6)–C(5)–S(3)	108·9 (2)
C(6)–C(5)–S(4)	109·6 (2)	C(6)–C(5)–C(4)	111·5 (2)
C(5)–C(6)–C(1)	119·5 (2)	C(7)–C(6)–C(1)	87·9 (2)
C(7)–C(6)–C(5)	122·3 (2)	C(8)–C(7)–C(6)	87·2 (2)
C(13)–C(7)–C(6)	120·7 (2)	C(13)–C(7)–C(8)	119·2 (2)
C(7)–C(8)–C(1)	89·1 (2)	C(10)–C(9)–S(1)	113·1 (4)
C(9)–C(10)–S(2)	110·2 (4)	C(12)–C(11)–S(3)	107·6 (3)
C(11)–C(12)–S(4)	110·1 (2)	C(14)–C(13)–C(7)	121·9 (2)
C(18)–C(13)–C(7)	120·7 (3)	C(18)–C(13)–C(14)	117·3 (3)
C(13)–C(14)–O(1)	118·8 (3)	C(15)–C(14)–O(1)	118·9 (3)

Selected torsion angles (°) (average e.s.d. 0·50°)

C(1)–C(2)–C(3)–C(4)	−59·42	C(2)–C(3)–C(4)–C(5)	65·94
C(3)–C(4)–C(5)–C(6)	−49·32	C(4)–C(5)–C(6)–C(1)	32·25
C(5)–C(6)–C(1)–C(2)	−29·16	C(6)–C(1)–C(2)–C(3)	40·85
C(1)–C(6)–C(7)–C(8)	21·19	C(6)–C(7)–C(8)–C(1)	−21·54
C(7)–C(8)–C(1)–C(6)	21·51	C(8)–C(1)–C(6)–C(7)	−21·40

substituents are in a normal orientation for a puckered conformation.

Except for the phenyl ring, all the other rings in the structure are not planar; however it is convenient to describe the overall structure in terms of the best least-squares plane (b.l.s.p.) of the rings involved. The dihedral angles between these planes are defined as the angles between the vectors which are perpendicular to the b.l.s.p.'s. Considering this, the b.l.s.p. of the six-membered ring forms a dihedral angle of 58 (1)° with the b.l.s.p. of the four-membered ring (folding angle 122°). The b.l.s.p.'s of the two dithiolane groups form a dihedral angle of 42 (1)° between each other, and these planes are related to the b.l.s.p. of the six-membered ring by dihedral angles of 100(1) and 74(1)°, respectively. The phenyl ring is practically planar and it is approximately perpendicular to the rest of the molecule. Its l.s.p. forms an angle of 89·0 (2)° with the b.l.s.p. of the four-membered ring.

The average C–C bond in the four-membered ring is 1·55 (1) Å and the average bond angle is 87·9 (2)°, in accordance with the values reported for similar systems (Adman & Margulis, 1968; Barnett & Davis, 1970; Benedetti, Corradini & Pedone, 1970; Cotton & Frenz, 1974; Brückner, Pitacco & Valentin, 1975). Distances and angles elsewhere in the molecule are not unusual. Shorter than normal bond lengths and a slight flattening in one of the dithiolane groups are probably due to the high temperature factors and the small disorder of C(9) and C(10). No unusually short intermolecular contacts were found in the crystal packing (Fig. 2).

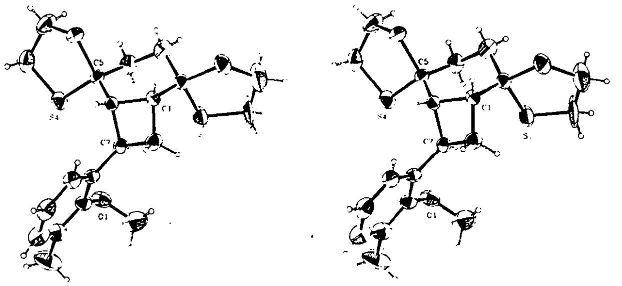

Fig. 1. Stereodrawing of (1) (*ORTEP*; Johnson, 1976).

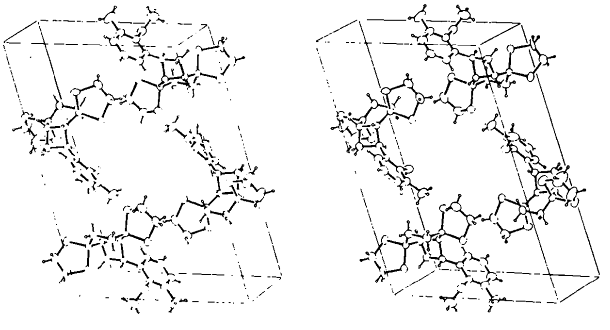

Fig. 2. Stereoview of the unit-cell packing of (1) (*ORTEP*).

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Structure of 5-Methyl-2′-deoxycytidine

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Abstract. $C_{10}H_{15}N_3O_4$, $M_r = 241{\cdot}2$, orthorhombic, $P2_12_12_1$, $a = 10{\cdot}454$ (1), $b = 11{\cdot}922$ (1), $c = 9{\cdot}057$ (1) Å, $V = 1128{\cdot}9$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}419$ Mg m^{-3}, Cu $K\alpha$ radiation, $\lambda = 1{\cdot}54178$ Å, $\mu = 0{\cdot}95$ mm^{-1}, $F(000) = 512$, room temperature, $R = 0{\cdot}029$ for 1186 observed reflections. The molecule has a typical C(2′)-*endo* (^2E) furanose ring associated with an *anti* base. The methyl substituent at C(5) causes a decrease of 2·6° in the endocyclic bond angle at C(5). The ring oxygen O(4′) is involved in an intermolecular hydrogen bond.

Introduction. Some of the cytosine residues in DNA are reversibly methylated at the C(5) position. Such a methylation causes a profound effect on the conformation of DNA (Behe & Feldsenfeld, 1980) and gene expression (Radin & Riggs, 1980; Ehrlich & Wang, 1981). Consequently, it is of interest to study the stereochemical effect of the substitution. Previous studies on the crystal structures of 5-methylcytosine (Takenaka, Kato & Sasada, 1980) and 5-methylarabinosylcytosine (Birnbaum & Gentry, 1983) have demonstrated a significant deformation of the pyrimidine ring on the substitution.

Experimental. Crystals grown from methanol/acetone, colorless plate, D_m not measured. Crystal dimensions 0·2 × 0·2 × 0·3 mm, Rigaku AFC-5 diffractometer, graphite-monochromated Cu $K\alpha$ radiation. Lattice parameters from 24 reflections ($50 < 2\theta < 58°$). $\omega/2\theta$ scan, $2\theta \leq 140°$, $0 \leq h \leq 12$, $0 \leq k \leq 14$, $0 \leq l \leq 11$, three standard reflections: no variation. 1199 independent reflections measured, 1186 with $I \geq 2\sigma(I)$ considered observed. No absorption correction. Structure solved by direct methods, H atoms located from a difference Fourier map and their positions and isotropic thermal parameters refined. Full-matrix least-squares refinement, anisotropic thermal parameters for non-H atoms, isotropic type I extinction correction (Becker & Coppens, 1974) with $g = 0{\cdot}52\ (2) \times 10^{-4}$, $\sum w(\Delta F)^2$ minimized, $w = 1$, $R = 0{\cdot}029$, $wR = 0{\cdot}029$, final $(\text{shift}/\sigma)_{\max} < 0{\cdot}3$, $-0{\cdot}15 \leq \Delta\rho \leq 0{\cdot}12$ e Å^{-3}. The final atomic parameters are given in Table 1.* Bond distances and angles are listed in Table 2.

All crystallographic computations were performed on a VAX11/780 computer using the program system *XTAL*2.2 (Hall & Stewart, 1987) with the scattering factors as included in the program.

Discussion. A perspective view of the molecule is shown in Fig. 1. The nucleoside adopts one of the most commonly observed conformations. The pseudorotation coordinates (Sato, 1983) of the furanose ring are $\Pi = 37{\cdot}9\ (3)°$ and $\Phi = 252{\cdot}7\ (4)°$ and, therefore, the

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* Lists of hydrogen-atom parameters, anisotropic thermal parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44672 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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