Table 1. *Selected geometric parameters (Å, °)*

O3—C3	1.364 (2)	C8—C14	1.494 (2)
O17—C17	1.216 (3)	C8—C9	1.5140 (19)
C5—C6	1.509 (2)	C9—C10	1.5122 (19)
C6—C7	1.496 (2)	C9—C11	1.546 (2)
C7—C8	1.324 (2)		
O3—C3—C4	117.94 (16)	C17—C13—C14	99.20 (13)
O3—C3—C2	122.73 (15)	C12—C13—C14	110.53 (12)
C4—C3—C2	119.33 (15)	C18—C13—C14	112.26 (14)
C8—C7—C6	124.03 (14)	C8—C14—C15	122.46 (15)
C7—C8—C14	125.80 (14)	C8—C14—C13	110.61 (12)
C7—C8—C9	122.88 (14)	C15—C14—C13	104.39 (13)
C14—C8—C9	111.27 (13)	C14—C15—C16	101.82 (15)
C13—C12—C11	110.18 (14)	C17—C16—C15	106.09 (15)
C17—C13—C12	117.01 (15)	O17—C17—C13	126.02 (18)
C17—C13—C18	106.44 (13)	O17—C17—C16	125.57 (18)
C12—C13—C18	110.91 (14)	C13—C17—C16	108.37 (16)

Structure solution was conducted by direct methods using *SHELXS*96 (Sheldrick, 1996) and the structure was refined using *SHELXL*97 (Sheldrick, 1997). H atoms were generated and refined as riding groups, except for H3 (bound to O3), which was located from a difference Fourier map.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1995). Molecular graphics: *CHAIN* (Sack, 1988). Software used to prepare material for publication: *ORTEP*III (Burnett & Johnson, 1996).

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N,*N*-Dimethyl-5-methoxymethyl-2′-deoxycytidine

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Abstract

In the title compound, $C_{13}H_{21}N_3O_5$, the pyrimidine ring adopts the antiperiplanar (*−ap*) conformation [χ = 193.54 (19)°]. The deoxyribose sugar ring has the C2′-*exo*–C3′-*endo* ($_2T^3$) twist conformation. The pseudorotational parameters of the deoxyribose sugar ring are P = 6.83 (2)° and τ_m = 38.27 (2)°. The exocyclic side chain at C5′ has the g^+ conformation [γ = 47.7 (3)°]. The 5-methoxymethyl group is distal to the deoxyribose sugar ring, with a C6—C5—C52—O52 torsion angle of −91.9 (3)°.

Comment

Our studies on 2′-deoxycytidine nucleoside analogues with selectivity against the *Herpes simplex* virus (HSV) have shown that substituents at the C5 position of the pyrimidine ring play an important role in biological activity (Gupta *et al.*, 1991, 1993; Stuart *et al.*, 1997). When deamination is prevented, 5-methoxymethyl-2′-deoxycytidine (MMdCyd) and (*E*)-5-(2-bromovinyl)-2′-deoxycytidine (BrVdCyd) are potent and selective anti-herpes agents (Aduma, Gupta, Stuart & Tourigny, 1990; Aduma, Gupta & De Clercq, 1990; Jia *et al.*, 1990*a*; Gupta *et al.*, 1991, 1993). Systematic investigations on the modification of the cytosine (N^4) moiety have indicated that substituents on the N^4 position have profound influence on biological activity (Zoghaib, Kamaly, Kumar *et al.*, 1996; Zoghaib, Kamaly, De Clercq *et al.*, 1996; Gupta, unpublished results). As part of this research programme, our studies have shown that loss of bio-activity is due to the conformation of the molecule (Jia *et al.*, 1990*b*; Gupta *et al.*, 1992; Audette *et al.*, 1997; Audette *et al.*, 1998).

N,*N*-Dimethyl-5-methoxymethyl-2′-deoxycytidine [*N*,*N*-dimethyl-MMdCyd], (I), was prepared in order to

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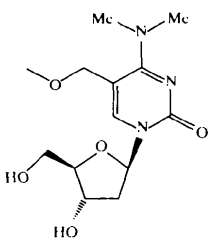
gain more information on the relationship between the alkyl substituents on the cytosine moiety, the steric conformation of the furanose ring and the conformations of the 5-methoxymethyl and 5′-CH_2OH side chains on the antiviral activity. *N,N*-Dimethyl-MMdCyd is devoid of anti-HSV activity (Zoghaib, 1996; Zoghaib, Kamaly, Kumar *et al.*, 1996). In this report, the molecular structure of *N,N*-dimethyl-MMdCyd is presented.



(I)

Selected bond lengths and angles of *N,N*-dimethyl-MMdCyd (Fig. 1) are summarized in Table 1; they are similar in range to those reported for other 2′-deoxycytidine nucleosides (Young & Wilson, 1975; Sato, 1988; Jia *et al.*, 1990*a*,*b*; Audette *et al.*, 1997; Audette *et al.*, 1998). Intermolecular hydrogen bonds occurring between symmetry-related molecules are summarized in Table 2.

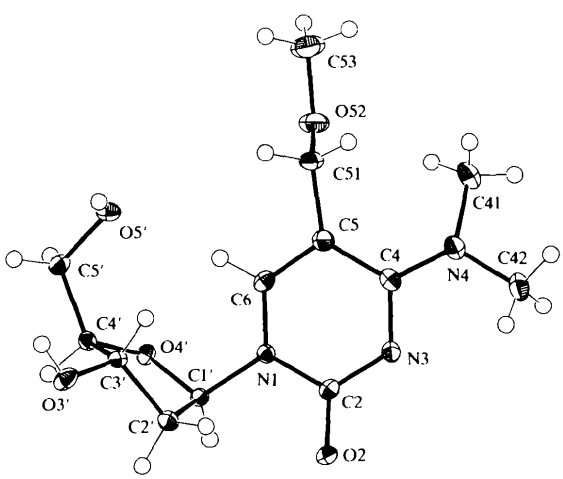


Fig. 1. A perspective *ORTEP*II (Johnson, 1976) plot of *N,N*-dimethyl-MMdCyd. All non-H atoms are drawn with displacement ellipsoids at the 50% probability level, and for clarity, all H atoms are shown as spheres of small arbitrary size.

In the title compound, the pyrimidine ring adopts the antiperiplanar (−*ap*) conformation, with χ = 193.54 (19)°. Interestingly, the glycosidic bond conformation is identical to N^4-methyl-MMdCyd [χ = 193.8 (2)], which is also devoid of anti-HSV activity (Jia *et al.*, 1990*b*). The *anti* conformation has also been found for other deoxycytidine nucleoside analogues (Young & Wilson, 1975; Jia *et al.*, 1990*a*; Audette *et al.*, 1997; Audette *et al.*, 1998). However, the χ values for other 2′-deoxycytidine nucleosides are higher ($\chi \sim$ 210–245°) compared to *N,N*-dimethyl-MMdCyd.

The deoxyribose sugar ring of *N,N*-dimethyl-MMdCyd adopts the C2′-*exo*–C3′-*endo* ($_2T^3$) twist conformation. The pseudorotational parameters (Altona & Sundaralingam, 1972) of the furanose ring are the pseudorotational phase angle P = 6.83 (2)° and puckering amplitude τ_m = 38.27 (2)°. A similar conformation for the deoxyribose moiety was also found for 3,4-etheno-MMdCyd, another inactive analogue of this series (Audette *et al.*, 1997). The $_2T^3$ conformation of *N,N*-dimethyl-MMdCyd differs from the C2′-*endo* (^2E) envelope conformation, most commonly found in 2′-deoxycytidine compounds (Young & Wilson, 1975; Sato, 1988; Jia *et al.*, 1990*a*; Audette *et al.*, 1998).

The exocyclic C5′—CH_2OH side chain of *N,N*-dimethyl-MMdCyd adopts the g^+ conformation [γ = 47.7 (3)°]. Although the g^+ conformation is the most common for the side chain at C5′ for cytidine and 2′-deoxycytidine nucleosides (Young & Wilson, 1975; Jia *et al.*, 1990*a*; Audette *et al.*, 1997; Audette *et al.*, 1998), some 2′-deoxycytidine analogues display the *t* conformation (Sato, 1988; Jia *et al.*, 1990*b*; Napper *et al.*, 1995).

The N^4-methyl groups of *N,N*-dimethyl-MMdCyd have a *cis*/*trans* orientation with respect to N^3, with an N3—C4—N4—C4*x* torsion angle of 159.5 (2)° for C41 (*trans*) and −11.8 (4)° for C42 (*cis*). The *cis* relationship between the N^4 substituent and N^3 appears to be a common feature among N^4-substituted 2′-deoxycytidine analogues (Takahashi *et al.*, 1988; Jia *et al.*, 1990*b*; Audette *et al.*, 1997; Audette *et al.*, 1998).

The 5-methoxymethyl substituent on the pyrimidine is distal to the deoxyribose sugar ring, and the C6—C5—C51—O52 torsion angle is −91.9 (3)°. This orientation was also found for the inactive analogue N^4-methyl-MMdCyd (Jia *et al.*, 1990*b*), as well as in both molecules of the active lead compound MMdCyd (Jia *et al.*, 1990*a*). In contrast, the 5-methoxymethyl substituent in 3,4-etheno-MMdCyd (an inactive analogue) is proximal to the deoxyribose sugar (Audette *et al.*, 1997).

MMdCyd and BrVdCyd are selectively phosphorylated (activated) by the virus-induced pyrimidine kinase (HSV-TK). Thus, the orientation of the deoxyribose sugar ring and disruption of the hydrogen-bonding capacity of the N^4 group in *N,N*-dimethyl-MMdCyd provide insights for its inactivity. Although the exocyclic C5′—CH_2OH side chain is in the favourable g^+ rotamer conformation (Gupta *et al.*, 1987; Gupta *et al.*, 1992; Jia *et al.*, 1990*a*; Stuart *et al.*, 1997), the $_2T^3$ twist conformation of the sugar ring results in negligible phosphorylation by the HSV-TK, and physiologically significant levels of the monophosphate are not formed in infected cells. In addition, the lack of the N^4 group's

capacity to be a hydrogen-bond donor possibly inhibits interaction of the compound with the HSV–TK.

Experimental

The title compound was prepared from 3′,5′-diacetyl-N^4,N^4-dimethyl-5-methoxymethyl-2′-deoxyuridine, using the triazolization procedure followed by treatment with methanolic ammonia (Jia *et al.*, 1990*a*; Zoghaib, 1996). High quality single crystals were obtained using the vapour diffusion method, with methanol as the solvent and diethyl ether as the precipitant, at 287 K.

Crystal data

$C_{13}H_{21}N_3O_5$
M_r = 299.33
Orthorhombic
$P2_12_12_1$
a = 4.906 (3) Å
b = 14.838 (5) Å
c = 19.488 (3) Å
V = 1418.6 (10) Å^3
Z = 4
D_x = 1.401 Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
λ = 0.70930 Å
Cell parameters from 25 reflections
θ = 8.30–26.26°
μ = 0.108 mm^{-1}
T = 123 (2) K
Rod
0.42 × 0.20 × 0.15 mm
Colourless

Data collection

Nonius CAD-4 diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.878, T_{max} = 0.984
1702 measured reflections
1702 independent reflections

1447 reflections with $I > 2\sigma(I)$
θ_{max} = 26.26°
$h = -1 \rightarrow 6$
$k = -2 \rightarrow 18$
$l = -7 \rightarrow 24$
3 standard reflections
frequency: 240 min
intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.037
$wR(F^2)$ = 0.090
S = 1.065
1702 reflections
195 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2 + 0.1106P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.188 e Å^{-3}
$\Delta\rho_{min}$ = −0.189 e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

C2—O2	1.242 (3)	C5—C51	1.514 (3)
C4—N4	1.341 (3)	C51—O52	1.424 (3)
N4—C41	1.459 (3)	O52—C53	1.426 (3)
N4—C42	1.460 (4)		
O2—C2—N3	123.4 (2)	C4—C5—C51	126.8 (2)
C4—N4—C41	124.0 (2)	O52—C51—C5	111.1 (2)
C4—N4—C42	121.6 (2)	C51—O52—C53	110.5 (2)
C41—N4—C42	113.9 (2)		
N3—C4—N4—C41	159.5 (2)	C1′—C2′—C3′—C4′	38.0 (2)
N3—C4—N4—C42	−11.8 (4)	C2′—C3′—C4′—O4′	−34.1 (2)
C6—C5—C51—O52	−91.9 (3)	C2′—C1′—O4′—C4′	7.9 (2)
C2—N1—C1′—O4′	−166.46 (19)	C3′—C4′—O4′—C1′	16.9 (2)
O4′—C1′—C2′—C3′	−29.1 (2)	C3′—C4′—C5′—O5′	47.7 (3)

Table 2. *Hydrogen-bonding geometry (Å, °)*

D—H···A	D—H	H···A	D···A	D—H···A
O3′—H3′1···N3^{i}	0.82	2.06	2.872 (3)	172.3
O5′—H5′···O2^{i}	0.82	1.90	2.713 (2)	169.8

Symmetry code: (i) $1-x, \frac{1}{2}+y, \frac{3}{2}-z$.

Determination of the absolute configuration of (I) was not possible in the present X-ray analysis, due to the absence of suitable anomalous scatterers within the molecule. However, the configuration chosen (Fig. 1) is consistent with both the configuration of the parent molecule (D-2′-deoxyuridine), as well as with the knowledge gained from previous chemical, crystallographic and NMR studies of this series of compounds (Jia *et al.*, 1990*a*,*b*; Zoghaib, 1996; Audette *et al.*, 1997; Audette *et al.*, 1998). Hydroxyl and methyl H atoms were located using difference maps, and all other H atoms were placed in calculated positions (*SHELXL*97; Sheldrick, 1997). All H atoms were refined using the riding model.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1992). Cell refinement: *SET*4 in *CAD*-4 *EXPRESS*. Data reduction: *Xtal*3.4 (Hall *et al.*, 1995). Program(s) used to solve structure: *Xtal*3.4. Program(s) used to refine structure: *SHELXL*97. Molecular graphics: *ORTEP*II (Johnson, 1976).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: DA1046). Services for accessing these data are described at the back of the journal.

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Self-assembled triple helices in the hydrogen-bonded structure of 2,2′-biphenol–4,4′-bipyridyl (1/1)†

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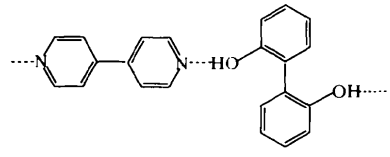
Abstract

In the hydrogen-bonded structure of the title compound, $C_{12}H_{10}O_2{\cdot}C_{10}H_8N_2$, the molecular components are linked by O—H···N hydrogen bonds having O···N distances of 2.793 (3) and 2.750 (3) Å into $C_2^2(16)$ chains which are coiled round 2_1 screw axes forming triple helices.

Comment

When bis-phenols form hydrogen-bonded adducts with di-tertiary amines, the supramolecular structures are generally based upon chains of alternating bis-donors and bis-acceptors of hydrogen bonds. When the molecular components have only very limited torsional flexibility, the chains are generally simple and uncoiled, while the presence of torsional degrees of freedom in the molecular components often permits the chains to coil (Coupar *et al.*, 1997; Ferguson, Bell *et al.*, 1997; Ferguson, Coupar & Glidewell, 1997). In 4,4′-biphenol, the distance between the two hydroxyl O atoms, and their mutual orientation, is independent of any rotation about the central C—C bond. Hence, when this phenol forms a hydrogen-bonded adduct with the rigid diamine 1,4-diazabicyclo[2.2.2]octane, the supramolecular structure consists of long, non-folded chains (Ferguson *et al.*, 1998). However, in the isomeric 2,2′-biphenol the essentially free rotation about the central C—C bond allows a range of inter-oxygen distances, and in most of its non-planar conformations this phenol will introduce bends into any chain of which it is a component. Hence, chains resulting from adduct formation are expected to be folded (Ferguson, Bell *et al.*, 1997). Here we report the structure of the 1:1 adduct, (I), formed between 2,2′-biphenol and 4,4′-bipyridyl in which the chains are coiled into triple helices.



(I)

Compound (I) crystallizes in the centrosymmetric space group $P2_1/n$ with one molecule of each component in the asymmetric unit (Fig. 1). The components are linked into continuous chains by means of O—H···N hydrogen bonds, but there is no evidence of any proton transfer from the phenol to the diamine. Within the asymmetric unit, atom O1 acts as a hydrogen-bond donor to N34 (Table 2). In addition, atom O2 at (x, y, z) acts as a donor to N44 at ($0.5 - x$, $-1.5 + y$, $0.5 - z$), while O2 at ($0.5 - x$, $-1.5 + y$, $0.5 - z$) acts in turn as donor to N44 at (x, $-3 + y$, z). The resulting chain, generated by the 2_1 screw axis at (0.25, y, 0.25), thus has a repeat period of three unit cells and so there are three identical but independent chains generated by this single screw axis. These chains are thus coiled together to form a triple helix (Fig. 2). Four such triple helices, two of each hand, run through each unit cell.

Such self-assembled multiple helices are not unprecedented in hydrogen-bonded adducts between phenols and poly-aza acceptors. Thus in adducts with hexamethylenetetramine, $(CH_2)_6N_4$, the bis-phenol 4,4′-isopropylidenediphenol, $Me_2C(C_6H_4OH)_2$, forms double helices and the tris-phenol 1,1,1-tris(4-hydroxyphenyl)-ethane, $CH_3C(C_6H_4OH)_3$, forms triple helices (Coupar *et al.*, 1997). On the other hand, the molecular components of compound (I) probably represent the simplest building blocks hitherto reported as capable of generating a multiple-helical structure by self-assembly.

† IUPAC name: 2,2′-biphenyldiol–4,4′-bipyridyl (1/1).