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## 1,10-Decanediol

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### Abstract

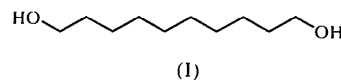
An all-*trans* conformation is observed in the hydrocarbon skeleton of the title compound,  $C_{10}H_{22}O_2$ , and both terminal hydroxyl groups are also *trans*. The centrosymmetric molecules are arranged in a zigzag manner to make a herring-bone motif, which can be regarded as a model structure of smectic C liquid crystals. These features are very similar to those of the homologues with an even number of C atoms, but different from those with an odd number.

### Comment

Crystal structures of many different kinds of monosubstituted long-chain compounds, for example *n*-higher alcohols, have been studied by several workers (*e.g.* Watanabe, 1961; Seto, 1962). However, there are few reports about  $\alpha,\omega$ -disubstituted *n*-alkanes.

These compounds have a simple linear hydrocarbon chain as a skeleton. The molecular shape could be regarded as a rod-like one, which is one of the typical features of liquid crystalline molecules. Such rod-like molecules in general construct a layer structure similar to the smectic phase found in liquid crystals. One of the present authors reported phase-transition phenomena of long chain  $\alpha,\omega$ -alkanediols from  $C_{13}$  to  $C_{24}$  with another researcher (Ogawa & Nakamura, 1999). In addition to this, we have determined crystal structures of five  $\alpha,\omega$ -alkanediols, 1,11-undecanediol (Nakamura *et al.*, 1999), 1,12-dodecanediol (Nakamura & Setodoi, 1997), 1,13-tridecanediol (Nakamura *et al.*, 1997), 1,14-tetradecanediol (Nakamura & Sato, 1999) and 1,16-hexadecanediol (Nakamura & Yamamoto, 1994). Although the crystal structure of 1,10-decanediol, (I), has already been reported (Wang *et al.*, 1994), it was derived from two-dimensional data; we have obtained a more

extensive single-crystal data set. The results are in good agreement.



The molecular structure of 1,10-decanediol, (I), is shown in Fig. 1. The hydrocarbon skeleton has an all-*trans* conformation and both terminal hydroxyl groups are also *trans* with respect to the skeleton. The centrosymmetric molecules form a layer structure perpendicular to the longest axis and make a herring-bone structure. The inclination angle of the long axis of the molecule to the layer plane is equal in each layer, but the direction of the long axis is opposite in alternate layers as is shown in Fig. 2. This structure could be regarded as a model structure of smectic C liquid crystals.

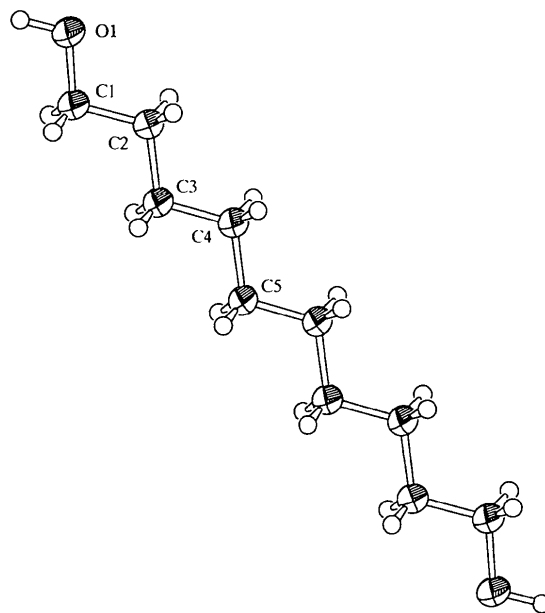


Fig. 1. The title molecule showing the crystallographic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

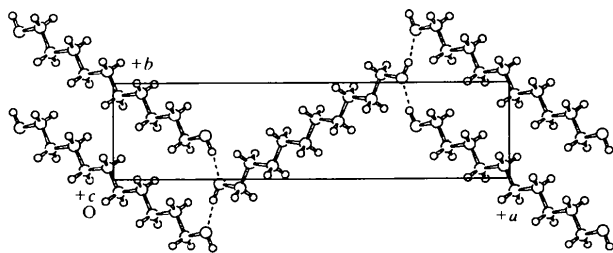


Fig. 2. The projection of the crystal structure along the *c* axis. Dashed lines indicate the hydrogen bonds.

These features are very similar to those of 1,12-dodecanediol, 1,14-tetradecanediol and 1,16-hexadecanediol and agree with those reported by Wang *et al.* (1994). In this structure, the molecules form interlayer hydrogen bonds. The interlayer hydrogen bonding O1...O1<sup>ii</sup> distance is 2.818 (1) Å. This value is in good agreement with those of 1,12-dodecanediol, 1,14-tetradecanediol and 1,16-hexadecanediol [2.823 (2), 2.831 (1) and 2.839 (2) Å, respectively]. The herring-bone motif has also been observed in  $\alpha,\omega$ -dibromoalkanes with an even number of C atoms, for example, 1,12-dibromododecane (Kupke *et al.*, 1981) and 1,16-dibromohexadecane (Kobayashi *et al.*, 1995). On the other hand, the homologous  $\alpha,\omega$ -alkanediols with an odd number of C atoms (1,11-undecanediol and 1,13-tridecanediol) have different molecular and crystal structures as has been reported in our previous papers.

Although the hydrocarbon skeleton is the all-*trans* conformation, one of the terminal hydroxyl groups is *gauche* with respect to the skeleton, whereas the other is *trans*. The *gauche* conformation of the hydroxyl group has been observed in 1-heptadecanol (Seto, 1962). The molecules lie parallel along the longest axis and form layers similar to the smectic A structure of liquid crystals. In this structure, the molecules form two different types of hydrogen bond, inter- and intralayer.

## Experimental

Commercially available 1,10-decanediol (Tokyo Kasei Kogyo Co. Ltd) was used after repeated recrystallizations. The single crystal used for the analysis was grown from a mixture of acetone and heptane by slow evaporation.

### Crystal data

C <sub>10</sub> H <sub>22</sub> O <sub>2</sub>	Cu K $\alpha$ radiation
$M_r = 174.28$	$\lambda = 1.5418 \text{ \AA}$
Monoclinic	Cell parameters from 25 reflections
$P2_1/a$	$\theta = 9.5\text{--}22.1^\circ$
$a = 21.148 (2) \text{ \AA}$	$\mu = 0.570 \text{ mm}^{-1}$
$b = 5.160 (2) \text{ \AA}$	$T = 298.2 \text{ K}$
$c = 4.940 (1) \text{ \AA}$	Cube
$\beta = 96.69 (1)^\circ$	$0.10 \times 0.10 \times 0.10 \text{ mm}$
$V = 535.4 (2) \text{ \AA}^3$	Colourless
$Z = 2$	
$D_x = 1.081 \text{ Mg m}^{-3}$	
$D_m = 1.089 \text{ Mg m}^{-3}$	
$D_m$ measured by flotation in aqueous KI solution	

### Data collection

Rigaku AFC-5R diffractometer	804 reflections with $I > 2\sigma(I)$
$\omega$ - $2\theta$ scans	$R_{\text{int}} = 0.011$
Absorption correction: $\psi$ scan (North <i>et al.</i> , 1968)	$\theta_{\text{max}} = 70^\circ$
$T_{\text{min}} = 0.875$ , $T_{\text{max}} = 0.945$	$h = -25 \rightarrow 25$
	$k = 0 \rightarrow 6$
	$l = -6 \rightarrow 6$

2187 measured reflections  
1281 independent reflections

3 standard reflections  
every 200 reflections  
intensity decay: 3.96%

### Refinement

Refinement on  $F$

$R = 0.039$   
 $wR = 0.063$   
 $S = 1.40$   
804 reflections  
55 parameters  
H atoms: see below  
 $w = 1/[\sigma^2(F_o) + 0.00126|F_o|^2]$

$(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.07 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.11 \text{ e \AA}^{-3}$   
Extinction correction: none  
Scattering factors from  
*International Tables for Crystallography* (Vol. C)

Table 1. Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

O1—C1	1.419 (1)	C3—C4	1.519 (2)
C1—C2	1.504 (2)	C4—C5	1.524 (1)
C2—C3	1.524 (2)	C5—C5'	1.518 (2)
O1—C1—C2	109.2 (1)	C3—C4—C5	113.4 (1)
C1—C2—C3	112.4 (1)	C4—C5—C5'	113.6 (1)
C2—C3—C4	113.3 (1)		

Symmetry code: (i)  $2 - x, -y, 2 - z$ .

Table 2. Contact distances ( $\text{\AA}$ )

O1...O1 <sup>ii</sup>	2.818 (1)	O1...C1 <sup>iii</sup>	3.459 (2)
O1...O1 <sup>iii</sup>	2.818 (1)	O1...C2 <sup>ii</sup>	3.551 (2)

Symmetry codes: (ii)  $\frac{1}{2} - x, \frac{1}{2} + y, -z$ ; (iii)  $\frac{1}{2} - x, y - \frac{1}{2}, -z$ .

All H atoms including hydroxyl-H atoms were fixed in idealized positions.

Data collection: *MSCI/AFD Diffractometer Control Software* (Molecular Structure Corporation, 1992). Cell refinement: *MSCI/AFD Diffractometer Control Software*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1995). Program(s) used to solve structure: *SAPI91* (Fan, 1991). Program(s) used to refine structure: *TEXSAN*. Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *TEXSAN*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: CF1316). Services for accessing these data are described at the back of the journal.

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## 1,14-Tetradecanediol

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### Abstract

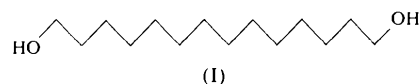
An all-*trans* conformation is observed in the hydrocarbon skeleton, C<sub>14</sub>H<sub>30</sub>O<sub>2</sub>, and both terminal hydroxyl groups are also *trans*. The centrosymmetric molecules are arranged in a zigzag manner to form a herring-bone motif, which can be regarded as a model structure for the liquid crystal smectic C phase. These features are very similar to those of the homologues with an even number of C atoms, but different from those with an odd number.

### Comment

Long chain aliphatic compounds have been studied from the point of view of basic models of both liquid crystals and polymers. These compounds have a simple straight hydrocarbon chain as a skeleton. The molecular shape can be regarded as rod-like, which is one of the typical features of liquid crystal molecules. Therefore, these compounds in general show a layer structure similar to that found in the smectic phase of liquid crystals.

Crystal structures of many different kinds of mono-substituted long chain compounds, for example the longer chain alcohols, have been studied (*e.g.* Watanabe,

1961; Seto, 1962). Recently, we reported crystal structures of four  $\alpha,\omega$ -alkanediols, namely 1,11-undecanediol (Nakamura *et al.*, 1999), 1,12-dodecanediol (Nakamura & Setodoi, 1997), 1,13-tridecanediol (Nakamura *et al.*, 1997) and 1,16-hexadecanediol (Nakamura & Yamamoto, 1994). Here, we present the crystal structure of 1,14-tetradecanediol, (I).



The molecular structure of (I) is shown in Fig. 1. The hydrocarbon skeleton has an all-*trans* conformation and both terminal hydroxyl groups are also *trans* with respect to the skeleton. The centrosymmetric molecules form a layer structure stacked along *c*. The inclination angle of the long axis of the molecule to the layer plane is equal in each layer, but the direction of the long axis is opposite in alternate layers (Fig. 2) because of the existence of a twofold screw axis parallel to *b*. Such herring-bone structures can be regarded as models of smectic C liquid crystals. These features are very similar to those of 1,12-dodecanediol and 1,16-hexadecanediol. The inclination angles of the molecules to the layer plane in 1,12-dodecanediol, 1,14-tetradecanediol and 1,16-hexadecanediol are 56.0(1), 55.8(1) and 55.9(1)°, respectively, *i.e.* no significant difference was observed. The molecules form interlayer hydrogen bonds, with an interlayer hydrogen-bonding distance O1...O1 = 2.831(1) Å. The herring-bone motif was also observed in 1,12-dibromododecane (Kupke *et al.*, 1981) and 1,16-dibromohexadecane (Kobayashi *et al.*, 1995).

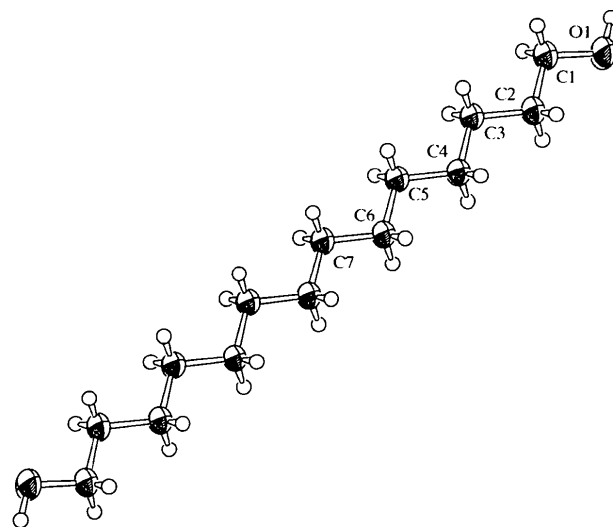


Fig. 1. An ORTEP (Johnson, 1976) view of the title molecule showing the crystallographic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.