

Octadecane-1,18-diol

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Key indicators

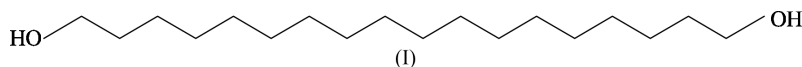
Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.045
 wR factor = 0.065
Data-to-parameter ratio = 10.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The skeleton of the title molecule, $\text{C}_{18}\text{H}_{38}\text{O}_2$, is all-*trans* and the molecules aggregate to form a layer structure along the c axis as in a smectic C liquid crystal. The inclination angle of the long axis of the molecule to the layer plane is the same in each layer, but the direction of the long axis is opposite in alternate layers. 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 long-chain compounds such as n -alkanes (Müller, 1928) and n -higher primary alcohols (e.g. Watanabe, 1961; Seto, 1962), have been studied by many researchers from the viewpoint of basic polymer science. According to those results, the compounds have a simple straight hydrocarbon chain as a skeleton and the molecular shape can be regarded as rod-like, which is one of the typical features of liquid crystal molecules. In addition, some long-chain compounds construct a layer structure in the crystal state, which is similar to that of a smectic phase of liquid crystals. Therefore, these compounds have been studied from a structural point of view as models for smectic liquid crystals.

We have already reported molecular and crystal structures of α,ω -alkanediols containing from 10 through 17 and 21 C atoms; these were investigated by Nakamura and co-workers: 1,10-decanediol (Nakamura & Sato, 1999a), 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, 1999b), 1,15-pentadecanediol (Nakamura *et al.*, 2000), 1,16-hexadecanediol (Nakamura & Yamamoto, 1994), 1,17-heptadecanediol (Nakamura *et al.*, 2001) and 1,21-henicosanediol (Nakamura *et al.*, 2000). The results showed a clear distinction in structure between the compounds with an even number of C atoms and those with an odd number of C atoms. In the α,ω -alkanediols with even number of C atoms, the hydroxyl groups located at both ends of a hydrocarbon skeleton showed an all-*trans* conformation with respect to the skeleton. These molecules were arranged making layers in a herring-bone fashion,



just like the chiral smectic C liquid crystals. On the other hand, in the α,ω -alkanediols with an odd number of C atoms, one hydroxyl group had *gauche* conformation with respect to the hydrocarbon skeleton, whereas another hydroxyl group had *trans* conformation. In this case, molecules made a layer structure which was very similar to that of the smectic A liquid

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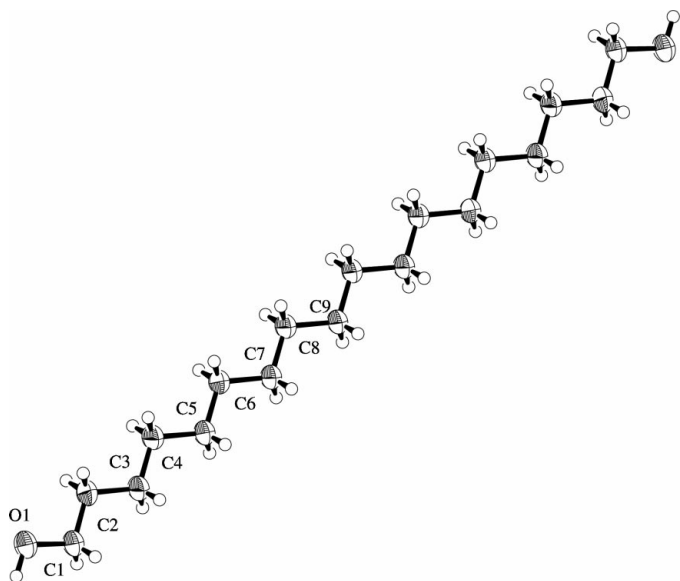


Figure 1
An ORTEP (Johnson, 1976) view of the title molecule showing the crystallographic numbering scheme. Displacement ellipsoids are shown at the 50% probability level.

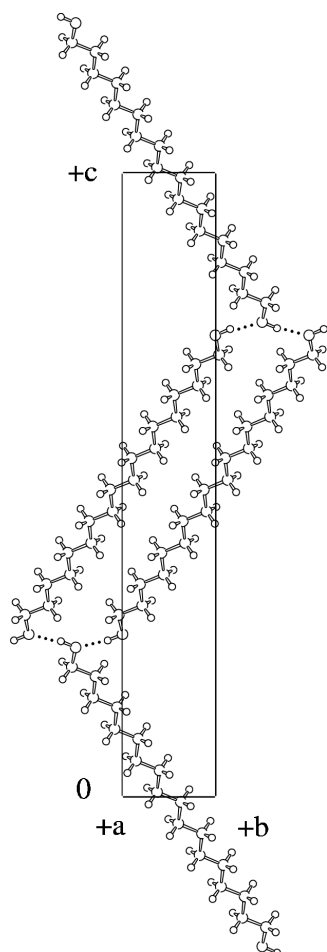


Figure 2
The *bc* projection of the crystal structure; dotted lines indicate the hydrogen bonds.

crystals. In addition, phase transition of α,ω -alkanediols from C13 through C24 was studied by means of a powder X-ray diffraction method and a linear relation of the longest axis of lattice constant *versus* number of C atoms was reported (Ogawa & Nakamura, 1999).

In the crystal structure of 1,18-octadecanediol, (I), shown in Fig. 1, an all-*trans* conformation was observed not only in the hydrocarbon skeleton but also in both terminal hydroxyl groups. The molecule is centrosymmetric and forms a layer structure stacked along the *c* axis. 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 of the molecule is opposite in alternate layers because of the existence of a twofold screw axis parallel to *b*. Such herring-bone structures can be regarded as a model structure of chiral smectic C liquid crystals. These features are very similar to those of 1,10-decanediol, 1,12-dodecanediol, 1,14-tetradecanediol and 1,16-hexadecanediol. The average value of inclination angles of the above compounds was about 56° , as found in the present structure. These molecules form interlayer hydrogen bonds, as shown in Fig. 2, with the interlayer hydrogen-bonding distance $O1 \cdots O1^i = 2.843(2) \text{ \AA}$ [symmetry code: (i) $3 - x, \frac{1}{2} + y, \frac{1}{2} - z$]. This value is in good agreement with those of other α,ω -alkanediols with an even number of C atoms.

Experimental

According to the conventional method, the title compound, (I), was synthesized from commercially available octadecanediolic acid (Tokyo Kasei Kogyo Co. Ltd) by esterification and reduction with $LiAlH_4$. The single crystal used for analysis was grown by very slow evaporation from a solution in a mixed solvent system comprising methanol, ethyl acetate and 1,3-dimethylbenzene (1:1:3 ratio).

Crystal data

$C_{18}H_{38}O_2$	$D_x = 1.047 \text{ Mg m}^{-3}$
$M_r = 286.50$	Cu $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 24 reflections
$a = 4.998(2) \text{ \AA}$	$\theta = 9.3\text{--}20.1^\circ$
$b = 5.220(2) \text{ \AA}$	$\mu = 0.50 \text{ mm}^{-1}$
$c = 34.853(2) \text{ \AA}$	$T = 298 \text{ K}$
$\beta = 92.04(2)^\circ$	Plate, colorless
$V = 908.8(5) \text{ \AA}^3$	$0.40 \times 0.20 \times 0.02 \text{ mm}$
$Z = 2$	

Data collection

Rigaku AFC-5R diffractometer	$R_{\text{int}} = 0.025$
ω - 2θ scans	$\theta_{\text{max}} = 70.5^\circ$
Absorption correction: ψ scans (North <i>et al.</i> , 1968)	$h = -2 \rightarrow 6$
$T_{\text{min}} = 0.929, T_{\text{max}} = 1.000$	$k = 0 \rightarrow 5$
2843 measured reflections	$l = -42 \rightarrow 42$
1802 independent reflections	3 standard reflections
991 reflections with $I > 2\sigma(I)$	every 150 reflections
	intensity decay: 2.6%

Refinement

Refinement on F	H-atom parameters not refined
$R = 0.045$	$w = 1/[\sigma^2(F_o) + 0.00053 F_o ^2]$
$wR = 0.065$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.94$	$\Delta\rho_{\text{max}} = 0.12 \text{ e \AA}^{-3}$
991 reflections	$\Delta\rho_{\text{min}} = -0.11 \text{ e \AA}^{-3}$
91 parameters	

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

Data collection and cell refinement: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); data reduction: *TEXSAN* (Molecular Structure Corporation, 1995); program(s) used to solve structure: *SAPI91* (Fan, 1991); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

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