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Nonadecane-1,19-diol

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.137
Data-to-parameter ratio = 10.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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In the molecular structure of the title compound, $C_{19}H_{40}O_2$, one hydroxyl group adopts a *gauche* conformation with respect to the hydrocarbon skeleton which is all-*trans*, whereas the other hydroxyl group adopts a *trans* conformation. In the crystal, the molecules lie parallel to the *b* axis, the longest axis, forming layers with thickness *b*/2 in which the long axis of the molecule is normal to the layer plane. The packing is similar to that in the smectic A phase of liquid crystals. These features are similar to those of the homologues with an odd number of C atoms, but different from those with an even number of C atoms.

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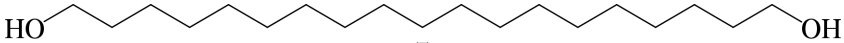
Comment

Long-chain aliphatic compounds have been studied by many researchers from the viewpoint of basic polymer science, as they have a simple chemical structure whose molecular skeleton is a straight hydrocarbon chain. Early crystallographic work on paraffins (Müller, 1928) demonstrated the rod-like conformation of these molecules in the crystalline state. This rod-like conformation is one of the typical features of liquid crystalline molecules. In addition, some long-chain aliphatic compounds form a layer structure in the crystalline state, which is similar to that of a smectic phase of liquid crystals. As a model for smectic liquid crystals, the structures of ten alkane-α,ω-diols containing from 10–18 and 21 C atoms have been investigated recently by Nakamura and co-workers: 1,10-decanediol (Nakamura & Sato, 1999*a*), 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*b*), 1,15-pentadecanediol (Nakamura, Uno, Watanabe *et al.*, 2000), 1,16-hexadecanediol (Nakamura & Yamamoto, 1994), 1,17-heptadecanediol (Nakamura *et al.*, 2001), octadecane-1,18-diol (Nakamura & Watanabe, 2001) and 1,21-henicosanediol (Nakamura, Uno & Ogawa, 2000). In addition, phase transitions in alkane-α,ω-diols with 13–24 C atoms were studied and a linear relation between the longest unit-cell axis and number of C atoms was reported (Ogawa & Nakamura, 1999).



(I)

Fig. 1 shows the molecular structure of nonadecane-1,19-diol, (I). One hydroxyl group adopts a *gauche* conformation with respect to the hydrocarbon skeleton which is all-*trans* [O1—C1—C2—C3 torsion angle of −63.2 (4)°], whereas the other hydroxyl group adopts a *trans* conformation [O2—

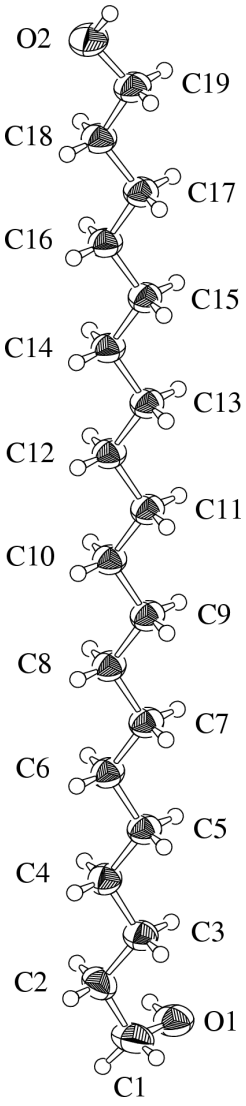


Figure 1
An *ORTEP*II (Johnson, 1976) view of the molecule of (I) showing the crystallographic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

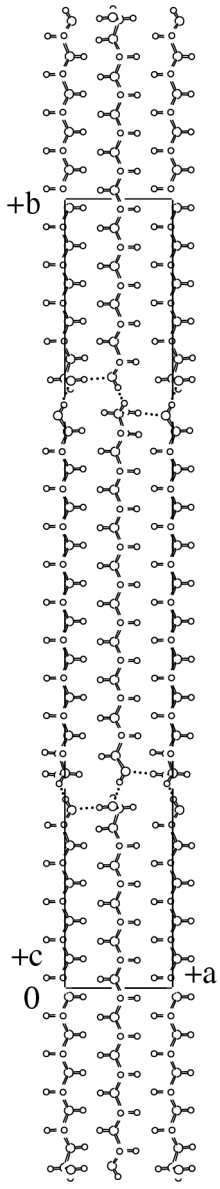


Figure 2
The projection of the crystal structure of (I) along the *c* axis. Dotted lines indicate the hydrogen bonding.

C19—C18—C17 torsion angle of 179.4 (2)°]. The projection of the crystal structure of nonadecane-1,19-diol, (I), along the *c* axis is shown in Fig. 2. The molecules lie parallel to the *b* axis, forming layers with a thickness of *b*/2 in which the long axis of the molecule is normal to the layer plane. The packing is similar to that in the smectic A phase of liquid crystals. The molecules also form two different types of O—H···O hydrogen bonds, one is interlayer and the other is intralayer. The donor–acceptor distances of interlayer and intralayer hydrogen bonds are 2.711 (2) and 2.779 (4) Å, respectively. These features are similar to those already reported for the homologues with an odd number of C atoms [torsion angles of *gauche* conformation: 1,11-undecanediol −63.3 (3)°, 1,13-tridecanediol −63.0 (3)°, 1,15-pentadecanediol −63.2 (4)°, 1,17-heptadecanediol −63.3 (3)° and 1,21-henicosanediol −65.1 (5)°; donor–acceptor distances of interlayer and intralayer hydrogen bonds: 1,11-undecanediol 2.710 (2) and 2.775 (3) Å, 1,13-tridecanediol 2.713 (2) and 2.776 (4) Å, 1,15-pentadecanediol 2.713 (2) and 2.777 (3) Å, 1,17-heptadecanediol 2.705 (2) and 2.782 (4) Å, and 1,21-henicosanediol 2.717 (3) and 2.778 (4) Å]. The C—C distances are in the range 1.498 (3)–1.521 (3) Å and C—C—C angles are in the range 112.5 (2)–115.3 (2)°.

The above observations contrast with the structures of alkane-α,ω-diols with an even number of C atoms, as already reported. In the molecular structure of the homologues with an even number of C atoms, both hydroxyl groups adopt a *trans* conformation with respect to the skeleton, the conformation of which is also all-*trans*. The centrosymmetric molecules form layers in which the long axis of the molecule is inclined to the layer plane and the layers are arranged in a zigzag manner among the neighbouring layers making a

herring-bone motif. The molecules form only interlayer hydrogen bonds. This kind of structure had been observed not only in alkane-α,ω-diols with an even number of C atoms but also in several examples of α,ω-alkanedibromides: 1,12-dibromododecane (Kuple *et al.*, 1981), 1,16-dibromohexadecane (Kobayashi *et al.*, 1995) and 1,18-dibromooctadecane (Nakamura *et al.*, 1993). All these packings are similar to that of the smectic C structure of liquid crystals.

Experimental

The title compound was synthesized as described previously by Ogawa & Nakamura (1999). The single crystal used for analysis was grown by slow evaporation from a solution containing a mixture of methanol, ethyl acetate and *n*-heptane (1:1:2).

Crystal data

$C_{19}H_{40}O_2$
M_r = 300.52
Orthorhombic, $P2_12_12_1$
a = 7.213 (5) Å
b = 52.870 (3) Å
c = 5.061 (3) Å
V = 1930 (1) Å^3
Z = 4
D_x = 1.034 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 22 reflections
θ = 9.1–15.2°
μ = 0.49 mm^{-1}
T = 296.2 K
Plate, colorless
0.60 × 0.30 × 0.04 mm

Data collection

Rigaku AFC-5*R* diffractometer
ω scans
Absorption correction: ψ (North *et al.*, 1968)
T_{min} = 0.757, T_{max} = 1.000
3390 measured reflections
2117 independent reflections
1367 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.014
θ_{max} = 70.6°
$h = -2 \rightarrow 8$
$k = 0 \rightarrow 64$
$l = -1 \rightarrow 5$
3 standard reflections every 150 reflections intensity decay: 3.0%

Refinement

Refinement on F^2
$R(F)$ = 0.040
$wR(F^2)$ = 0.137
S = 1.42
2110 reflections
197 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + \{0.05[\mathrm{Max}(F_o^2,0) + 2F_c^2]/3\}^2]$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}
Extinction correction: Zachariasen (1967), type 2, Gaussian isotropic
Extinction coefficient: 0.043 (5)

The methylene H atoms were located at idealized positions and were allowed to ride on the parent C atoms. The hydroxyl H atoms were located in difference syntheses and the positional parameters were allowed to refine for the final refinements. All H-atom isotropic displacement parameters were set at $1.2U_{eq}$ of the parent atom.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 2000); program(s) used to solve structure: *SAPI*91 (Fan, 1991); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

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