Molecular Structure Corporation (1995). *TEXSAN. Single Crystal Structure Analysis Software*. Version 1.7-1. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Nakamura, N. & Sato, T. (1999). *Acta Cryst.* **C55**, 1687–1689.
Nakamura, N. & Setodoi, S. (1997). *Acta Cryst.* **C53**, 1883–1885.
Nakamura, N., Setodoi, S. & Ikeya, T. (1999). *Acta Cryst.* **C55**, 789–791.
Nakamura, N., Tanihara, Y. & Takayama, T. (1997). *Acta Cryst.* **C53**, 253–255.
Nakamura, N. & Yamamoto, T. (1994). *Acta Cryst.* **C50**, 946–948.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
Ogawa, Y. & Nakamura, N. (1999). *Bull. Chem. Soc. Jpn*, **72**, 943–946.
Seto, T. (1962). *Mem. Coll. Sci. Univ. Kyoto Ser. A*, **30**, 89–107.
Wang, J., Leveiller, F., Jacquemain, D., Kjaer, K., Als-Nielsen, J., Lahav, M. & Leiserowitz, L. (1994). *J. Am. Chem. Soc.* **116**, 1192–1204.
Watanabe, A. (1961). *Bull. Chem. Soc. Jpn*, **34**, 1728–1734.

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1,14-Tetradecanediol

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Abstract

An all-*trans* conformation is observed in the hydrocarbon skeleton, $C_{14}H_{30}O_2$, 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 monosubstituted 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 α,ω-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).

(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 (Kuple *et al.*, 1981) and 1,16-dibromohexadecane (Kobayashi *et al.*, 1995).

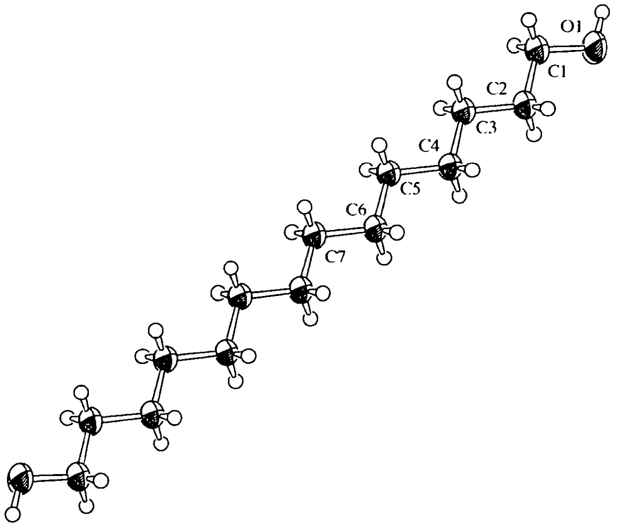

Fig. 1. An *ORTEP*II (Johnson, 1976) view of the title molecule showing the crystallographic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

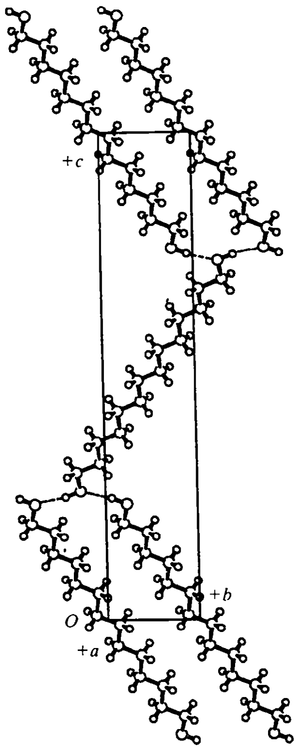

Fig. 2. The projection of the crystal structure along the *a* axis. Dashed lines indicate the hydrogen bonds.

In contrast, those homologues with an odd number of C atoms (1,11-undecanediol and 1,13-tridecanediol) have different molecular and crystal structures, as was reported in our previous papers. Although the hydrocarbon skeleton of these molecules has the all-*trans* conformation, one of the terminal hydroxyl groups is *gauche* with respect to the skeleton, whereas the other is *trans*. The molecules lie parallel along the longest axis and form layers similar to the smectic A structure of liquid crystals. In a given layer, neighbouring molecular planes defined by the hydrocarbon skeleton are nearly perpendicular to each other. The molecules form two different types of hydrogen bond, namely interlayer and intralayer hydrogen bonds. The *gauche* conformation of the hydroxyl group was observed in 1-heptadecanol by Seto (1962).

Experimental

According to the conventional method, the title compound was synthesized from commercially available tetradecanedioic acid by esterification and reduction with $LiAlH_4$. Single crystals were grown from a benzene solution by slow evaporation.

Crystal data

$C_{14}H_{30}O_2$
$M_r = 230.39$
Monoclinic
$P2_1/n$
$a = 4.976\,(1)$ Å
$b = 5.1968\,(8)$ Å
$c = 27.955\,(3)$ Å
$\beta = 93.82\,(1)°$
$V = 721.2\,(2)$ Å^3
$Z = 2$
$D_x = 1.061$ Mg m^{-3}
$D_m = 1.07$ Mg m^{-3}
D_m measured by flotation in aqueous KI

Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å
Cell parameters from 24 reflections
$\theta = 31.5–32.5°$
$\mu = 0.524$ mm^{-1}
$T = 298.2$ K
Plate-like
$0.5 \times 0.4 \times 0.1$ mm
Colourless

Data collection

Rigaku AFC-5*R* diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.819$, $T_{\max} = 0.949$
1529 measured reflections
1392 independent reflections

1030 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.029$
$\theta_{\max} = 70°$
$h = 0 \rightarrow 6$
$k = 0 \rightarrow 5$
$l = -33 \rightarrow 33$
3 standard reflections every 150 reflections intensity decay: 5.4%

Refinement

Refinement on *F*
$R = 0.050$
$wR = 0.097$
$S = 1.77$
1030 reflections
73 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o) + 0.0025|F_o|^2]$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.15$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

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

O1—C1	1.417 (1)	C4—C5	1.520 (1)
C1—C2	1.502 (2)	C5—C6	1.518 (2)
C2—C3	1.522 (1)	C6—C7	1.521 (1)
C3—C4	1.519 (2)	C7—C7$^{\rm i}$	1.519 (2)
O1—C1—C2	109.5 (1)	C4—C5—C6	113.6 (1)
C1—C2—C3	112.6 (1)	C5—C6—C7	113.6 (1)
C2—C3—C4	113.50 (10)	C6—C7—C7$^{\rm i}$	113.7 (1)
C3—C4—C5	113.4 (1)		

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

Table 2. *Contact distances (Å)*

O1···O1$^{\rm i}$	2.831 (1)	O1···C1$^{\rm ii}$	3.469 (2)
O1···O1$^{\rm ii}$	2.831 (1)	O1···C2$^{\rm i}$	3.545 (2)

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

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992). Cell refinement: *MSC/AFC 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*. 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: OB1010). Services for accessing these data are described at the back of the journal.

References

Fan, H.-F. (1991). *SAPI91. Structure Analysis Program with Intelligent Control.* Rigaku Corporation, Tokyo, Japan.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Kobayashi, H., Yamamoto, T. & Nakamura, N. (1995). *Cryst. Res. Technol.* **30**, 375–380.
Kuple, S., Seidei, I., Szulzewsky, K., Steger, U. & Steger, E. (1981). *Cryst. Res. Technol.* **16**, 349–356.
Molecular Structure Corporation (1992). *MSC/AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Molecular Structure Corporation (1995). *TEXSAN. Single Crystal Structure Analysis Software*. Version 1.7. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Nakamura, N. & Setodoi, S. (1997). *Acta Cryst.* C**53**, 1883–1885.
Nakamura, N., Setodoi, S. & Ikeya, T. (1999). *Acta Cryst.* C**55**, 789–791.
Nakamura, N., Tanihara, Y. & Takayama, T. (1997). *Acta Cryst.* C**53**, 253–255.
Nakamura, N. & Yamamoto, T. (1994). *Acta Cryst.* C**50**, 946–948.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Seto, T. (1962). *Mem. Coll. Sci. Univ. Kyoto Ser. A*, **30**, 89–107.
Watanabe, A. (1961). *Bull. Chem. Soc. Jpn*, **34**, 1728–1734.

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4-Ethoxy-*N*-(6-methylquinolin-2-ylmethylene)aniline

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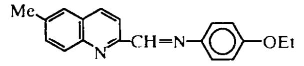
Abstract

The crystal structure of the title Schiff base, $C_{19}H_{18}N_2O$, has been determined. The 6-methylquinoline group and formimidoyl moiety are almost planar, and the dihedral angle between the planes of ethoxyphenyl and 6-methylquinoline is 44.02 (8)°. The crystal structure is stabilized by intramolecular and intermolecular hydrogen bonds of the C—H···N type forming a chain extending in the *a* direction.

Comment

It is interesting to note that several Schiff bases have physical properties which impart to them liquid-crystal behaviour (Gray, 1962; Arora *et al.*, 1970). The formation of Schiff bases may proceed readily in many cases under relatively mild conditions. It is therefore not surprising that biochemistry, biomedical research, immunochemistry *etc.* have found uses for the reaction of amines (Sandler & Karo, 1986). In this paper we report the structure of 4-ethoxy-*N*-(6-methylquinolin-2-ylmethylene)aniline, (I).



(I)

Fig. 1 shows a view of the title compound with the atom-numbering scheme. The C9═N1 bond length of 1.268 (2) Å is typical of a double bond as has been observed in a similar structure [1.270 (3) and 1.276 (3) Å; Cannadine *et al.*, 1996]. The bond lengths and angles in the title compound are in agreement with related structures reported earlier (Abu-Surrah *et al.*, 1997; Işık *et al.*, 1998).

The formimidoyl and methyl groups are almost coplanar with the quinoline moiety, the maximum

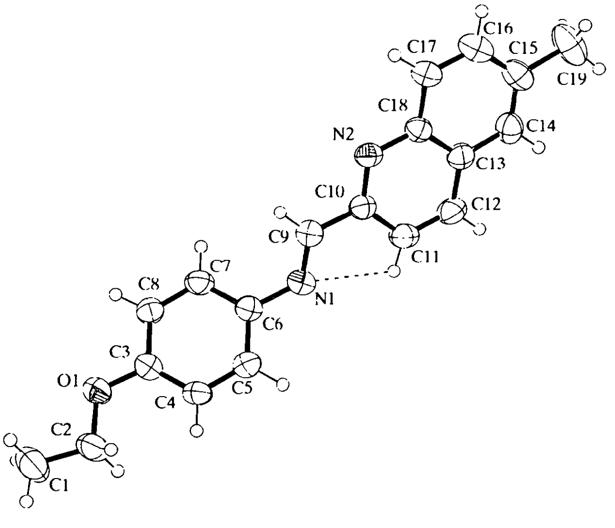


Fig. 1. An *ORTEP*III (Burnett & Johnson, 1996) drawing of the title compound showing the atomic numbering scheme. Displacement ellipsoids of non-H atoms are shown at the 50% probability level; H atoms are shown as small spheres of arbitrary size. The intramolecular hydrogen bond is shown as a dashed line.