Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

1,24-Dibromotetracosane

Naotake Nakamura* and Akira Ohishi

Department of Applied Chemistry, College of Science and Engineering, Ritsumeikan University, 1-1-1 Nojihigashi, Kusatsu, Shiga 525-8577, Japan

Correspondence e-mail:
nakamura@se.ritsumei.ac.jp

Received 28 June 2005
Accepted 5 July 2005
Online 9 July 2005

In the title compound, $C_{24}H_{48}Br_2$, the molecule is centrosymmetric and the molecular skeleton including both terminal Br atoms has an all-*trans* conformation. The molecules form layers with a thickness of $c/2$. These features are similar to the smectic C_A phase of liquid crystals.

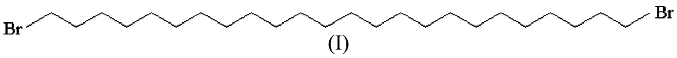
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.007 Å
R factor = 0.056
wR factor = 0.108
Data-to-parameter ratio = 16.2

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

Comment

Normal long-chain compounds can be regarded as having a rod-like shape, and the molecules in the crystalline state form a layered structure similar to those of the smectic liquid crystalline phase. Moreover, some of these long-chain compounds exhibit a high-temperature rotator phase just below their melting points, in which molecules have motional freedom to some degree, comparable with that in liquid crystals. Thus, these long-chain compounds have been studied as model compounds for smectic liquid crystals.



(I)

Many researchers have analyzed the crystal structures of many different kinds of normal long-chain aliphatic

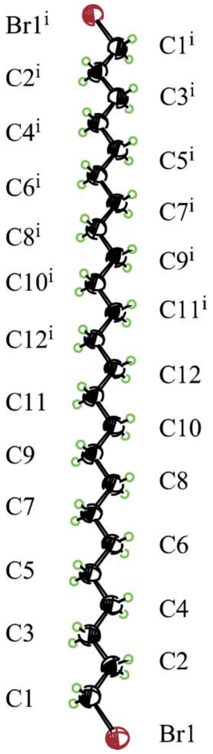


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry code: (i) $-x$, $1 - y$, $2 - z$].

doi:10.1107/S1600536805021379

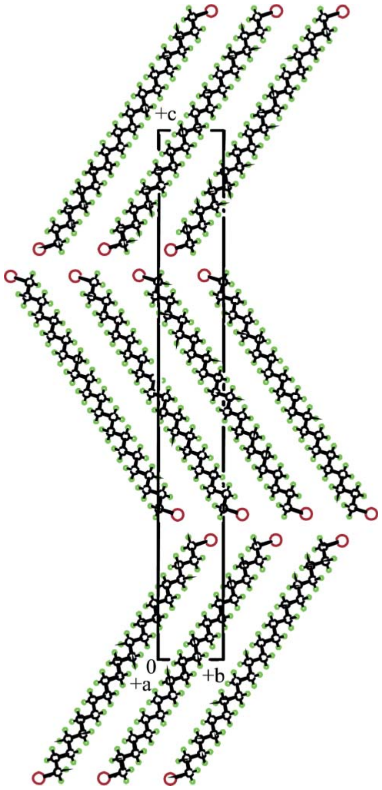


Figure 2
The projection of the crystal structure of (I) along the *a* axis.

compounds. Recently, we have systematically analysed the crystal structures of the alkane-α,ω-diols containing 10–19 and 21–23 C atoms (Nakamura *et al.*, 2001*a*; Uno *et al.*, 2002) and the alkane-α,ω-dithiols containing 12, 19–21 and 23 C atoms (Nakamura *et al.*, 2001*b*,*c*, 2004, 2005*a*,*b*). In the present paper, we report the results of the crystal structure analysis of the title compound, (I), in order to elucidate the effect of the terminal groups in normal long-chain compounds in constructing a layer structure.

The molecular structure of (I) is shown in Fig. 1. The molecule is centrosymmetric and all torsion angles are close to ±180°, that is, the molecular structure including both terminal Br atoms has an all-*trans* conformation. The layers are arranged in a zigzag manner between the neighboring layers, forming a herringbone motif similar to the smectic C_A phase of liquid crystals, as shown in Fig. 2. The layers are stacked closely in such a way that the α-CH$_2$ groups are allowed to fit into the grooves formed by Br atoms, with the nearest contact Br1$\cdots$Br1^i = 3.754 (2) Å [symmetry code: (i) $4 - x, y - \frac{1}{2}, \frac{3}{2} - z$], agreeing closely with the van der Waals contact of 3.75 Å (Rowland & Taylor, 1996). Such a close packing is observed in the even-numbered alkane-α,ω-diols containing 4–19 and 21–23 C atoms (Thalladi *et al.*, 2000) and the α,ω-dichloroalkanes containing 16, 20 and 26 C atoms (Takamizawa *et al.*, 1992; Nakamura & Shimizu, 2004). Fig. 3 shows the projection of the crystal structure of (I) along the *b* axis. The molecules form layers with a thickness of *c*/2. In the layer, the long axes of the molecules are inclined to the *ab* plane. This layer structure is similar to that of the triclinic structure of the even-numbered *n*-alkanes containing 6–22C atoms (Nyburg & Gerson, 1992). It is considered that the arrangement in the layer is influenced by the steric and electrostatic repulsion of Br atoms at both ends.

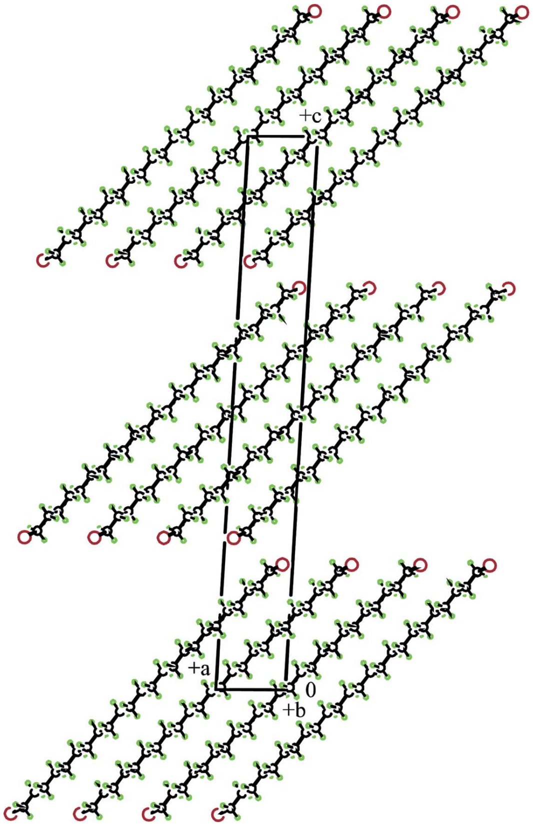


Figure 3
The projection of the crystal structure of (I) along the *b* axis.

The main features of the structure of (I) are similar to those of the homologous series with an even number of C atoms, *viz*. 1,12-dibromododecane (Kulpe *et al.*, 1981), 1,14-dibromotetradecane (Uno & Nakamura, 2003), 1,16-dibromohexadecane (Kobayashi *et al.*, 1995), 1,18-dibromooctadecane (Nakamura *et al.*, 1993), 1,20-dibromoicosane (Nakamura & Ohishi, 2004) and 1,26-dibromohexacosane (Takamizawa *et al.*, 1992).

Experimental

Thin plate-like crystals of (I) were grown by slow evaporation of a solution in a mixture of ethyl acetate and ethanol (2:1). The well developed face of the crystal is (001).

Crystal data

$C_{24}H_{48}Br_2$
M_r = 496.45
Monoclinic, $P2_1/c$
a = 5.482 (3) Å
b = 5.381 (2) Å
c = 43.859 (2) Å
β = 93.07 (2)°
V = 1291.9 (9) Å^3
Z = 2
D_x = 1.276 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 24 reflections
θ = 9.2–17.1°
μ = 3.99 mm^{-1}
T = 296 (1) K
Plate, colourless
0.51 × 0.41 × 0.01 mm

Data collection

Rigaku AFC-5*R* diffractometer
ω scans
Absorption correction: numerical (*ABSCOR*; Higashi, 1999)
$T_{\min} = 0.175$, $T_{\max} = 0.961$
4250 measured reflections
2374 independent reflections
1525 reflections with $F^2 > 2\sigma(F^2)$

$R_{\rm int} = 0.040$
$\theta_{\max} = 70.8°$
$h = -1 \rightarrow 6$
$k = -1 \rightarrow 6$
$l = -53 \rightarrow 53$
3 standard reflections every 150 reflections intensity decay: 14.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.108$
$S = 1.00$
2374 reflections
143 parameters
All H-atom parameters refined

$w = 1/[0.0001F_o^2 + 8.45\sigma^2(F_o) + 0.525]/(4F_o^2)$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 1.07$ e Å^{-3}
$\Delta\rho_{\min} = -1.26$ e Å^{-3}
Extinction correction: Larson (1970)
Extinction coefficient: 19.0 (2)

Table 1
Selected geometric parameters (Å, °).

Br1—C1	1.926 (5)	C7—C8	1.520 (6)
C1—C2	1.493 (6)	C8—C9	1.518 (6)
C2—C3	1.506 (7)	C9—C10	1.521 (6)
C3—C4	1.520 (6)	C10—C11	1.509 (6)
C4—C5	1.514 (6)	C11—C12	1.526 (6)
C5—C6	1.526 (6)	C12—C12$^{\rm i}$	1.506 (8)
C6—C7	1.516 (6)		
Br1—C1—C2—C3	179.3 (3)	C6—C7—C8—C9	−179.5 (4)
C1—C2—C3—C4	−179.9 (5)	C7—C8—C9—C10	180.0 (4)
C2—C3—C4—C5	−179.2 (4)	C8—C9—C10—C11	−179.8 (4)
C3—C4—C5—C6	180.0 (4)	C9—C10—C11—C12	−179.8 (4)
C4—C5—C6—C7	−179.2 (4)	C10—C11—C12—C12$^{\rm i}$	−179.7 (4)
C5—C6—C7—C8	−179.3 (4)	C11—C12—C12$^{\rm i}$—C11$^{\rm i}$	180.0 (4)

Symmetry code: (i) $-x, -y+1, -z+2$.

H atoms were positioned geometrically and treated as riding, with C—H distances of 0.95 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(parent). The intensity decay was somewhat high (14.0%) because a longer time was needed to collect the reflection data.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *CrystalStructure* (Molecular Structure Corporation & Rigaku, 2001); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

The authors express their gratitude to Mr K. Uno and Mr H. Shimizu for their support. This work was supported by MEXT.HAITEKU(2005).

References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.

Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Higashi, T. (1999). *NUMABS*. Rigaku Corporation, Tokyo, Japan.

Kobayashi, H., Yamamoto, T. & Nakamura, N. (1995). *Cryst. Res. Technol.* **30**, 275–280.

Kulpe, S., Seidel, I., Szulzewsky, K., Steger, U. & Steger, E. (1981). *Cryst. Res. Technol.* **16**, 349–356.

Larson, A. C. (1970). *Crystallographic Computing*, edited by F. R. Ahmed, S. R. Hall & C. P. Huber, pp. 291–294. Copenhagen: Munksgaard.

Molecular Structure Corporation (1992). *MSC/AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

Molecular Structure Corporation & Rigaku (2001). *CrystalStructure*. Version 3.10. MSC, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA, and Rigaku Corporation, 3-9-12 Akishima, Tokyo 196-8666, Japan.

Nakamura, N. & Ohishi, A. (2004). *Acta Cryst.* E**60**, o1408–o1410.

Nakamura, N. & Shimizu, H. (2004). *Acta Cryst.* E**60**, o131–o133.

Nakamura, N., Shimizu, H. & Ogawa, Y. (2004). *Acta Cryst.* E**60**, o1684–o1686.

Nakamura, N., Shimizu, H. & Ogawa, Y. (2005*a*). *Acta Cryst.* E**61**, o450–o452.

Nakamura, N., Shimizu, H. & Ogawa, Y. (2005*b*). *Acta Cryst.* E**61**, o1046–o1048 .

Nakamura, N., Uno, K. & Ogawa, Y. (2001*a*). *Acta Cryst.* E**57**, o1091–o1093.

Nakamura, N., Uno, K. & Ogawa, Y. (2001*b*). *Acta Cryst.* E**57**, o505–o507.

Nakamura, N., Uno, K. & Ogawa, Y. (2001*c*). *Acta Cryst.* E**57**, o508–o510.

Nakamura, N., Yamamoto, T., Kobayashi, H. & Yoshimura, Y. (1993). *Cryst. Res. Technol.* **28**, 953–957.

Nyburg, S. C. & Gerson, A. R. (1992). *Acta Cryst.* B**48**, 103–106.

Rowland, R. S. & Taylor, R. (1996). *J. Phys. Chem.* **100**, 7384–7391.

Takamizawa, K., Kodama, M., Matsunaga, S. & Shiokawa, K. (1992). *Eng. Sci. Rep. Kyushu Univ.* **13**, 341–347.

Thalladi, V. R., Boese, R. & Weiss, H. C. (2000). *Angew. Chem. Int. Ed.* **39**, 918–922.

Uno, K. & Nakamura, N. (2003). *Acta Cryst.* E**59**, o708–o710.

Uno, K., Nakamura, N. & Ogawa, Y. (2002). *Acta Cryst.* A**58** (Supplement), C–338.