

in the fibers. The strain applied to the fibers has been modeled by an integrated texture-stress model inside the program as well.

[1] <http://www.ing.unitn.it/~luttero/maud> [2] Ischia G., Wenk H.-R., Lutterotti L., Berberich F., *J. Appl. Cryst.*, 2005, **38**, 377.

**Keywords:** structure determination, texture, polymer

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##### Novel Structure of 1,1'-Disubstituted Ferrocene Derivative

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Some of the 1,1'-disubstituted ferrocene derivatives (bMAF-*n*, *n* is the carbon number in the flexible spacer) show liquid crystallinity. It was reported that bMAF-5 had S-typed molecular structure [1]. The S-shaped one of the other derivative was already reported by the other workers [2]. Recently, new U-typed one was found out in bMAF-10 [3].

In this study, the crystal structure of bMAF-2 was analyzed by single crystal X-ray diffraction method. All measurements were made by Rigaku AFC-5R diffractometer with graphite monochromatized CuK $\alpha$  radiation. The crystal structure obtained in this study was a monoclinic with space group *C2/c*. The residual R and wR converged on 0.036 and 0.067, respectively. The feature of the structure was very unique, because the two substituent had a bent structure around a *gauche* conformation. This molecular structure was given a name to Z-shape, which was different from those of bMAF-5 (S-shape) and 10 (U-shape).

Liquid crystallinity will be discussed from structural point of view.

[1] Nakamura N., et al, *Mol. Cryst. Liq. Cryst.*, 2005, *in press*. [2] Khan A.M., et al., *Liq. Cryst.*, 1989, **5**, 285. [3] Nakamura N., et al, *Chem. Lett.*, 2004, **33**, 358.

**Keywords:** ferrocene compounds, liquid crystal, crystal structure

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##### Crystal Structure of 1,24-Dibromotetracosane

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The crystal structure of 1,24-dibromotetracosane was analyzed by single crystal X-ray diffraction method. The compound crystallized in a monoclinic system (*a* = 5.482 (3)Å, *b* = 5.381 (2)Å, *c* = 43.859 (2)Å,  $\beta$  = 93.07 (2)°, *Z* = 2) with a space group *P2<sub>1</sub>/c*. The molecule is centrosymmetric and its skeleton has an all-*trans* conformation including both terminal Br atoms. In the crystal, the molecules form layers with a thickness of *c*/2. In the layer, the molecules inclined to the basal plane of Br atoms. The layers are arranged in a zigzag manner between the neighboring layers making a herringbone motif just like the smectic C<sub>A</sub> structure of liquid crystals.

The molecular and crystal structures of 1,24-dibromotetracosane are similar to those of the homologs with an even number of C atoms, *vis.* 1,12-dibromododecane[1], 1,14-dibromotetradecane[2], 1,16-dibromo-hexadecane[3], 1,18-dibromooctadecane[4], 1,20-dibromoicosane[5], and 1,26-dibromohexacosane[6].

[1] Kulpe S., et al, *Cryst. Res. Technol.*, 1981, **30**, 349. [2] Uno K., et al, *Acta Cryst.*, 2003, **E59**, o708. [3] Kobayashi H., et al, *Cryst. Res. Technol.*, 1995, **30**, 275. [4] Nakamura N., et al, *Cryst. Res. Technol.*, 1993, **28**, 953. [5] Nakamura N., et al, *Acta Cryst.*, 2004, **E60**, o1408. [6] Takamizawa K., et al, *Eng. Sci. Rep. Kyushu Univ.*, 1992, **13**, 341.

**Keywords:** alkyl halide, crystal structure, liquid crystal

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##### Crystal Structure of Monosubstituted Ferrocene Derivatives

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A series of monosubstituted ferrocene derivatives,  $\omega$ -[4-(4-methoxyphenoxy-carbonyl)phenoxy-carbonyl]alkyl 4-ferrocenyl benzoate (abbreviated hereafter as MPAF-*n*, *n* = 1~11, where *n* is the number of carbon atoms in the methylene unit) were prepared in our laboratory [1].

In the present study, the crystal and molecular structures of MPAF-10 were determined by X-ray diffraction method using a single crystal. All measurements were made by Rigaku AFC-5R diffractometer with graphite monochromatized CuK $\alpha$  radiation. The crystal structure obtained in this study was orthorhombic (*a*=8.176(6), *b*=88.253(7), *c*=10.140(9)Å, *Z*=8) with space group *Pbca*. The residual R and wR converged on 0.056 and 0.128, respectively. Good of fitness is 1.000.

This compound shows liquid crystallinity. This molecule bends a little around an ester group located in the ferrocene side. The feature of the molecule is not favorable for the liquid crystalline compound. Two molecules, however, associate head to head manner making a rod-like shape. Therefore, this compound exhibits liquid crystallinity.

[1] Hanasaki T., Ueda M., Nakamura N., *Mol. Cryst. Liq. Cryst.*, 1993, **237**, 329.

**Keywords:** liquid crystal, ferrocene compounds, crystal structure

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##### Crystal Structure of a Liquid Crystalline Ferrocene Derivative

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A series of 1,1'-disubstituted ferrocene derivative, 1,1'-bis[ $\omega$ -[4-(4-methoxyphenoxy-carbonyl)phenoxy]alkoxy-carbonyl]ferrocene (abbreviated hereafter as bMAF-*n*, where *n* is the number of carbon atoms in the methylene unit) was prepared, and some of them (bMAF-3,5~12) exhibited liquid crystallinity[1,2]. In this study, the crystal structures of bMAF-3 were determined by the X-ray diffraction method in order to gain an understanding of the interrelation between the crystal structure and some physical properties. The single crystals of the compounds were obtained from a solution with a mixed solvent by the slow evaporation method. The measurement was made on a Rigaku AFC-5R diffractometer with graphite monochromatized Cu-K $\alpha$  radiation. The calculation was performed using the *Crystal-Structure* crystallographic software package. The crystal structure was mono-clinic system (*a*=5.857(4)Å, *b*=24.105(3)Å, *c*=14.069(4)Å,  $\beta$ =93.15(4)°, *Z*=2) with space group *P2<sub>1</sub>*. In generally, rod-like molecules has advantageous structure to show liquid crystallinity. The molecular structures of bMAF-3 could be regarded as rod-like. In fact, they have the advantage of showing liquid crystallinity, and they give rise to liquid crystallinity.

[1] Hanasaki T., Ueda M., Nakamura N., *Mol. Cryst. Liq. Cryst.*, 1994, **250**, 257. [2] Nakamura N., Mizoguchi R., Ueda M., Hanasaki T., *Mol. Cryst. Liq. Cryst.*, 1998, **312**, 127.

**Keywords:** liquid crystal, ferrocene, rod-like

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##### Layer and Molecular Orientation in Electroclinic Liquid Crystals: Dynamic $\mu$ -Diffraction

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