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

P.11.09.1

Acta Cryst. (2005). A**61**, C392

Novel Structure of 1,1'-Disubstituted Ferrocene Derivative

Masako Nishikawa, Naotake Nakamura, *Department of Applied Chemistry, College of Science and Engineering, Ritsumeikan University, 1-1-1, Nojihigashi, Kusatsu, Shiga 525-8577, Japan.* E-mail: rc007016@se.ritsumei.ac.jp

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 monocromatized CuKα 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

P.11.09.2

Acta Cryst. (2005). A**61**, C392

Crystal Structure of 1,24-Dibromotetracosane

Akira Ohishi, Naotake Nakamura, *Department of Applied Chemistry,College of Science and Engineering, Ritsumeikan University, 1-1-1 Nojihigashi, Kusatsu, Shiga 525-8577, Japan.* E-mail: rc001006@se.ritsumei.ac.jp

The crystal structure of 1,24-dibromotetracsane 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, β = 93.07 (2)°, Z = 2) with a space group $P2_1/c$. 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_A 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-dibeomotetradecane[2], 1,16-dibromo -hexadecasne[3], 1,18-dibromooctadecane[4], 1,20-dibromoicosane[5], and 1,26-dibromohexsacosane[6].

[1] Kulpe S., et al, *Cryst. Res. Technol.*, 1981, **30**, 349. [2] Uno K., et al, *Acta Cryst.*, 2003, **E59**, o708. [3] Kobayasi 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: alkyle halide, crystal structure, liquid crystal

P.11.09.3

Acta Cryst. (2005). A**61**, C392

Crystal Structure of Monosubstituted Ferrocene Derivatives

Naotake Nakamura, T. Okabe, T. Takahashi, *Department of Applied Chemistry, College of Science and Engineering, Ritsumeikan University, 1-1-1, Nojihigashi, Kusatsu, Shiga 525-8577, Japan.* E-mail: nakamura@se.ritsumei.ac.jp

A series of monosubstituted ferrocene derivatives, ω-[4-(4-methoxyphenoxy-carbonyl)phenoxycarbonyl]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 monocrochromatixed CuKα 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 bents a little around a 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

P.11.09.4

Acta Cryst. (2005). A**61**, C392

Crystal Structure of a Liquid Crystalline Ferrocene Derivative

Keisuke Nakazaki, Naotake Nakamura, *Department of Applied Chemistry,College of Science and Enginnering, Ritsumeikan University, 1-1-1 Nojihugashi, Kusatsu, Shiga 525-8577, JAPAN.* E-mail: rc007003@se.ritsumei.ac.jp

A series of 1,1'-disubstituted ferrocene derivative, 1,1'-bis[ω-[4-(4-methoxyphenoxy-carbonyl)phenoxy]alkoxycarbonyl]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-5*R* diffractometer with graphite monochromatized Cu-*Kα* 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, *β*=93.15(4)°, *Z*=2) with space group $P2_1$. 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

P.11.09.5

Acta Cryst. (2005). A**61**, C392-C393

Layer and Molecular Orientation in Electroclinic Liquid Crystals: Dynamic μ-Diffraction

Atsuo Iida[a], Yumiko Takahashi[b], Yoichi Takanishi[c], Ken Ishikawa[c], Hideo Takezoe[c], *[a]Photon Factory, Institute of Materials Structure Science. [b]Department of Physics, Nihon University. [c]Department of*