Crystal Structure of a Liquid Crystalline Ferrocene Derivative

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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-$K\alpha$ 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, 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.

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