Crystal Structure of Monosubstituted Ferrocene Derivatives

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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.

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