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Syntheses and Physical Properties of Ferrocene Derivatives (XII) Crystal Structure of a Liquid Crystalline Ferrocene Derivative, ω-[4-(4-methoxy-phenoxycarbonyl)phenoxycarbonyl] hexyl 4-ferrocenylbenzoate

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Syntheses and Physical Properties of Ferrocene Derivatives (XII) Crystal Structure of a Liquid Crystalline Ferrocene Derivative, ω-[4-(4-methoxyphenoxycarbonyl)phenoxycarbonyl] hexyl 4-ferrocenylbenzoate

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The structure of a liquid crystalline monosubstituted ferrocene derivative was determined by the single crystal X-ray structure analysis. The title compound, ω-[4-(4-methoxyphenoxycarbonyl) phenoxycarbonyl]hexyl 4-ferrocenylbenzoate has a characteristic chemical structure in which a flexible spacer (hexyl chain) is located between the ferrocenyl and mesogenic groups. The flexible spacer is an all-*trans* conformation. In order to form a rod-like structure, the molecule is slightly bent around the ester group neighboring the ferrocenylbenzoate group. This rod-like molecular geometry may play an important role in the appearance of the liquid crystal phase and lead to efficient packing, because it is generally known that the derivatives having a bulky ferrocenyl group are not suitable for liquid crystalline compounds. By the way, two cyclopentadienyl rings exhibit an eclipsed conformation rather than a staggered one. The molecules are arranged in layers just like those in the smectic phase of the liquid crystals. The structure obtained is discussed with those of homologues having different flexible spacer lengths and related ferrocene derivatives containing a different mesogenic group, already reported previously.

Keywords: Crystal Structure; Metallocene; Ferrocene Derivatives; Metallomesogen; Liquid Crystal

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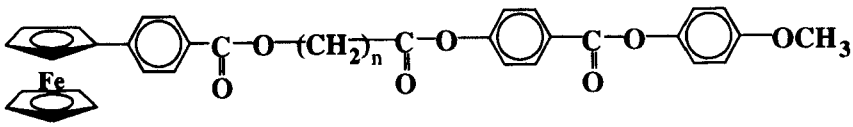
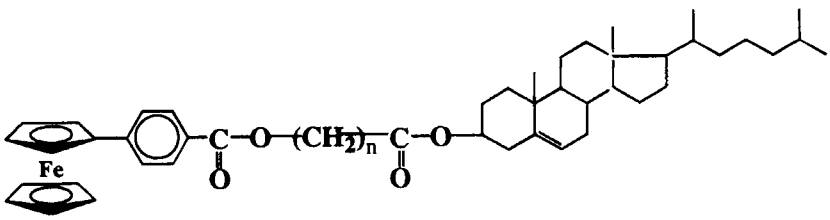
INTRODUCTION

The liquid crystalline compounds containing transition metal, that is metallomesogens have been of great interest in recent years. The metallomesogen has attracted attention because it is expected to develop interesting electric, magnetic, chromatic properties and so on. In our laboratory, several different kinds of metallomesogen were synthesized and we investigated their thermal properties, dielectric properties, crystal structures, Mössbauer effect and so on [1–13]. Especially, two series of monosubstituted ferrocene derivatives were studied from a viewpoint of liquid crystallinity in detail. One is a series of [4-[ω-(cholesteryloxycarbonyl)alkoxycarbonyl]phenyl]ferrocene (abbreviated hereafter as CAPF-*n*, where *n* is the number of a methylene unit), and 8 of the CAPF-*n* exhibited liquid crystallinity, where *n*=2, 4, 6, 8, 9, 10, 11 and 15 [1–2]. The other is the series of ω-[4-(4-methoxyphenoxycarbonyl)phenoxycarbonyl]alkyl 4-ferrocenylbenzoate (abbreviated hereafter as MPAF-*n*, where *n* is the number of carbon atoms in a methylene unit). MPAF-*n* was synthesized into 9 kinds of homologues (*n*=1~7, 10 and 11) and we observed liquid crystallinity for 4 kinds of MPAF-*n*, where *n*=4, 6, 10 and 11 [3]. The general structures of CAPF-*n* and MPAF-*n* are shown in Figure 1.



MPAF-*n*



CAPF-*n*

FIGURE 1 General chemical structures of MPAF-*n* and CAPF-*n*

In 1993, a paper describing the crystal structure of the liquid crystalline monosubstituted ferrocene derivative was published by other workers [14]. In succes-

sion, the molecular and crystal structure of CAPF-6 was determined and the mechanism of the liquid crystal phase transition was discussed by one of the present authors and his coworker [8]. After that, no structure analyses of CAPF-*n* except CAPF-6 have been made, because it was too difficult to obtain the high-quality single crystals of CAPF-*n*. Therefore, we reported the results obtained by small-angle X-ray diffraction measurements using powder samples in order to discuss the liquid crystal structure of CAPF-*n* [5, 7]. Recently, we published the molecular and crystal structure of three kinds of MPAF-*n*, that is, MPAF-2 [12], MPAF-3 [11] and MPAF-4 [10]. According to these results, it was clarified that the molecular and crystal structure of MPAF-2 and those of MPAF-4 are very similar to each other, though the former shows no liquid crystallinity while the latter shows liquid crystallinity. It was considered that this difference of the appearance of liquid crystallinity is caused by the steric hindrance in the phenylbenzoate group introduced as a mesogenic group [12]. The structural feature of MPAF-3 is a sharp bent one, caused by two *gauche* conformations in the flexible spacer. This suggests that it is difficult for this bent structure to show liquid crystallinity for MPAF-3. In fact, no liquid crystallinity was observed in MPAF-3 as was already reported in our previous paper [3]. We have discussed liquid crystallinity from the viewpoints of each molecular and crystal structure, space groups and so on in our previous papers [10–12].

MPAF-6 displays the liquid crystalline phase between 294 and 318 K in the heating process and between 323 and 293 K in the cooling process [3]. In this paper, we will discuss the relation between the molecular and crystal structure and the liquid crystallinity of MPAF-6 in detail with reference to those of CAPF-6.

EXPERIMENTAL

The sample, MPAF-6, was synthesized in accordance with the method mentioned in our previous paper [3]. The compound obtained was confirmed to be MPAF-6 using ^{1}H-NMR (JEOL, JNMGX-400) spectra. The single crystal of the compound was obtained by the slow evaporation method employed a solution with a mixed solvent of benzene and methanol (1:3). The density of this single crystal was measured by the flotation method in KI aq. The orange plate-like crystals having approximate dimensions of 0.4 × 0.3 × 0.05 mm were chosen and mounted on a glass fiber. All measurements were made on a Rigaku AFC-5R diffractometer with graphite monochromatized Cu-Kα radiation (λ=1.54178 Å).

The unit cell parameters and an orientation matrix for data collection were obtained by a least-squares refinement of the setting angle of 25 reflections, with

2θ between 19.80 and 39.21 °. The data were collected at a temperature of 25±1°C, using the ω-2θ-scan technique to maximize the 2θ value of 120.1 °.

5471 reflections were measured, of which 5051 were unique (R_{int}=0.070). The intensity of three representative reflections were measured after every 150 reflections. Over the course of data collection, the standards decreased by 9.1 %. We judged that a linear correction factor was applied to the data to account for this phenomenon. The data were corrected for Lorentz and polarization effects and for absorption (ψ scan [15]; minimum and maximum transmission factors were 0.6456 and 0.9927, respectively).

The structure was solved by direct methods (SAPI 91) [16] and expanded using the Fourier technique. All non-hydrogen atoms were refined anisotropically and the hydrogen atoms were introduced at their theoretical positions and allowed to ride with the carbon atoms to which they are attached. The final refinement was made by full-matrix least-squares based on 3089 observed reflections ($I > 3.0\sigma(I)$). The refinement was concluded with final reliability factors:

$$R = \Sigma(|F_0| - |F_C|)/\Sigma|F_0| = 0.074$$

$$R_w = (\Sigma W(|F_0| - |F_C|)^2/\Sigma WF_0^2)^{1/2} = 0.099$$

where the weighted scheme $W = 1 / [\sigma^2(F_0) + 0.00063F_0^2]$. Moreover, the goodness of the fit indicator is estimated to be 2.40.

All calculations were performed using the teXsan [17] crystallographic software package of Molecular Structure Corporation.

Final data may be obtained from the Cambridge Crystallographic Data Center, 12 Union Road, Cambridge, CB2 1EZ, UK.

RESULTS AND DISCUSSION

Data regarding collection and refinement are summarized in Table I. Fractional atomic coordinates and equivalent isotropic factors are given in Table II.

The value of the measured density (1.279 g/cm^3) coincides with that of the calculated one (1.376 g/cm^3) within an experimental error. Reliability factors, R, R_W and the S factor, are suitable values for consideration of the molecular and crystal structure in organic compounds. With respect to unit cell parameter, the length of the c-axis increases approximately 4.8 Å and 2.5 Å for MPAF-2 and MPAF-4, respectively, as the number of carbon atoms in the flexible methylene unit increase.

The molecular structures labeling the number of atoms, over view and side view of the cyclopentadienyl rings are presented in an ORTEP II [18] drawing in Figure 2. The molecular geometry is almost extended and linear in shape, in

other words, the rod-like feature. The lists of the bond distances and bond angles are shown in Table III. Moreover, the defined least-squares planes and dihedral angles are given in Table IV.

TABLE I Summarized data regarding collection and refinement

Empirical formula	$C_{38}H_{36}O_7Fe$
Formula weight	660.55
Crystal system	monoclinic
Space group	$P2_1/a$
Lattice parameter	
a / Å	7.746(6)
b / Å	10.547(4)
c / Å	39.019(5)
β / °	90.72(4)
Volume / $Å^3$	3187(2)
Z value	4
D_{calc} / gcm^{-3}	1.376
D_{meas} / gcm^{-3}	1.279
Measured reflections	5471
Independent reflections	5051
Observed reflections ($I>3.0\sigma(I)$)	3089
R	0.074
R_W	0.099
S	2.40

TABLE II Fractional atomic coordinates and equivalent isotropic temperature factors

Atom	*x*	*y*	*z*	B_{eq}
Fe(1)	0.1789(2)	0.01527(9)	0.06391(3)	4.00(3)
O(1)	0.4591(7)	-0.0750(5)	0.2491(1)	5.1(1)
O(2)	0.6170(9)	-0.2298(6)	0.2256(1)	6.8(2)
O(3)	0.1922(9)	-0.0383(5)	0.4929(1)	5.9(1)
O(4)	0.3454(10)	-0.2051(6)	0.4751(1)	7.2(2)
O(5)	0.2168(7)	-0.0796(5)	0.6534(1)	4.7(1)
O(6)	0.0587(9)	-0.2527(6)	0.6421(1)	7.2(2)
O(7)	0.1398(9)	-0.1254(6)	0.7930(1)	6.3(2)
C(1)	0.382(1)	0.0890(6)	0.0931(2)	4.4(2)
C(2)	0.259(1)	0.1849(6)	0.0833(2)	4.8(2)
C(3)	0.238(1)	0.1953(7)	0.0476(2)	5.4(2)

Atom	*x*	*y*	*z*	B_{eq}
C(4)	0.348(1)	0.1045(7)	0.0324(2)	5.1(2)
C(5)	0.435(1)	0.0376(7)	0.0594(2)	4.5(2)
C(6)	0.064(1)	-0.1106(8)	0.0954(2)	6.3(2)
C(7)	-0.057(1)	-0.0231(9)	0.0843(3)	5.9(2)
C(8)	-0.068(1)	-0.0275(9)	0.0489(3)	6.2(2)
C(9)	0.043(2)	-0.1190(10)	0.0380(2)	6.8(3)
C(10)	0.133(1)	-0.1725(7)	0.0663(3)	6.7(3)
C(11)	0.4311(10)	0.0400(7)	0.1248(2)	4.5(2)
C(12)	0.514(1)	0.0773(7)	0.1285(2)	6.1(2)
C(13)	0.547(1)	0.1311(8)	0.1602(2)	6.2(2)
C(14)	0.504(1)	0.0664(7)	0.1902(2)	4.4(2)
C(15)	0.434(1)	0.0525(7)	0.1873(2)	4.9(2)
C(16)	0.400(1)	0.1055(7)	0.1555(2)	4.7(2)
C(17)	0.535(1)	-0.1346(8)	0.2226(2)	4.9(2)
C(18)	0.473(1)	-0.1434(9)	0.2814(2)	5.5(2)
C(19)	0.376(1)	-0.0.718(9)	0.3078(2)	5.7(2)
C(20)	0.383(1)	-0.1390(8)	0.3417(2)	5.6(2)
C(21)	0.289(1)	-0.0712(9)	0.3703(2)	5.8(2)
C(22)	0.305(1)	-0.1338(8)	0.4051(2)	5.1(2)
C(23)	0.225(1)	-0.0624(9)	0.4338(2)	6.1(2)
C(24)	0.263(1)	-0.1135(7)	0.4685(2)	4.7(2)
C(25)	0.194(1)	-0.0778(7)	0.5275(2)	4.8(2)
C(26)	0.105(1)	-0.1845(8)	0.5369(2)	5.2(2)
C(27)	0.093(1)	-0.2126(8)	0.5713(2)	5.5(2)
C(28)	0.164(1)	-0.1333(7)	0.5955(2)	4.2(2)
C(29)	0.257(1)	-0.0258(7)	0.5848(2)	4.5(2)
C(30)	0.269(1)	-0.0024(7)	0.5502(2)	5.1(2)
C(31)	0.139(1)	-0.1630(7)	0.6317(2)	4.7(2)
C(32)	0.192(1)	-0.0959(7)	0.6892(2)	4.5(2)
C(33)	0.272(1)	-0.1904(7)	0.7070(2)	5.1(2)
C(34)	0.253(1)	-0.1980(8)	0.7416(2)	5.7(2)
C(35)	0.152(1)	-0.1085(8)	0.7585(2)	4.8(2)
C(36)	0.071(1)	-0.0141(7)	0.7400(2)	5.1(2)
C(37)	0.094(1)	-0.0080(7)	0.7051(2)	4.9(2)
C(38)	0.045(1)	-0.034(1)	0.8118(2)	7.8(3)

TABLE III The list of bond lengths and bond angles of MPAF-6

Atoms	*Bond Distance / Å*	*Atoms*	*Bond Distance / Å*
Fe(1) – C(1)	2.044(8)	C(7) – C(8)	1.38(1)
Fe(1) – C(2)	2.035(7)	C(8) – C(9)	1.37(1)
Fe(1) – C(3)	2.056(7)	C(9) – C(10)	1.41(1)
Fe(1) – C(4)	2.036(8)	C(11) – C(12)	1.40(1)
Fe(1) – C(5)	2.012(8)	C(11) – C(16)	1.405(10)
Fe(1) – C(6)	2.023(8)	C(12) – C(13)	1.38(1)
Fe(1) – C(7)	2.045(9)	C(13) – C(14)	1.40(1)
Fe(1) – C(8)	2.04(1)	C(14) – C(15)	1.37(1)
Fe(1) – C(9)	2.026(9)	C(14) – C(17)	1.47(1)
Fe(1) – C(10)	2.014(8)	C(15) – C(16)	1.38(1)
O(1) – C(17)	1.351(9)	C(18) – C(19)	1.49(1)
O(1) – C(18)	1.453(9)	C(19) – C(20)	1.50(1)
O(2) – C(17)	1.194(10)	C(20) – C(21)	1.52(1)
O(3) – C(24)	1.358(9)	C(21) – C(22)	1.51(1)
O(3) – C(25)	1.414(9)	C(22) – C(23)	1.49(1)
O(4) – C(24)	1.187(9)	C(23) – C(24)	1.48(1)
O(5) – C(31)	1.358(9)	C(25) – C(26)	1.37(1)
O(5) – C(32)	1.425(8)	C(25) – C(30)	1.35(1)
O(6) – C(31)	1.206(9)	C(26) – C(27)	1.38(1)
O(7) – C(35)	1.361(9)	C(27) – C(28)	1.37(1)
O(7) – C(38)	1.42(1)	C(28) – C(29)	1.407(10)
C(1) – C(2)	1.42(1)	C(28) – C(31)	1.461(10)
C(1) – C(5)	1.423(10)	C(29) – C(30)	1.387(10)
C(1) – C(11)	1.45(1)	C(32) – C(33)	1.36(1)
C(2) – C(3)	1.40(1)	C(32) – C(37)	1.35(1)
C(3) – C(4)	1.42(1)	C(33) – C(34)	1.37(1)
C(4) – C(5)	1.43(1)	C(34) – C(35)	1.40(1)
C(6) – C(7)	1.38(1)	C(35) – C(36)	1.38(1)
C(6) – C(10)	1.42(1)	C(36) – C(37)	1.38(1)
Atoms	*Bond Angle/°*	*Atoms*	*Bond Angle /°*
C(17) – O(1) – C(18)	113.8(6)	C(20) – C(21) – C(22)	114.7(7)
C(24) – O(3) – C(25)	119.9(6)	C(21) – C(22) – C(23)	114.9(7)
C(31) – O(5) – C(32)	118.1(6)	C(22) – C(23) – C(24)	115.1(7)
C(35) – O(7) – C(38)	117.7(7)	O(3) – C(24) – O(4)	122.9(7)

Atoms	*Bond Distance / Å*	*Atoms*	*Bond Distance / Å*
O(1) – C(17) – O(2)	123.6(8)	O(3) – C(24) – C(23)	110.6(7)
O(1) – C(17) – C(14)	111.3(7)	O(4) – C(24) – C(23)	126.4(7)
O(2) – C(17) – C(14)	125.1(7)	O(5) – C(31) – O(6)	121.6(7)
O(1) – C(18) – C(19)	108.3(7)	O(5) – C(31) – C(28)	113.6(6)
C(18) – C(19) – C(20)	110.8(8)	O(6) – C(31) – C(28)	124.9(7)
C(19) – C(20) – C(21)	114.3(8)		

TABLE IV The defined planes and these dihedral angles between least-squares planes

Plane No	*Least-Squares Planes*
Plane 1	substituted CP-ring
Plane 2	unsubstituted CP-ring
Plane 3	phenyl ring (C11~C16)
Plane 4	phenyl ring (C25~C30)
Plane 5	phenyl ring (C32~C37)
Plane 6	C(17), O(1), O(2)
Plane 7	C(24), O(3), O(4)
Plane 8	C(31), O(5), O(6)
Planes	*Dihedral Angle / °*
Plane 1 – Plane 2	2.79
Plane 1 – Plane 3	17.73
Plane 1 – Plane 6	166.14
Plane 4 – Plane 5	68.81
Plane 6 – Plane 7	7.38
Plane 6 – Plane 8	67.12
Plane 7 – Plane 8	67.39

1. Molecular structure

In order to discuss the molecular structure more exactly, it might be better to divide this molecular structure into three parts, that is ferrocenyl moiety, flexible spacer and mesogenic group.

In ferrocenyl moiety, two cyclopentadienyl rings (plane 1 and plane 2) run in parallel conformation to each other with a dihedral angle of 2.79 °. Also, the two cyclopentadienyl rings have not a staggered conformation but an eclipsed one.

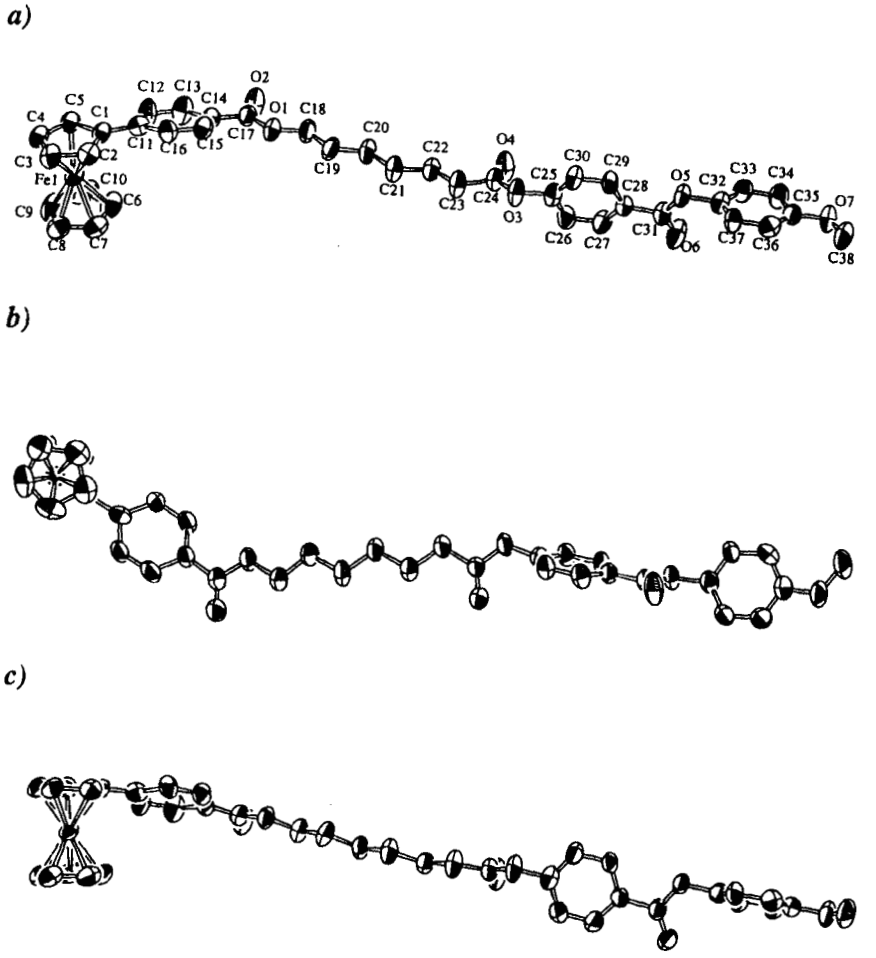


FIGURE 2 *ORTEP*II view of the molecular structure, showing the crystallographic numbering scheme. Thermal ellipsoids are drawn at 50% probability. a) showing the crystallographic numbering scheme, b) over view onto the cyclopentadienyl rings, c) side view onto the cyclopentadienyl rings

Ferrocene molecules have a staggered conformation [21]. In addition to this fact, the staggered conformation is widely observed in disubstituted ferrocene derivatives [19–20], while the eclipsed one is found in monosubstituted ferrocene derivatives [22] except MPAF-3. Therefore, MPAF-3 is one of the remarkable example. The average values of Fe-C and C-C bond distances are calculated to be 2.03 Å and 1.41 Å, respectively, and all C-C-C bond angles in two cyclopentadienyl rings are estimated to be 108.0 °. These values are in good agreement

with those of ferrocene within an experimental error [21]. The dihedral angle of the substituted cyclopentadienyl rings (plane 1) and the adjacent phenyl ring (plane 3) is 17.73 °, and that of the plane (plane 1) and the neighboring ester function (plane 6) is 166.14 °.

In the flexible spacer, the hexyl chain (C18-C23) is regarded as an all-*trans* conformation with 180 ° torsion angles differing by less than 5 °. The mean values of the C-C bond distances and C-C-C bond angles are 1.50 Å and 114.0 °, respectively. The chain length, that is, the spacer length is estimated to be 6.33 Å long. As is well known, the length of the C-C-C unit obtained in the extended normal paraffins are 2.54 Å long. Using this value, the length of the hexyl chain is calculated to be 6.35 Å long by 2.54 × 2.5. This value (6.35 Å) is nearly equal to the estimated value (6.33 Å). Therefore, the structure of the spacer is fully extended and just like that of normal paraffin. To add to this fact, it has to be noted that the hexyl spacer is coplanar with both neighboring ester functions.

In the mesogenic group, the bond distances and angles in the phenylbenzoate group are in agreement with those in the homologous compounds and other compounds having similar structures already reported [23–24]. The dihedral angle of two phenyl rings (plane 4 and plane 5) is 68.81 ° and the C28-C31-O5-C32 torsion angle is equal to 176.7(7) °. With respect to similar compounds having a phenylbenzoate group [23–24], it is clear that the corresponding dihedral angle indicates an inherent value in each case. The length of the mesogenic group (C24----C35) is calculated as 11.36 Å long.

As a result, the whole molecular length (C3----C38) is estimated to be 30.56 Å long. The molecule is slightly bent at the C17 atom (C1----C17----C38). This slightly bent structure may play a very important role in giving rise to liquid crystallinity described later. The whole molecular structure is exceedingly similar to that of MPAF-2 [12] and MPAF-4 [10].

2. Crystal structure

The crystal structures projected from the *a-c* plane and *b-c* plane are shown in Figure 3 and Figure 4, respectively.

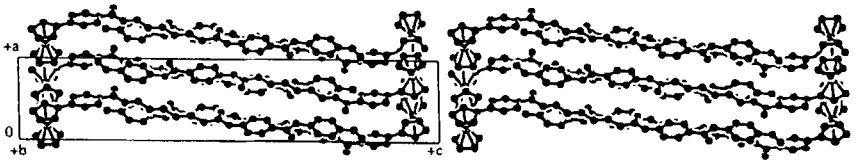


FIGURE 3 Crystal structure of MPAF-6, the projection of the *a-c* plane

As is mentioned above, the molecule is slightly bent around the ester group located at the nearest neighbor of the phenyl ferrocenyl group. This slightly bent structure contributes effectively to the highly compact packing of the crystal lattice. The mesogenic groups in the molecules are packed in anti-parallel fashion along the long crystallographic *c*-axis. That is, the two molecules array anti-parallel form as a pair, and these pairs pile up along short crystallographic axes. As a result, the molecules make up a layer structure. Also, this structure is able to lead to the most effective crystal packing, namely the superfluous space around unsubstituted cyclopentadienyl ring may be compensated. It is very interesting that ferrocenyl moiety builds in a head-to-head manner between the layers. This fact may indicate that there is some kind of interaction between ferrocenyl moieties and this interaction is one of the primary factors to make up the layer structure. The layer structures of α,ω-alkanediols [25–28] are different from each other depending on the number of carbon atoms of the hydrocarbon chain. The compounds with even carbon atoms have an all-*trans* conformation throughout the whole molecule, while one of the two hydroxyl groups in the odd members adopts the *gauche* conformation. As a result, the even carbon-number compounds show the smectic C-like structure and the odd carbon-members show the smectic A-like one. As mentioned above, the interaction of molecular terminal groups should play an important role in making the layer structure. Thereby, the interaction of ferrocenyl moiety located in the molecular terminal may contribute to the molecular arrangement in the liquid crystalline phase and this crystal structure strongly suggests that the liquid crystal phase of this compound may be smectic.

From the projection of the *b-c* plane (Figure 4), three carbonyl oxygen atoms in one molecule orient toward three other carbonyl oxygen ones in the neighboring molecule in order to make up the network of dipole interactions. The interaction in the direction of the molecular short axes generates from not only the mesogen but also the carbonyl oxygen atoms as the dipole interaction. Generally, an intensity of the dipole interaction is expressed by the position and orientation of the corresponding dipole. It may be considered that this effect may contribute to the appearance of liquid crystallinity and to build up the layer structure in the liquid crystalline phase.

3. Comparison of MPAF-6 and CAPF-6

The structure of CAPF-6 and that of MPAF-6 are different from each other in some respects. Figure 5 presented the molecular and crystal structure of CAPF-6 [8]. In the molecular structure of CAPF-6, the most characteristic point is that there are two crystallographically independent molecules (A and B) in the unit cell and one of them has one *gauche* conformation in the flexible hexyl chain.

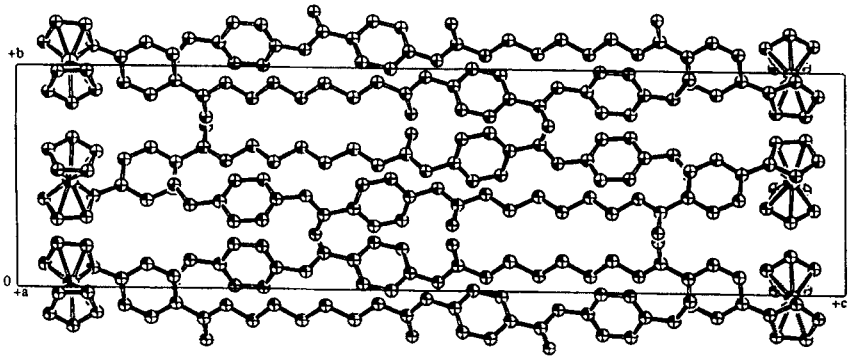


FIGURE 4 Crystal structure of MPAF-6, the projection of the *b-c* plane

CAPF-6 contains the cholesterylester function as a mesogen. As the cholesterylester function is a large and bulky atomic group as well as having ferrocenyl moiety, it may be difficult to make up the rod-like molecular feature for CAPF-6. Therefore, the *gauche* conformation in the flexible alkyl spacer contributes to making up a linear shape as a set of A and B molecules. As a result, this *gauche* conformation in the flexible spacer enables CAPF-6 to show liquid crystallinity in spite of the unstable conformation in steric hindrance. On the other hand, the mesogenic phenylbenzoate group in MPAF-6 is superior in planarity compared with that of the cholesterylester function in CAPF-6. As a result, MPAF-6 makes up rod-like features itself.

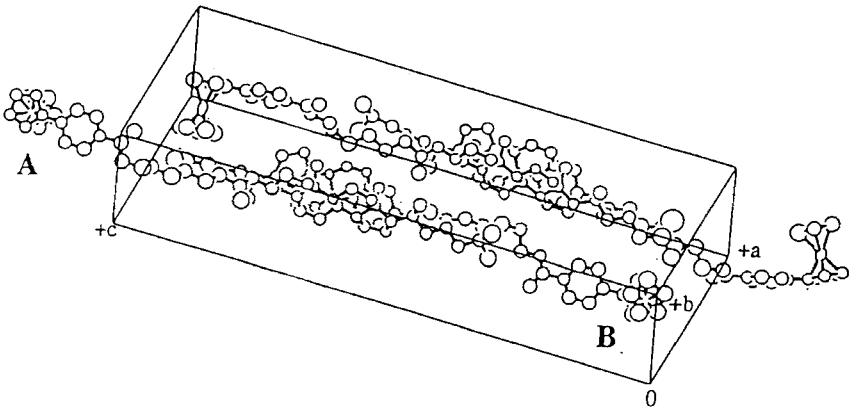


FIGURE 5 Crystal structure of CAPF-6

In crystal structure, CAPF-6 arrayed the head-to-tail type between A and B, and built up the layer structure with the two molecules (A and B) overlapping in anti-parallel fusion. However, the degree of overlapping in CAPF-6 is a little looser compared with that of MPAF-6. According to the projection of the *a-c* plane in CAPF-6, it is clear that each tetracyclic core in the cholesterylester group overlaps with the neighboring tetracyclic cores. This suggests that the interaction in the direction of the molecular short axes is generated by the cholesteryl function. On the other hand, the interaction in MPAF-6 is generated by not only the mesogenic phenylbenzoate group but also by the three carbonyl oxygen atoms.

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