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Crystal Structure of the 4-Cyanophenyl 4-Perfluorohexylbenzoate

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Crystal Structure of the 4-Cyanophenyl 4-Perfluorohexylbenzoate

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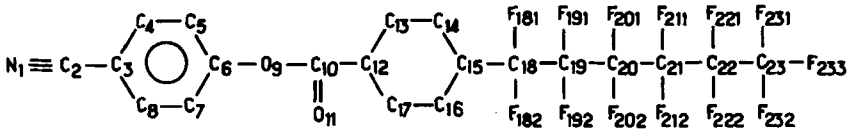
The title compound crystallizes with four molecules in the asymmetric unit. They adopt a slightly bent conformation with quite extended perfluorinated aliphatic chain. The molecular arrangement is characterized by the segregation of the cores 4-cyanophenyl 4-benzoate on one side and the perfluorinated aliphatic chains on the other side. The molecules give bilayer sheets, parallel to the xoy plane, the thickness of bilayers being equal to the c parameter. The interactions between the sheets are quite weak.

Keywords: Liquid crystal, smectic A, perfluorinated chain, crystal structure

INTRODUCTION

Liquid crystals play an important role in a wide variety of electrooptical devices and their development is currently of great interest[1]. Recently, liquid crystals incorporating fluorine atoms show very interesting results for these displays[2,3]. There are numerous ways to introduce fluorine into liquid crystals but here we limit the brief discussion to smetic materials in which one of the tails is a perfluorinated alkyl chain. These materials show a smectic A phase with a monolayer (S_{A1}), a partial bilayer (S_{Ad}) or a bilayer arrangement (S_{A2}) of the molecules[4–10]. The mean difference between fluoro and hydrocarbon chain liquid crystals is that the former does not exhibit the nematic phase but favors the interdigitated arrangement in the smectic phases than the later. So the 4-cyanophenyl series shows a nematic phase for short chains and nematic and smectic A phases for the long one ($n > 10$). The studied compound, 4-cyanophenyl 4-perfluorohexylbenzoate displays the following phase sequence:

$$K \xrightarrow{101^\circ} S_{A2} \xrightarrow{123^\circ} I$$



and the structural characterization shows that the S_A phase is a bilayered one (S_{A2}). In order to clarify the precise relationship between the S_{A2} structure and the molecular interactions, we intended to perform the crystal structure of the present compound.

TABLE 1

Crystal Data

$C_{20}H_8NF_{13}O_2$	$M_x = 541.6\,g\,cm^{-3}$
Triclinic	space group $P\bar{1}$ ($Z = 8$)
$a = 5.926(6)$Å	$\alpha = 80.60(1)°$
$b = 19.665(7)$	$\beta = 87.00(5)$
$c = 36.67(7)$	$\gamma = 88.65(8)$
$v = 4208$ Å^3	$d_c = 1.709\,g\,cm^{-3}$
$\lambda(CuK\alpha) = 1.5417$ Å	$\mu(CuK\alpha) = 1.8\,mm^{-1}$

CRYSTAL DATA AND X-RAY MEASUREMENT

Colourless crystals were obtained with some difficulties by evaporation from toluene solutions. They were fragile, soft and often twinned. The crystal is lamellar, with dimensions $0.4 \times 0.25 \times 0.025$. The unit cell parameters were obtained by a least-squares fit of the setting angles of 25 reflections, with θ between 18 and 39°. The crystal data are given in Table 1.

There are four independent molecules per asymmetric unit, i.e., 144 non-hydrogen atoms. The data were collected on a CAD-4 Enraf Nonius diffractometer for the monochromatized CuKα radiation with $(\sin\theta/\lambda)_{max} < 0.45°$, $(-5 \leq h \leq 5)$, $(-19 \leq k \leq 19)$ and $(-36 \leq 1 \leq 36)$ using the $\omega - 2\theta$ scan mode. The scan range was $(1.8 + 0.15\tan\theta°)$ and the detector width $(1.8 + 0.5\tan\theta)$ mm; 9130 reflections were measured (Rint = 0.024) of which 4908 were unique and 4222 observed ($I \geq 3\sigma(I)$); experimental absorption corrections was performed: minimum and maximum transmission factors are 0.94 and 0.99 respectively.

STRUCTURE ANALYSIS AND REFINEMENT

The structure was solved by direct methods using the Mithril package[11]. Because of the poor quality of the crystal, the limitation of the reflection sphere ($\theta < 45°$) and the great number of non-hydrogen atoms per asymmetric unit, several successive Fourier synthese were necessary to locate the 144 non-hydrogen atoms. The structure could then be refined only by using constraints[12] on C—C (1.53 ± 0.02) and C—F (1.33 ± 0.02) Å on the end of perfluorinated chains, with the SHELX76 program[13]. The hydrogen atoms were introduced at the theoretical positions[14] and allowed to ride with the carbon atoms to which they are attached. The refinement was resumed with unit weights. The final reliability factor is $R = 0.098$.

RESULTS AND DISCUSSION

Atomic parameters (x, y, z, Ueq) are given in Table 2. For the sake of clarity, the same numbering has been used for the four independent identical molecules of the asymmetric unit. The SNOOPI drawing[15] and atom numbering of one of the molecules is presented in Figure 1.

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TABLE 2

Atomic Coordinates x, y, z ($\times 10^4$) and Ueq ($\times 10^3$), $Ueq = 1/3\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* a_i a_j$

		X	Y	Z	Ueq
Mole 1	N 1	4781(20)	1427(6)	5513(3)	124(17)
	C 2	4716(21)	1273(7)	5221(4)	95(17)
	C 3	4655(24)	1000(7)	4872(3)	80(17)
	C 4	6444(22)	1115(6)	4619(3)	79(16)
	C 5	6552(23)	833(6)	4301(3)	77(16)
	C 6	4744(24)	418(6)	4249(3)	71(15)
	C 7	2852(20)	325(6)	4487(3)	82(17)
	C 8	2874(24)	619(6)	4814(3)	87(17)
	O 9	4588(13)	110(4)	3932(2)	80(9)
	C 10	6396(23)	−247(7)	3809(3)	78(16)
	O 11	8213(15)	−274(5)	3931(2)	103(12)
	C 12	5721(18)	−618(5)	3508(3)	54(17)
	C 13	3742(20)	−474(6)	3330(3)	74(17)
	C 14	3176(19)	−831(6)	3049(3)	76(14)
	C 15	4682(19)	−1339(6)	2950(3)	66(13)
	C 16	6702(19)	−1466(5)	3133(3)	67(14)
	C 17	7210(18)	−1117(6)	3406(3)	67(13)
	C 18	4055(16)	−1775(6)	2670(3)	70(15)
	C 19	5111(22)	−1509(5)	2281(3)	79(17)
	C 20	4423(17)	−1879(5)	1967(3)	76(16)
	C 21	5714(24)	−1678(6)	1593(3)	108(21)
	C 22	4831(29)	−1949(8)	1260(3)	192(39)
	C 23	6350(31)	−1783(8)	913(4)	191(45)
	F181	1810(12)	−1767(4)	2641(2)	115(10)
	F182	4774(12)	−2419(3)	2769(2)	103(9)
	F191	4579(13)	−838(3)	2187(2)	105(10)
	F192	7359(12)	−1560(5)	2301(2)	108(10)
	F201	2243(13)	−1744(6)	1907(2)	170(15)
	F202	4676(19)	−2541(4)	2067(2)	169(16)
	F211	5854(24)	−999(5)	1513(2)	206(21)
	F212	7829(17)	−1898(8)	1631(3)	238(24)
	F221	2963(21)	−1594(13)	1186(5)	352(40)
	F222	4908(33)	−2620(7)	1352(3)	281(29)
	F231	6534(34)	−1130(8)	799(3)	283(32)
	F232	8256(29)	−2127(13)	963(5)	338(41)
	F233	5479(22)	−2044(7)	646(3)	243(24)
Mole 2	N 1	−91(18)	1945(7)	5093(3)	131(18)
	C 2	−57(22)	2100(8)	5384(4)	110(20)
	C 3	−73(27)	2334(7)	5728(4)	88(18)
	C 4	1814(23)	2692(6)	5317(3)	80(17)
	C 5	1767(20)	2964(5)	6135(3)	66(14)
	C 6	−110(23)	2871(6)	6365(3)	60(14)
	C 7	−1990(23)	2509(6)	6300(3)	70(16)
	C 8	−1974(21)	2252(6)	5979(4)	84(17)
	O 9	4(12)	3120(3)	6702(2)	71(9)
	C 10	−1650(21)	3587(6)	6799(3)	66(15)
	O 11	−3226(14)	3768(4)	6618(2)	89(10)
	C 12	−1118(19)	3799(5)	7158(3)	63(13)
	C 13	−2645(18)	4243(5)	7305(3)	74(14)
	C 14	−2188(21)	4469(6)	7624(3)	81(15)
	C 15	−268(19)	4270(5)	7797(3)	69(14)
	C 16	1236(19)	3820(6)	7662(3)	83(15)
	C 17	829(19)	3604(6)	7331(3)	83(15)
	C 18	303(23)	4551(6)	8145(3)	87(18)
	C 19	−727(23)	4111(7)	8496(3)	85(18)

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TABLE 2 (*Continued*)

		X	*Y*	*Z*	*Ueq*
	C 20	−57(26)	4286(6)	8868(3)	98(21)
	C 21	−1357(26)	3995(8)	9227(3)	130(29)
	C 22	−266(40)	3973(9)	9598(4)	293(76)
	C 23	−2007(37)	3896(11)	9925(4)	265(84)
	F181	−497(13)	5189(3)	8137(2)	110(10)
	F182	2552(13)	4552(3)	8188(2)	107(10)
	F191	−2964(14)	4153(5)	8494(2)	131(12)
	F192	−92(14)	3452(4)	8502(2)	120(11)
	F201	−2(25)	4957(5)	8848(2)	218(23)
	F202	2099(21)	4052(9)	8918(4)	246(25)
	F211	−3285(25)	4370(11)	9208(5)	339(39)
	F212	−2129(25)	3382(6)	9202(3)	209(23)
	F221	574(34)	4599(9)	9580(3)	305(35)
	F222	961(39)	3390(12)	9613(9)	462(71)
	F231	−3178(45)	4479(14)	9862(9)	491(73)
	F232	−3020(39)	3306(11)	9931(4)	307(39)
	F233	−699(31)	3828(10)	10210(4)	302(35)
Mole 3	N 1	−4528(20)	3138(7)	4643(4)	154(21)
	C 2	−4710(20)	3464(7)	4873(4)	96(18)
	C 3	−4759(21)	3906(6)	5157(3)	69(15)
	C 4	−6710(20)	4317(6)	5212(3)	73(15)
	C 5	−6849(20)	4677(6)	5496(3)	79(15)
	C 6	−5062(21)	4649(6)	5723(3)	67(14)
	C 7	−3058(20)	4271(6)	5676(3)	75(15)
	C 8	−2985(21)	3894(6)	5377(3)	82(16)
	O 9	−5004(13)	5040(4)	6009(2)	75(9)
	C 10	−6626(23)	4968(6)	6271(3)	65(16)
	O 11	−8155(16)	4579(4)	6292(2)	86(12)
	C 12	−6382(22)	5412(6)	6556(3)	67(14)
	C 13	−4497(24)	5799(6)	6556(3)	76(16)
	C 14	−4301(21)	6253(6)	6803(3)	78(16)
	C 15	−6054(23)	6300(5)	7064(3)	68(15)
	C 16	−7918(24)	5903(6)	7078(3)	86(17)
	C 17	−8117(19)	5462(6)	6817(3)	73(14)
	C 18	−6016(16)	6823(5)	7328(3)	74(17)
	C 19	−5223(23)	6509(5)	7708(2)	89(19)
	C 20	−5377(24)	6911(6)	8024(3)	130(25)
	C 21	−4275(32)	6683(6)	8381(3)	305(70)
	C 22	−5062(31)	7006(7)	8720(3)	200(51)
	C 23	−3267(36)	6856(9)	9014(4)	293(84)
	F181	−4629(16)	7335(4)	7192(2)	114(12)
	F182	−8090(12)	7103(4)	7372(2)	132(11)
	F191	−3176(14)	6275(5)	7668(2)	147(13)
	F192	−6450(19)	5955(5)	7834(2)	157(17)
	F201	−4652(37)	7524(7)	7888(3)	263(36)
	F202	−7463(24)	7135(11)	8068(4)	329(36)
	F211	−2131(27)	6788(19)	8262(10)	657(96)
	F212	−4440(24)	6014(5)	8456(2)	190(19)
	F221	−4892(23)	7680(6)	8593(3)	186(18)
	F222	−7052(32)	6725(14)	8842(14)	596(99)
	F231	−1618(40)	7122(15)	8775(9)	576(89)
	F232	−4223(29)	7100(7)	9295(3)	257(28)
	F233	−3550(32)	6198(7)	9155(3)	293(31)
Mole 4	N 1	456(20)	3866(6)	4492(4)	139(19)
	C 2	468(22)	3415(7)	4325(4)	98(18)
	C 3	470(22)	2912(6)	4076(3)	73(15)

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TABLE 2 (*Continued*)

	X	*Y*	*Z*	*Ueq*
C 4	−1379(22)	2870(6)	3860(3)	94(17)
C 5	−1346(20)	2448(6)	3618(3)	82(15)
C 6	580(21)	2046(6)	3578(3)	70(14)
C 7	2346(21)	2047(6)	3791(3)	82(15)
C 8	2326(21)	2461(3)	4051(3)	91(16)
O 9	768(16)	1649(4)	3279(2)	86(11)
C 10	−954(30)	1293(7)	3191(4)	80(20)
O 11	−2711(17)	1202(5)	3361(2)	102(13)
C 12	−388(22)	1043(6)	2831(3)	65(15)
C 13	1561(21)	1213(6)	2616(3)	77(16)
C 14	1975(21)	993(6)	2284(3)	76(16)
C 15	367(24)	579(6)	2166(3)	72(16)
C 16	−1531(22)	399(6)	2380(3)	74(16)
C 17	−1974(22)	620(6)	2713(3)	77(16)
C 18	763(22)	354(7)	1788(2)	71(16)
C 19	−388(17)	815(5)	1471(3)	87(19)
C 20	100(26)	707(7)	1075(3)	189(38)
C 21	−1516(28)	962(8)	776(3)	205(44)
C 22	−446(36)	1084(9)	380(3)	268(58)
C 23	−2314(34)	1069(10)	106(5)	292(76)
F181	−3(14)	−286(3)	1802(2)	108(11)
F182	3021(12)	347(4)	1694(2)	101(9)
F191	−2593(13)	795(5)	1555(2)	137(13)
F192	160(16)	1456(4)	1483(2)	140(14)
F201	418(33)	37(6)	1082(3)	223(27)
F202	2246(24)	867(13)	979(4)	356(47)
F211	−3115(47)	491(15)	875(11)	600(83)
F212	−2335(20)	1552(6)	851(2)	186(17)
F221	733(52)	1646(13)	403(16)	705(99)
F222	560(26)	486(10)	343(3)	276(28)
F231	−1138(35)	1263(12)	−207(4)	326(40)
F232	−3275(30)	1681(9)	128(3)	283(31)
F233	−3156(51)	455(13)	242(11)	577(99)

As expected the cyano groups show significantly greater thermal motion factors than the other atoms of the 4-cyanophenyl moiety[16]. This thermal motion increases from the beginning to the end of the chains, especially from the C(20) to the C(23) atoms and the fluorine atoms which are bound to the above carbon atoms for the perfluorinated chains. The bond lengths are given in Table 3. The SNOOPI drawing of the four molecules of the asymmetric unit is shown in Figure 2. The molecules 1 to 4 can be

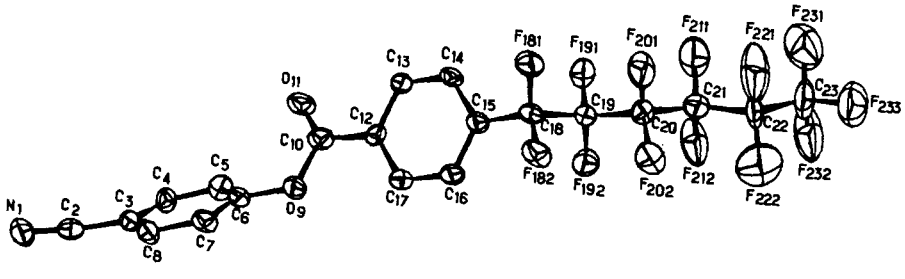

FIGURE 1 SNOOPI drawing of one molecule.

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TABLE 3

Bond Lengths (Å (for the Four Independent Molecules.

	Mole 1	Mole 2	Mole 3	Mole 4
N 1–C 2	1.163(17)	1.159(19)	1.141(20)	1.156(19)
C 2–C 3	1.470(18)	1.411(19)	1.460(18)	1.453(18)
C 3–C 4	1.369(18)	1.416(20)	1.419(17)	1.398(18)
C 3–C 8	1.356(19)	1.412(19)	1.355(17)	1.403(17)
C 4–C 5	1.367(16)	1.358(16)	1.353(16)	1.312(17)
C 5–C 6	1.402(19)	1.357(17)	1.376(16)	1.387(17)
C 6–C 7	1.381(17)	1.389(18)	1.403(17)	1.340(17)
C 6–O 9	1.405(13)	1.409(12)	1.400(13)	1.444(13)
C 7–C 8	1.415(16)	1.353(17)	1.420(16)	1.351(16)
O 9–C 10	1.364(15)	1.399(14)	1.316(15)	1.335(18)
C 10–O 11	1.184(16)	1.187(14)	1.190(16)	1.187(19)
C 10–C 12	1.497(16)	1.494(15)	1.484(17)	1.502(17)
C 12–C 13	1.373(16)	1.392(15)	1.368(18)	1.380(17)
C 12–C 17	1.387(15)	1.363(16)	1.381(16)	1.401(18)
C 13–C 14	1.399(15)	1.359(16)	1.383(16)	1.368(16)
C 14–C 15	1.401(16)	1.351(16)	1.387(17)	1.398(18)
C 15–C 16	1.400(16)	1.371(16)	1.362(19)	1.356(18)
C 15–C 18	1.509(16)	1.529(15)	1.528(14)	1.530(14)
C 16–C 16	1.354(15)	1.385(16)	1.407(16)	1.372(17)
C 18–C 19	1.541(15)	1.535(16)	1.519(13)	1.531(14)
C 18–F181	1.339(12)	1.326(14)	1.330(12)	1.340(15)
C 18–F182	1.326(14)	1.350(16)	1.347(12)	1.364(15)
C 19–C 20	1.536(14)	1.532(16)	1.506(14)	1.514(15)
C 19–F191	1.342(11)	1.326(16)	1.296(16)	1.326(12)
C 19–F192	1.338(15)	1.337(15)	1.330(15)	1.318(13)
C 20–C 21	1.535(15)	1.525(17)	1.493(17)	1.508(19)
C 20–F201	1.334(13)	1.313(16)	1.301(18)	1.323(18)
C 20–F202	1.301(12)	1.358(21)	1.312(21)	1.332(21)
C 21–C 22	1.531(18)	1.530(21)	1.531(17)	1.537(18)
C 21–F211	1.324(15)	1.343(23)	1.331(27)	1.336(33)
C 21–F212	1.323(18)	1.319(20)	1.304(16)	1.312(20)
C 22–C 23	1.512(20)	1.531(27)	1.544(24)	1.537(26)
C 22–F221	1.310(23)	1.330(27)	1.335(17)	1.339(35)
C 22–F222	1.307(20)	1.337(31)	1.338(31)	1.329(26)
C 23–F231	1.290(22)	1.318(35)	1.333(34)	1.317(25)
C 23–F232	1.307(26)	1.317(31)	1.304(21)	1.332(27)
C 23–F233	1.312(20)	1.320(25)	1.323(22)	1.327(35)

analyzed as made as moieties: the 4 cyanophenyl-4 benzoate moiety and the perfluorinated chain, each of which is quite linear. There is a bend at the C(18) level: the N(1)···C(18)···C(23) angles are close to 157, 153, 151 and 138° respectively for molecules 1 to 4, close to the 145° observed in the perfluoroheptyl analogue (16).

The perfluorinated alkyl chains are more or less extended with most of the C—C—C—C torsion angles differing by less than 20° from 180°. The cyano group is slightly out of the plane of the first phenyl ring (C(3) to C(8)): 0.31, 0.24, 0.16 and 0.34 Å respectively for the nitrogen atom N(1) of molecules 1 to 4 as observed for the 4-perfluoroheptyl analogue (16). The 4-cyanophenyl 4-benzoate axis (C(13)···C(18)) of the four molecules are quite parallel. The perfluorinated chains are only roughly parallel. The cyano groups of molecules 1 and 2 on one side and molecules 3 and 4 on the other side are antiparallel. The angles between the φ_0 benzene ring (C(3) to C(8))

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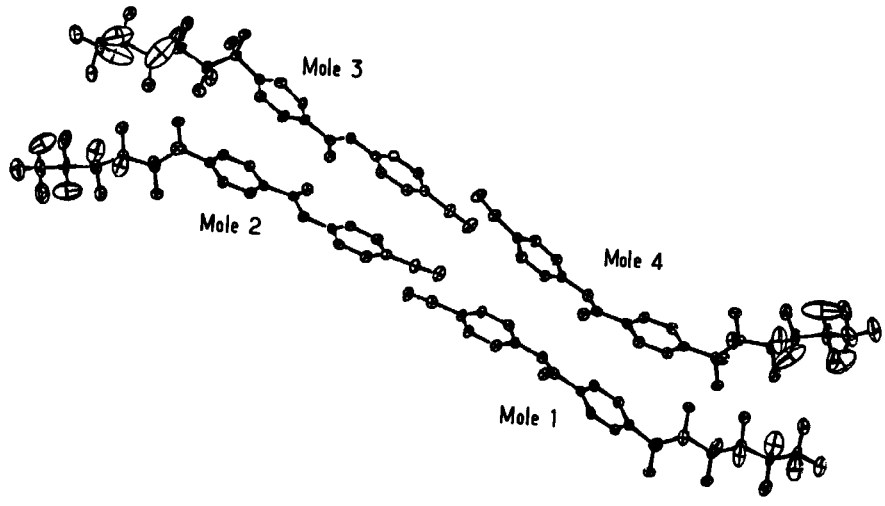

FIGURE 2 SNOOPI drawing of the four independent molecules.

and the φ_1 one (C(12) to C(17)) defined as φ_0/φ_1 are 56, 52, 49 and 54°. Finally, the four molecules of the asymmetric unit, have very similar conformations and differ slightly in the conformation of their perfluorinated alkyl chains. The significant torsion angles of the four independent molecule of the asymmetric unit are as follows.

	mole 1	mole 2	mole 3	mole 4
C(5)–C(6)–C(9)–C(10)	49(1)	125(1)	58(1)	−43(2)
C(6)–O(9)–C(10)–O(11)	−7(1)	3(1)	2(1)	−8(1)
C(6)–O(9)–C(10)–C(12)	171(1)	−178(1)	178(1)	170(1)
O(11)–C(10)–C(12)–C(13)	−168(1)	2(1)	172(1)	173(1)
C(14)–C(15)–C(18)–C(19)	99(1)	88(1)	−99(1)	−95(1)
C(15)–C(18)–C(19)–C(20)	−175(1)	173(1)	−171(1)	172(1)
C(18)–C(19)–C(20)–C(21)	−172(1)	167(1)	−169(1)	158(2)
C(19)–C(20)–C(21)–C(22)	−171(1)	160(1)	−163(1)	157(2)
C(20)–C(21)–C(22)–C(23)	−174(2)	160(2)	−164(2)	160(2)

The molecular arrangement (Figure 3) shows that the four molecules of the asymmetric unit are roughly parallel. The crystal cohesion partly results from strong dipolar interactions between antiparallel polar cyano groups, like those found in other mesogenic compounds (17). Moreover, there are numerous weak interactions between roughly parallel perfluorinated side-chains, in agreement with the high thermal motions of such chains. The molecular arrangement results in bilayer sheets, parallel to the $x0y$ plane, the thickness of which is close to the length of the c parameter. This arrangement looks like a smectic A_2 one, as observed in perfluoroheptyl homologue (16). The interactions between the sheets are very weak.

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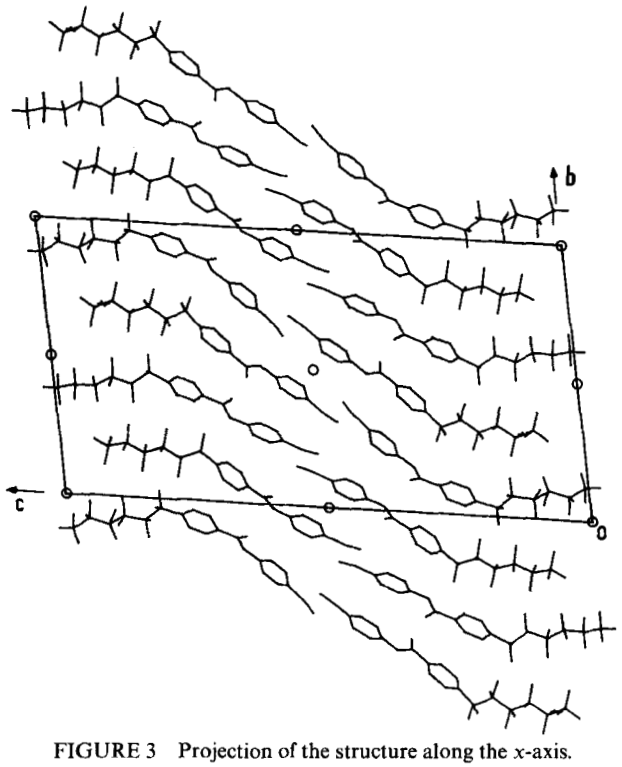

FIGURE 3 Projection of the structure along the *x*-axis.

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