The molecular and crystal structure of *N*-(4-*n*-butyloxybenzylidene)-4'-ethylaniline (4O.2) and *N*-(4-*n*-heptyloxybenzylidene)-4'-hexylaniline (7O.6)

Wolfgang Thyen[a]; Frauke Heineman[a]; Peter Zugenmaier[a]

[a] Institut für Physikalische Chemie der Technischen Universität Clausthal, Clausthal-Zellerfeld,
Germany

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by WOLFGANG THYEN, FRAUKE HEINEMANN
and PETER ZUGENMAIER*

Institut für Physikalische Chemie der Technischen Universität Clausthal,
Arnold-Sommerfeld-Straße 4, D-38678 Clausthal-Zellerfeld, Germany

The crystal and molecular structure of N-(4-n-butyloxybenzylidene)-4'-ethylaniline (4O.2) and the homologue N-(4-n-heptyloxybenzylidene)-4'-hexylaniline (7O.6) have been solved (at room temperature) by direct methods. The crystals of both compounds belong to the triclinic system with space group P$\bar{1}$ with two molecules per unit cell. 4O.2: $a = 5.531(2)$, $b = 7.592(3)$, $c = 19.746(7)$ Å, $\alpha = 86.66(2)$, $\beta = 88.15(2)$, $\gamma = 90.29(2)°$; 7O.6: $a = 5.420(2)$, $b = 8.307(3)$, $c = 28.057(7)$ Å, $\alpha = 91.69(2)$, $\beta = 89.76(2)$, $\gamma = 108.02(2)°$. The structures were refined by full-matrix least-squares calculations to $R = 0.036$ for 2297 observed reflections for 4O.2 and to $R = 0.037$ for 2150 reflections for 7O.6. The conformations in the asymmetric units of the two compounds differ considerably: The planes of the two phenyl rings of 4O.2, forming the mesogenic core of the molecule, are twisted at 61·2° to each other and the butoxy group contains a *gauche* conformation. In contrast the heptoxy chain of 7O.6 forms an all *trans*-conformation which lies almost in one plane with the two coplanar phenyl rings. The hexyl group also exists in an extended form, in a plane which is rotated against the plane of the mesogenic unit. The packing in the crystalline state of the two homologues exhibits a layered structure along c^*; in 4O.2 these layers are separated, but in 7O.6 they are interdigitated. The compensation of the dipole moments of the C–O–C and C=N–C bonds occurs similarly in both structures: molecular orientations parallel to the a, c-plane in which the long axes of the molecules points in the same direction are packed in antiparallel fashion along b^*.

1. Introduction

Since the discovery of the liquid crystalline (LC) state more than one hundred years ago, a correlation between the formation of definite liquid crystalline phases and the constitution, as well as the conformation, of the molecules of LC compounds is yet missing [1–9].

The structure determination of the crystalline state seems to be one path to obtain general information about conformation and packing of the molecules, but it is an open question whether this knowledge enables the type and properties of smectic phases formed from the crystals to be predicted. Despite some doubts on the interpretation of data obtained in such a way, essentially the interactions, as well as the steric conditions, which are manifested in the crystal structure are also valid to a high degree with respect to the formation of the LC states.

*Author for correspondence.

A large scale of systematic investigation is needed to obtain detailed knowledge in this field of liquid crystal research. Although in the past 15 years many studies have been undertaken—30–40 papers are published on this subject per year—the available data are not yet sufficient for the derivation of general ideas or laws. Besides, many of the known structure determinations have been carried out on crystal precursors of nematic, smectic A and smectic C phases. In most of these cases, the 'smectic precursors' form layered structures, while the 'nematic precursors' possess imbricated structures. This statement may be regarded as of limited general validity, since these fluid LC phases and the crystals have long range orientational order as the only common property.

In our opinion, the basis for such investigations has to involve the closest similarity of the crystal and liquid crystal structures. This requirement then might lead to some conclusions concerning a comparison between both. Therefore, it seems to us very promising to compare the structures of the crystals and liquid crystals of highly ordered smectic phases.

2. Experimental, structure solution and refinement

The compounds have been synthesized according to standard procedures and recrystallized several times for purification [10–12]. Crystals suitable for an X-ray determination were obtained by slow crystallization from ethanol (4O.2) and petroleum (7O.6) at room temperature. Data collection was performed with a CAD4 instrument and data processing and refinement with the MoLEN package (Enraf-Nonius, Delft). Basic crystallographic data are represented in table 1. The figures representing conformation and packing in the structures were produced with SCHAKAL 92 [13].

3. Results and discussion

3.1. *Molecular geometry and conformation*

3.1.1. *Molecular geometry*

The molecular conformation, the bond lengths and bond angles of the homologues 4O.2 and 7O.6 agree closely with literature data found for the homologues 4O.8 and 8O.4 [7, 8], as well as for the low temperature modification of 1O.4 (MBBA) [9].

Figures 1 and 2 represent the molecular structure and the numbering of atoms for 4O.2 and 7O.6, respectively. In tables 2–4† and 5–7† the fractional coordinates, bond lengths and bond angles have been collected for both compounds.

The mean values of the bond distances for the two molecules differ little—4O.2: ring A (C1 to C6) $1\cdot387(12)$ Å, ring B (C8 to C13) $1\cdot385(4)$ Å; 7O.6: ring A (C1 to C6) $1\cdot384(9)$ Å, ring B (C8 to C13) $1\cdot383(10)$ Å—as do the bond angles, with $120\cdot0(1\cdot4)°$ for 4O.2 and $120\cdot0(1\cdot9)°$ for 7O.6 for all aromatic carbon atoms.

The C=N and C–N distances in the azomethine group within the mesogen are $1\cdot276(2)$ Å and $1\cdot415(2)$ Å for 4O.2 and $1\cdot255(4)$ Å and $1\cdot406(4)$ Å for 7O.6, respectively. The mean values for the C–C bond distances and C–C–C angles in the alkyl and alkoxy chains are found to be $1\cdot497(21)$ Å and $113\cdot5(4)°$ for 4O.2 and $1\cdot504(18)$ Å and $113\cdot9(8)°$ for 7O.6.

† Tables 3, 4, 6 and 7 have been deposited with the British Library, copies of these tables which comprise 4 pages may be obtained from the British Library, Lending Division, by quoting the number SUP 16527 according to the procedure described at the end of the issue.

Table 1. Summary of crystallographic data.

|	4O.2	7O.6
Molecular formula	$C_{19}H_{23}NO$	$C_{26}H_{37}NO$
Formula weight (g mol^{-1})	281·40	379·59
Crystal system	Triclinic	Triclinic
Space group	P$\overline{1}$	P$\overline{1}$
a/Å	5·531(2)	5·420(2)
b/Å	7·592(3)	8·307(3)
c/Å	19·746(7)	28·057(7)
α	86·66(2)°	91·69(2)°
β	88·15(2)°	89·76(2)°
γ	90·29(2)°	108·02(2)°
Cell volume/Å^{-3}	827·3(5)	1161·6(7)
D_{cal}/g cm^{-3}	1·134	1·090
Z	2	2
Number of reflections used for lattice parameter refinement	19	16
Scan range	$8° < \theta < 16°$	$10° < \theta < 17°$
$F(000)$	304	416
$\mu(MoK_\alpha)$/cm^{-1}	0·6	0·6
$\lambda(MoK_\alpha)$/Å	0·71073	0·71073
Points scanned	2297	2150
Significant Is ($\sigma > 3$)	1511	1288
Parameters refined	190	253
Scan range/θ	1–23°	1–20°
R	0·036	0·037
R_w	0·047	0·048
High peak in final diff. map/eÅ^{-3}	0·09(3)	0·08(2)
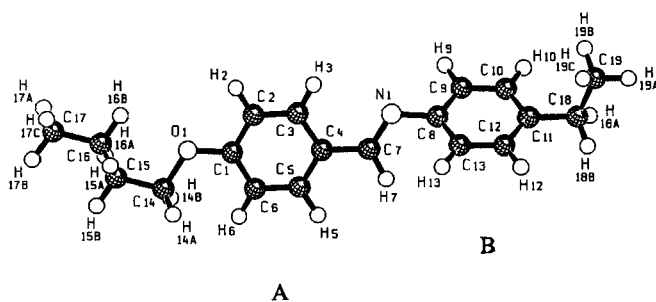
Figure 1. The molecular structure of 4O.2 with the numbering scheme.
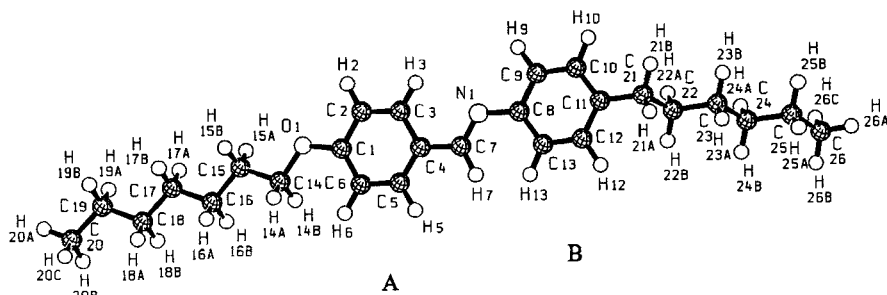

Figure 2. The molecular structure of 7O.6 with the numbering scheme.

Table 2.   Atomic coordinates and equivalent isotropic displacement factors of 4O.2.

	x	y	z	$B_{eq}/\text{Å}^2$
O(1)	0·0925(2)	− 0·2980(2)	0·26919(6)	4·65(3)
N(1)	0·3656(3)	− 0·2569(2)	− 0·04770(7)	4·09(3)
C(1)	0·0969(3)	− 0·2797(2)	0·19983(8)	3·69(4)
C(2)	0·2970(3)	− 0·3523(2)	0·16737(9)	3·90(4)
C(3)	0·3211(3)	− 0·3405(2)	0·09814(9)	3·86(4)
C(4)	0·1429(3)	− 0·2583(2)	0·05865(9)	3·67(4)
C(5)	− 0·0585(3)	− 0·1908(3)	0·09220(9)	4·09(4)
C(6)	− 0·0818(3)	− 0·1977(2)	0·16212(9)	4·10(4)
C(7)	0·1654(3)	− 0·2396(2)	− 0·01488(9)	4·01(4)
C(8)	0·3668(3)	− 0·2420(2)	− 0·11947(8)	3·70(4)
C(9)	0·5559(3)	− 0·1518(3)	− 0·15422(9)	4·14(4)
C(10)	0·5673(3)	− 0·1386(3)	− 0·22413(9)	4·47(5)
C(11)	0·3938(3)	− 0·2168(2)	− 0·26195(9)	4·08(4)
C(12)	0·2064(3)	− 0·3075(3)	− 0·22688(9)	4·29(4)
C(13)	0·1909(3)	− 0·3204(3)	− 0·15664(9)	4·13(4)
C(14)	− 0·1156(4)	− 0·2347(3)	0·3054(1)	5·31(5)
C(15)	− 0·0780(4)	− 0·2766(3)	0·3797(1)	5·90(6)
C(16)	0·1327(5)	− 0·1807(4)	0·4065(1)	7·16(7)
C(17)	0·1777(6)	− 0·2269(5)	0·4805(1)	10·5(1)
C(18)	0·4126(4)	− 0·2111(3)	− 0·3384(1)	5·25(5)
C(19)	0·6033(5)	− 0·3329(4)	− 0·3651(1)	7·20(7)
H(2)	0·429	− 0·412	0·197	5·1†
H(3)	0·476	− 0·394	0·074	5·2†
H(5)	− 0·198	− 0·135	0·063	5·4†
H(6)	− 0·232	− 0·142	0·187	5·5†
H(7)	0·008	− 2·208	− 0·042	5·4†
H(9)	0·694	− 0·094	− 0·126	5·7†
H(10)	0·708	− 0·066	− 0·250	5·8†
H(12)	0·073	− 0·370	− 0·255	5·6†
H(13)	0·047	− 0·389	− 0·131	5·7†
H(14A)	− 0·275	− 0·296	0·289	7·2†
H(14B)	− 0·134	− 0·096	0·295	7·2†
H(15A)	− 0·047	− 0·415	0·388	7·9†
H(15B)	− 0·238	− 0·248	0·408	7·9†
H(16A)	0·099	− 0·040	0·401	9·9†
H(16B)	0·291	− 0·204	0·377	9·9†
H(17A)	0·325	− 0·154	0·498	13·4†
H(17B)	0·022	− 0·195	0·512	13·4†
H(17C)	0·212	− 0·361	0·490	13·4†
H(18A)	0·454	− 0·078	− 0·357	7·1†
H(18B)	0·239	− 0·242	− 0·357	7·1†
H(19A)	0·613	− 0·325	− 0·418	9·2†
H(19B)	0·777	− 0·300	− 0·347	9·2†
H(19C)	0·565	− 0·466	− 0·348	9·2†

† These atoms were not refined; isotropic temperature factors are used. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as

$$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + ab\cos\gamma \cdot B(1,2) + ac\cos\beta \cdot B(1,3)$$
$$+ bc\cos\alpha \cdot B(2,3)].$$

Table 5. Atomic coordinates and equivalent isotropic displacement factors of 7O.6.

	x	y	z	$B_{eq}/\text{Å}^2$
O(1)	0·3817(4)	0·1914(3)	0·52199(7)	6·75(6)
N(1)	0·1646(4)	0·3171(3)	0·30656(8)	6·29(7)
C(1)	0·3977(5)	0·2417(4)	0·4758(1)	5·53(8)
C(2)	0·1676(5)	0·1777(4)	0·4498(1)	6·26(9)
C(3)	0·1616(5)	0·2181(4)	0·4028(1)	5·90(8)
C(4)	0·3835(5)	0·3205(3)	0·3798(1)	5·36(8)
C(5)	0·6093(5)	0·3812(4)	0·4066(1)	6·40(9)
C(6)	0·6215(5)	0·3436(4)	0·4541(1)	6·04(9)
C(7)	0·3736(5)	0·3591(4)	0·3298(1)	6·02(8)
C(8)	0·1536(5)	0·3474(4)	0·2576(1)	5·64(8)
C(9)	− 0·0832(5)	0·2674(4)	0·2352(1)	6·58(9)
C(10)	− 0·1172(6)	0·2843(4)	0·1872(1)	6·72(9)
C(11)	0·0851(5)	0·3824(4)	0·1592(1)	6·00(8)
C(12)	0·3197(6)	0·4652(4)	0·1824(1)	6·65(9)
C(13)	0·3552(6)	0·4492(4)	0·2300(1)	6·36(9)
C(14)	0·6089(5)	0·2440(4)	0·5516(1)	6·15(9)
C(15)	0·5291(5)	0·1690(4)	0·5996(1)	6·03(8)
C(16)	0·7500(5)	0·2146(4)	0·6361(1)	5·94(8)
C(17)	0·6642(5)	0·1397(4)	0·6846(1)	6·17(9)
C(18)	0·8774(5)	0·1784(4)	0·7219(1)	6·27(9)
C(19)	0·7849(6)	0·1060(4)	0·7700(1)	6·62(9)
C(20)	0·9926(6)	0·1583(4)	0·8081(1)	8·1(1)
C(21)	0·0534(6)	0·3959(4)	0·1066(1)	6·89(9)
C(22)	0·1994(6)	0·2956(4)	0·0771(1)	6·32(9)
C(23)	0·1655(5)	0·3018(4)	0·2325(1)	6·43(9)
C(24)	0·3197(6)	0·2075(4)	− 0·0055(1)	6·43(9)
C(25)	0·2895(6)	0·2116(4)	− 0·0588(1)	7·0(1)
C(26)	0·4448(7)	0·1165(5)	− 0·0868(1)	8·2(1)
H(2)	− 0·008	0·102	0·466	8·0†
H(3)	− 0·018	0·170	0·383	8·1†
H(5)	0·779	0·455	0·389	8·5†
H(6)	0·802	0·393	0·475	8·0†
H(7)	0·558	0·425	0·314	7·7†
H(9)	− 0·244	0·193	0·257	8·9†
H(10)	− 0·303	0·219	0·171	9·0†
H(12)	0·482	0·541	0·161	8·7†
H(13)	0·542	0·515	0·247	9·7†
H(14A)	0·677	0·385	0·556	8·5†
H(14B)	0·759	0·203	0·538	8·5†
H(15A)	0·458	0·028	0·596	7·8†
H(15B)	0·374	0·209	0·614	7·8†
H(16A)	0·820	0·354	0·640	8·5†
H(16B)	0·901	0·171	0·623	8·5†
H(17A)	0·588	− 0·002	0·679	8·4†
H(17B)	0·508	0·181	0·696	8·4†
H(18A)	0·956	0·320	0·725	8·3†
H(18B)	1·030	0·133	0·709	8·3†
H(19A)	0·716	− 0·037	0·766	9·1†
H(19B)	0·619	0·142	0·781	9·1†
H(20A)	0·929	0·105	0·842	10·4†
H(20B)	1·157	0·118	0·799	10·4†
H(20C)	1·061	0·298	0·813	10·4†
H(21A)	0·127	0·534	0·096	9·1†
H(21B)	− 0·146	0·355	0·096	9·1†

Table 5. *(Continued)*.

	x	y	z	$B_{eq}/\text{Å}^2$
H(22A)	0·125	0·158	0·086	8·7†
H(22B)	0·398	0·337	0·086	8·7†
H(23A)	0·229	0·440	0·015	8·9†
H(23B)	− 0·034	0·254	0·015	8·9†
H(24A)	0·265	0·073	0·005	9·3†
H(24B)	0·523	0·262	0·003	9·3†
H(25A)	0·339	0·342	− 0·070	10·1†
H(25B)	0·086	0·151	− 0·068	10·1†
H(26A)	0·419	0·117	− 0·124	11·5†
H(26B)	0·647	0·172	− 0·079	11·5†
H(26C)	0·393	− 0·019	− 0·077	11·5†

† These atoms were not refined; isotropic temperature factors are used. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as

$$(4/3)\cdot[a^2\cdot B(1,1) + b^2\cdot B(2,2) + c^2\cdot B(3,3) + ab\cos\gamma\cdot B(1,2) + ac\cos\beta\cdot B(1,3) + bc\cos\alpha\cdot B(2,3)].$$

3.1.2. *Molecular conformation*

The molecular conformation of 4O.2 and 7O.6 differ considerably in their crystalline structures. For reasons of visual comparison, the two molecules are drawn atop of each other with greatest possible overlapping of some parts of the molecules (see figures 3 and 4); black represents the shape of 4O.2 and white the shape of 7O.6.

In 4O.2, the planes formed by the two benzene rings (*A* and *B*) are twisted by − minus sign 61·20(4)°; in 7O.6, this angle amounts to 4·6(10)° only, and is comparable with the values found for 8O.4 with 2·2° and for 4O.8 with 13·3° and 29·2° for the two molecules in the asymmetric unit, respectively. The different conformations are reflected by the changes in torsion angles made with the C7=N1 bond included (cf. table 8).

The two structures also deviate in some torsion angles of the alkyl and alkoxy side groups as is clearly visible in figure 3 and stated in table 8. The bond C15–C16 is placed *gauche* to O1–C14 in 4O.2 and *trans* in 7O.6, with torsion angles τ (O1–C14–C15–C16) to 64·5° and − 179·4°, respectively. Changes in the torsion angles in the alkyl groups occur for τ (C10–C11–C18–C19) with 74° in 4O.2, which corresponds to τ (C10–C11–C21–C22) − 108·4° in 7O.6.

All the other bonds of the alkoxy and alkyl groups are in a *trans* position for 7O.6 leading to a coplanarity of the carbon atoms of the alkoxy group and the two benzene rings and a twist angle of the carbon atoms of the hexyl group of about 70° from the above mentioned plane. The conformation of 4O.2 resembles the conformation of the low temperature modification of 1O.4 (MBBA) [9] and differs from that of 7O.6. However, the shape of 7O.6 shows some similarities to that of the homologues 4O.8 and 8O.4 which were described in the literature some time ago [7, 8]. As represented in figure 4, the mesogenic cores and alkoxy groups of the different molecules might be superimposed, but the alkyl groups differ for the various molecules. The angles between the planes of the benzene ring *B* and the carbon atoms of the alkyl groups amount to 111·1(1)° for 7O.6, to − 116·4° for 8O.4 and to − 61·4° and 64·9° for the two independent molecules of 4O.8.

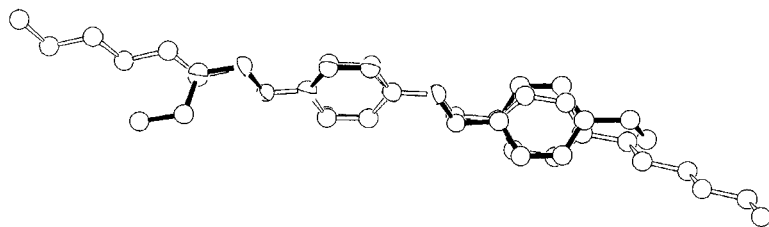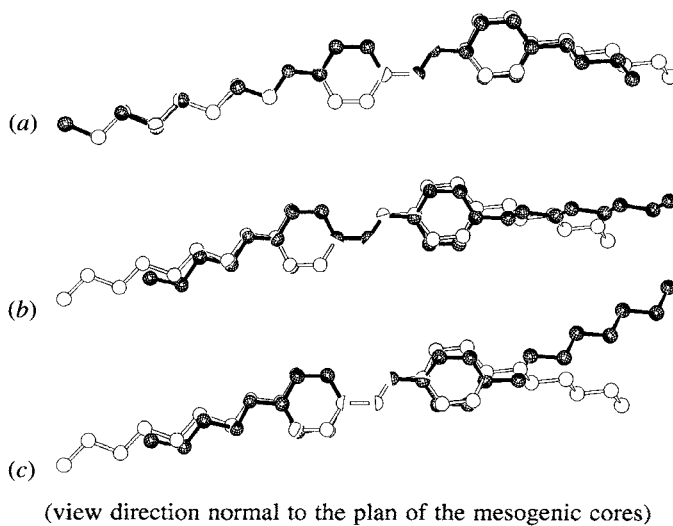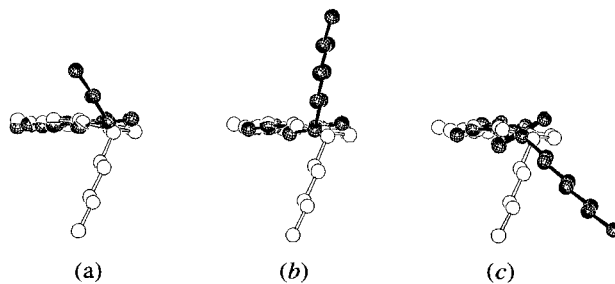Figure 3.   Superposition of the molecules 4O.2 (black) and 7O.6 (white).

(a)

(b)

(c)

(view direction normal to the plan of the mesogenic cores)

(a)   (b)   (c)

(view direction along the axis of the mesogenic core)

Figure 4.   Superposition of the molecule of 7O.6 (white) with 8O.4 (*a*), the first independent molecule of 4O.8 (*b*) and the second independent molecule of 4O.8 (*c*) (black drawings) in two different directions of view for comparison of the twist angle of the mesogenic core and the plane of the alkyl chain. Data for 8O.4 and 4O.8 [7, 8].
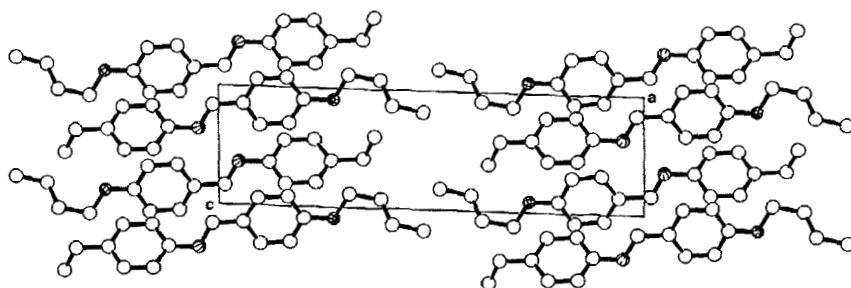
Figure 5.   Schematic representation of the packing of the 4O.2 molecules. Projection along the [010] direction.
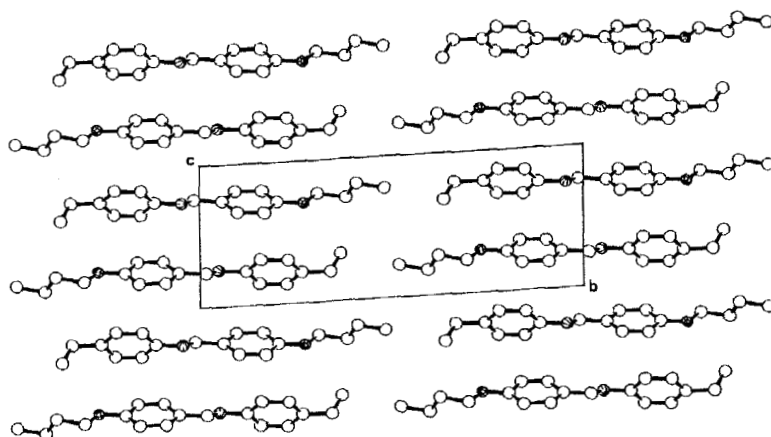
Figure 6.   Schematic representation of the packing of the 4O.2 molecules. Projection along the [100] direction.

3.2. *Molecular packing*

3.2.1. *Packing of 4O.2*

Figures 5–10 represent the packing in the crystal structures of 4O.2 and 7O.6 from different directions of view.

The crystal structure of 4O.2 reveals an arrangement of the molecules in layers (see figure 5, 6 and 7) similar to that in smectic liquid crystalline phases; these lie parallel to the a, b-plane, piled up in c^*-direction. Neighbouring molecules overlap almost completely in one layer with minimal interdigitation of layers. Within a layer the molecules form an almost ideal hexagonal packing, with four adjacent molecules pointing in opposite direction and two in the same direction.

Parallel to the a, c-plane, sheets are formed containing parallel arranged molecules of the same orientation opposing the direction of the molecules of the adjacent sheet. The dipole moments of the $C=N-C$ and $C-O-C$ bonds are in opposite directions out of the a, c-plane, as a result of the conformation of the single molecule. A compensation of dipole moments of one kind is not possible within one sheet, but is realized by the piling up of the sheets in the b^*- direction through the antiparallel orientation of the molecules in neighbouring sheets.

The twisting of the 4O.2 benzene rings along the molecular axes hinders shifting of the molecules along the c-direction. In this respect the geometry of 4O.2 differs from
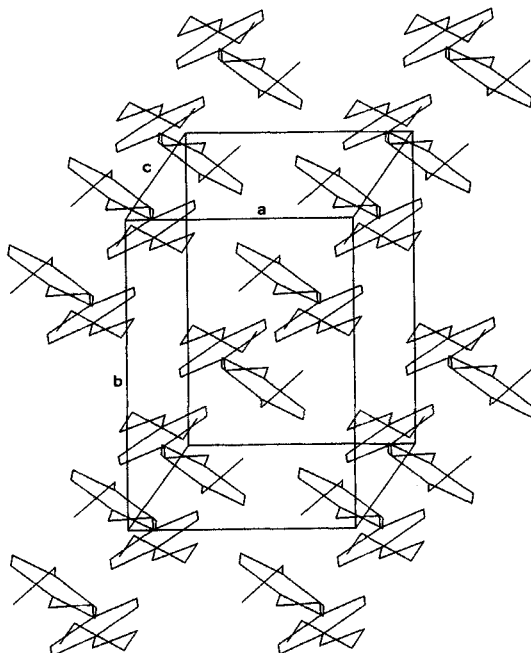
Figure 7. Schematic representation of the packing of the 4O.2 molecules. Projection along *c* and slightly rotated around *a* and *b*.

Table 8. Selected torsion angles (°) for non-hydrogen atoms in 4O.2 and 7O.6.

	4O.2	7O.6
C(3)–C(4)–C(7)–N(1)	− 17·0(3)	6·7(4)
C(4)–C(7)–N(1)–C(8)	177·9(2)	− 177·3(3)
C(7)–N(1)–C(8)–C(13)	− 43·3(3)	− 11·0(4)
O(1)–C(14)–C(15)–C(16)	64·5(2)	− 179·4(2)
C(10)–C(11)–C(18)–C(19)	74·0(3)	
C(10)–C(11)–C(21)–C(22)		− 108·4(3)

that of 7O.6, 8O.4 and 4O.8, where the two benzene rings are almost coplanar and slipping of molecules may occur more easily.

This difference may be understood if one takes into account that the crystal modification of 4O.2 described here, changes to another crystal form as revealed by DSC experiments. Exclusively, this second modification, not yet solved, undergoes the transition to the G phase. Hence, a simple relationship between the crystal structure and the packing of the molecules in the G phase cannot be established with the data presented, but will be dealt with in a further paper.

3.2.2. *Packing of 7O.6*

The crystal structure of 7O.6 shows some differences to that of 4O.2, but resembles those found for 4O.8 and 8O.4.

The molecules are placed in sheets parallel to the *a, b*-plane and piled up in *c**-direction (see figures 8–10). The overlap of the mesogenic cores and the alkoxy
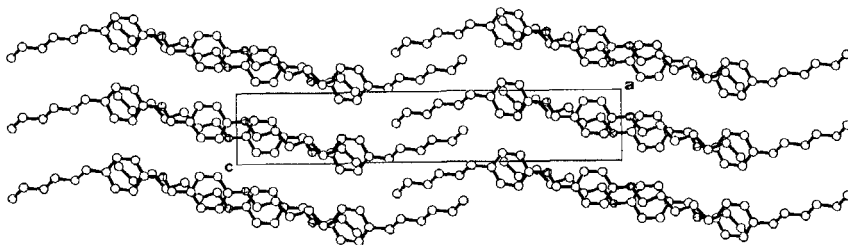
Figure 8. Schematic representation of the packing of the 7O.6 molecules. Projection along the [010] direction.
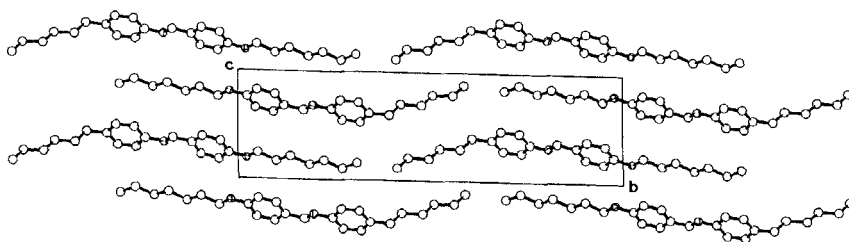

Figure 9. Schematic representation of the packing of the 7O.6 molecules. Projection along the [100] direction.

groups of adjacent molecules results in a protrusion of the hexyl groups on both sides of the layers and an interdigitation of neighbouring layers.

Molecules within the layers pack a distorted hexagonal antiparallel arrangement. The molecules with parallel orientation lie in sheets parallel to the a, c-plane and are piled up in the b^* direction. Since the molecules in adjacent sheets point in opposite directions, an overall antiparallel packing arrangement is obtained, quite similar to that for 4O.2, 4O.8 and 8O.4.

The dipole moments of the C=N–C and the C–O–C bonds for 7O.6 point out of the a, c-plane in one direction, in contrast to 4O.2; this is caused by the flat shape of the part of the molecules containing the two benzene rings, the azomethine group and the alkoxy chain.

The almost flat shape of the molecules leads to the impression that slipping of molecules may occur easily, and in this way new structures may be formed by crystalline–crystalline or crystalline–smectic phase transitions.

4. Conclusions

In the search for similarities between crystal and liquid crystalline structures, the problems are clearly revealed through a comparison of the homologues 7O.6 and 8O.4 on the one hand, and 4O.8 on the other. All three structures possess very similar conformations and packings, yet 4O.8 forms a smectic B crystal phase, and 7O.6 and 8O.4 G phases.
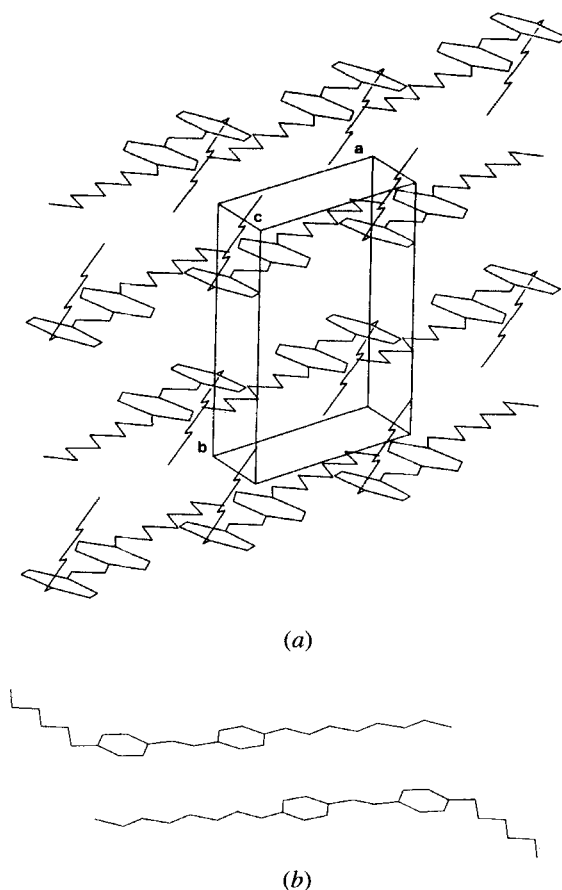
(*a*)

(*b*)

Figure 10. Schematic representation of the packing of the 7O.6 molecules. Projection along *c* and slightly rotated around *a* and *b*, (*a*). A part of the molecular arrangement shown in a different projection, (*b*).

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