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Crystal structures of 4-cyano-4′-hexylbiphenyl (6CB) and 4-cyano-4′-heptylbiphenyl (7CB) in relation to odd–even effects

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Crystal structures of 4-cyano-4′-hexylbiphenyl (6CB) and 4-cyano-4′-heptylbiphenyl (7CB) with low melting points (13.5 and 30°C, respectively) have been determined at − 73 and − 33°C, respectively, and compared with previously reported structures of other homologues ($n = 2$–5, 8–11). In the crystal of 7CB, chains and cores stack alternately, where core regions are largely overlapped with distances of 3.575(2) and 3.597(2) Å for N (in CN) … C (in phenyl), showing almost the same packing mode as those of 9CB and 11CB. In the crystal of 6CB, CN groups are antiparallel between neighbouring molecules though the interatomic distances are much longer—N … C, 3.673(3) and 3.563(3) Å—than in 8CB and 10CB (3.28–3.43 Å), resulting in a quite different packing mode from those of 8CB and 10CB, which had been found to be similar, with CN–CN interactions. Systematic comparison of the homologous series ($n = 2$–11) reveals odd–even effects, CN–phenyl and CN–CN interactions for odd and even members, respectively, in the crystal structures, except for 5CB and 6CB.

1. Introduction

Structural studies using STM observation [1], computer simulation [2], etc. have been carried out on 4-cyano-4′-alkylbiphenyls (nCB) or 4-cyano-4′-alkoxybiphenyls (nOCB) because of their simple molecular structures, as well as their practical importance. Both series have typical liquid crystalline phase sequences depending on the chain lengths [3]: for nCB, crystal–nematic–isotropic ($n = 5, 6, 7$), crystal–smectic A (SmA)–nematic–isotropic ($n = 8, 9, 11$) and crystal–SmA–isotropic ($n = 10, 12$); for nOCB, crystal–nematic–isotropic ($n = 5, 6, 7$), crystal–SmA–nematic–isotropic ($n = 8, 9$) and crystal–SmA–isotropic ($n = 10, 12$). X-ray diffraction studies [4] showed that the mesophases have interdigitated structures with overlapping of core regions due to the strong dipole moment of the CN group.

In order to obtain precise information on intermolecular interaction, attempts have been made to find the relationships between crystal structures and mesophase behaviour. Crystal structures have been reported for $n = 1$–9 of nOCB [5–10]. In the course of systematic crystal structure determination for higher homologues ($n = 7$–10, 12), crystalline polymorphs were found; especially for each of 7OCB and 8OCB, at least 4 solid states were found [8, 9]. The square-plate crystal form, which has a distinct smectic-like structure composed of bilayers with two-dimensional infinite networks of closely arranged CN groups, appears in common for $n \geqslant 7$. This form is metastable for $n = 7$ and 8 but stable at room temperature for $n \geqslant 9$. Thus, it was concluded that distinct smectic-like bilayer structures with infinite networks of closely arranged CN groups are dominant for higher nOCB homologues [10].

For the nCB series, crystal structures were determined for $n = 2$–5 [11–14] and $n = 8$–11 [15–18], while those of 6CB and 7CB with low melting points (13.5 and 30°C, respectively) have remained undetermined until recently. This paper describes the crystal structures of 6CB and 7CB determined at low temperature (at − 73 and − 33°C, respectively), which allow us a thorough comparison within the nCB series, as well as between the nCB and nOCB series.

2. Experimental

2.1. *General*

Both compounds studied were purchased from Merck Ltd., UK. Plate and needle crystals of 6CB and 7CB, respectively, were obtained from an ethanol/ethyl acetate solution kept in a freezer (− 16°C). Melting peaks of single crystals, measured on a Seiko DSC-22C calorimeter, were simple and sharp at 13.5 and 30.0°C, respectively, in good agreement with reported values, showing that the crystals are thermodynamically stable phases.

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2.2 *X-ray analysis of crystal structure*

Cell parameter measurements and reflection data collection were done on an AFC-7R four-circle diffractometer using CuK$_\alpha$ radiation monochromated by graphite ($\lambda = 1.54184$ Å). The 2θ-ω mode was applied up to $2\theta = 120°$. Three standard reflections were measured after every 150 reflections; no significant variation was observed. All the diffraction data were corrected for Lorentz and polarization factors. Detailed experimental conditions and crystal data are summarized in table 1*.

The structures were solved by applying SHELXS86 [19] and refined by full-matrix least-squares method on F^2 by using SHELXL93 [20]. All the non-hydrogen atoms were refined anisotropically. The hydrogen atoms, calculated geometrically (C–H distance: 0.98 and 0.97 Å for primary, 0.98 and 0.99 Å for secondary and 0.95 and 0.94 Å for aromatic at 200 and 240 K, respectively), were included in structure–factor calculations but not refined. An extinction correction was applied for 7CB (extinction coefficient, 0.0100(7)). The atomic scattering factors were taken from International Tables for Crystallography [21]. Final results of refinements are summarized in table 1. Final atomic coordinates for 6CB and 7CB are listed in tables 2 and 3, respectively.

Table 1. Experimental details, crystal data, and final results of refinements.

Parameter	6CB	7CB
T/K	200	240
Formula	$C_{19}H_{21}N$	$C_{20}H_{23}N$
Formula weight	263.37	277.39
Crystal shape	plate	needle
Crystal size/mm	0.4 × 0.4 × 0.1	0.4 × 0.08 × 0.08
L.s. for cell const.[a]	$25(56 < 2\theta < 57°)$	$25(56 < 2\theta < 57°)$
Crystal system	triclinic	triclinic
Space group	$P1$	$P1$
a/Å	12.427(4)	11.438(2)
b/Å	12.724(3)	15.800(2)
c/Å	10.857(2)	9.674(2)
α/°	100.74(2)	99.000(12)
β/°	112.54(2)	107.164(11)
γ/°	75.89(2)	91.062(11)
V/Å^3	1529.5(7)	1646.0(4)
Z	4	4
d_x/Mg m^{-3}	1.144	1.119
μ/mm^{-1}	0.496	0.483
F (000)	568	600
No. of unique refl.	4539	4874
No. of obsd. refl. (> 2σ(I))	3512	3376
S	1.073	1.015
$R1$[b]	0.0469	0.0468
R_w2[c]	0.1367	0.1524
$(\Delta/\sigma)_{max}$	0.009	0.009
$\Delta\rho$/e Å^{-3}	0.18, – 0.14	0.18, – 0.16

[a] Number of reflections with the 2θ range in parentheses.

[b] $R1 = \Sigma \| F_o| - |F_c\| / \Sigma |F_o|$ for observed reflections.

[c] $R_w2 = [\Sigma w(F_o^2 - F_o^2)^2 / \Sigma w(F_o^2)^2]^{0.5}$ for all reflections, where $w = 1/[\sigma^2(F_o^2) + (0.0657P)^2 + 0.3732P]$ for 6CB and $w = 1/[\sigma^2(F_o^2) + (0.0784P)^2 + 0.3260P]$ for 7CB with $P = (F_o^2 + 2F_c^2)/3$.

Table 2. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for 6CB. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
N(1A)	295(2)	10153(2)	1834(2)	68(1)
C(1A)	540(2)	10934(2)	1717(2)	55(1)
C(2A)	847(2)	11917(2)	1581(2)	52(1)
C(3A)	1200(2)	12666(2)	2682(2)	62(1)
C(4A)	1477(2)	13611(2)	2550(2)	59(1)
C(5A)	1418(2)	13848(2)	1315(2)	48(1)
C(6A)	1066(2)	13073(2)	226(2)	56(1)
C(7A)	784(2)	12125(2)	343(2)	56(1)
C(8A)	1702(2)	14878(2)	1178(2)	48(1)
C(9A)	2007(2)	15666(2)	2252(2)	72(1)
C(10A)	2287(2)	16616(2)	2137(2)	72(1)
C(11A)	2267(2)	16846(2)	931(2)	50(1)
C(12A)	1952(2)	16067(2)	– 142(2)	56(1)
C(13A)	1676(2)	15112(2)	– 34(2)	55(1)
C(14A)	2538(2)	17893(2)	759(2)	55(1)
C(15A)	3138(2)	18577(2)	2037(2)	53(1)
C(16A)	3457(2)	19574(2)	1779(2)	53(1)
C(17A)	3981(2)	20291(2)	3055(2)	56(1)
C(18A)	4372(2)	21266(2)	2856(2)	59(1)
C(19A)	4905(2)	21946(2)	4168(2)	75(1)
N(1B)	– 971(2)	– 4422(2)	– 6527(2)	75(1)
C(1B)	– 403(2)	– 3767(2)	– 6018(2)	58(1)
C(2B)	294(2)	– 2932(2)	– 5383(2)	51(1)
C(3B)	1079(2)	– 2968(2)	– 4067(2)	56(1)
C(4B)	1696(2)	– 2132(2)	– 3458(2)	55(1)
C(5B)	1557(2)	– 1248(2)	– 4123(2)	48(1)
C(6B)	781(2)	– 1242(2)	– 5454(2)	53(1)
C(7B)	156(2)	– 2065(2)	– 6075(2)	55(1)
C(8B)	2172(2)	– 320(2)	– 3442(2)	48(1)
C(9B)	2471(2)	– 28(2)	– 2070(2)	52(1)
C(10B)	2996(2)	863(2)	– 1444(2)	53(1)
C(11B)	3236(2)	1520(2)	– 2157(2)	49(1)
C(12B)	2949(2)	1220(2)	– 3531(2)	55(1)
C(13B)	2430(2)	330(2)	– 4160(2)	55(1)
C(14B)	3765(2)	2527(2)	– 1524(2)	53(1)
C(15B)	4246(2)	2701(2)	– 4(2)	51(1)
C(16B)	4775(2)	3724(2)	539(2)	51(1)
C(17B)	5180(2)	3960(2)	2050(2)	56(1)
C(18B)	5750(2)	4961(2)	2575(2)	65(1)
C(19B)	6173(3)	5194(2)	4083(2)	93(1)

*Further data for band lengths, band angles, displacement parameters, hydrogen coordinates and structure factors for both 6CB and 7CB have been deposited as *Supplementary Material*, available from the British Library Document Supply Centre, Boston Spa, Wetherby, Yorkshire LS23 7BQ, UK (publication number 90484). For further details refer to any published issue of the Journal.

Table 3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å $\times 10^3$) for 7CB. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	X	y	z	U_{eq}
N(1A)	12098(2)	6534(2)	4854(2)	92(1)
C(1A)	11383(2)	6005(2)	4115(3)	65(1)
C(2A)	10497(2)	5338(1)	3180(2)	54(1)
C(3A)	10435(2)	4537(1)	3586(2)	55(1)
C(4A)	9574(2)	3904(1)	2689(2)	51(1)
C(5A)	8767(2)	4051(1)	1371(2)	47(1)
C(6A)	8851(2)	4858(1)	985(2)	54(1)
C(7A)	9701(2)	5495(1)	1869(2)	56(1)
C(8A)	7839(2)	3376(1)	414(2)	46(1)
C(9A)	7492(2)	3301(1)	– 1115(2)	56(1)
C(10A)	6593(2)	2701(1)	– 2009(2)	58(1)
C(11A)	5971(2)	2144(1)	– 1442(2)	50(1)
C(12A)	6331(2)	2212(1)	80(2)	51(1)
C(13A)	7239(2)	2809(1)	987(2)	50(1)
C(14A)	4963(2)	1523(1)	– 2465(2)	57(1)
C(15A)	4269(2)	973(1)	– 1774(2)	54(1)
C(16A)	3242(2)	392(1)	– 2899(2)	56(1)
C(17A)	2475(2)	– 123(1)	– 2240(2)	57(1)
C(18A)	1446(2)	– 697(1)	– 3360(2)	56(1)
C(19A)	625(2)	– 1174(1)	– 2718(2)	57(1)
C(20A)	– 409(2)	– 1730(2)	– 3881(3)	66(1)
N(1B)	7110(2)	6656(2)	4624(2)	80(1)
C(1B)	6401(2)	6106(2)	3968(2)	59(1)
C(2B)	5511(2)	5416(1)	3146(2)	51(1)
C(3B)	5768(2)	4823(2)	2073(3)	63(1)
C(4B)	4910(2)	4170(1)	1266(3)	59(1)
C(5B)	3773(2)	4079(1)	1503(2)	47(1)
C(6B)	3543(2)	4678(1)	2607(2)	50(1)
C(7B)	4390(2)	5336(1)	3410(2)	50(1)
C(8B)	2821(2)	3405(1)	596(2)	47(1)
C(9B)	2740(2)	3096(1)	– 866(2)	53(1)
C(10B)	1805(2)	2511(1)	– 1741(2)	56(1)
C(11B)	897(2)	2203(1)	– 1221(2)	50(1)
C(12B)	1002(2)	2491(1)	245(2)	56(1)
C(13B)	1936(2)	3076(1)	1134(2)	54(1)
C(14B)	– 154(2)	1603(1)	– 2238(2)	57(1)
C(15B)	– 859(2)	1072(1)	– 1538(2)	55(1)
C(16B)	– 1856(2)	460(1)	– 2654(2)	55(1)
C(17B)	– 2520(2)	– 119(1)	– 1971(2)	57(1)
C(18B)	– 3485(2)	– 757(1)	– 3069(2)	58(1)
C(19B)	– 4156(2)	– 1324(2)	– 2377(3)	63(1)
C(20B)	– 5081(3)	– 1986(2)	– 3482(3)	82(1)

3. Results

3.1. *Molecular structures*

Figure 1 shows the molecular structures of 6CB and 7CB, with atomic numbering schemes. Both crystals contain two crystallographically independent molecules, A and B. The bond angles, C4–C5–C6, C9–C8–C13 and C10–C11–C12, are slightly smaller (116.0(2)–117.9(2)°) than 120° in both crystals, as was observed in higher homologues [16–18]. The dihedral angles between the rings of the biphenyl moieties are 2.09(12)° (6CB-A), 28.44(9)° (6CB-B), 35.93(8)° (7CB-A) and 30.26(10)° (7CB-B). All the alkyl chains have all-*trans* conformation and the dihedral angles between the plane of the C–C–C backbones and attached benzene rings are 10.16(15)° (6CB-A), 7.3(2)° (6CB-B), 7.20(10)° (7CB-A) and 19.16(11)° (7CB-B).

3.2. *Crystal packings*

Figure 2 shows the crystal structure of 6CB, viewed along the a and c axes. Distances between CN groups are 3.563(3) Å for N1B(x, y, z)… C1B($-x, -y-1, -z-1$) and 3.673(3) Å for N1A(x, y, z)… C1A($-x, -y+2, -z$), longer than those of 8CB (C… N: 3.283(3), 3.336(3) Å). The CN group is relatively close to the biphenyl moiety with interatomic distances of 3.482(2) Å for C13A(x, y, z)… N1B($-x, -y+1, -z-1$) and 3.500(2) Å for N1A(x, y, z)… C6B($x, y+1, z+1$). As a consequence, 6CB does not have a distinct smectic-like layer structure.

The crystal structure of 7CB is shown in figure 3, viewed along the a and a skewed direction. A CN group is close to a ring of the biphenyl moiety of an adjacent molecule with interatomic distances of 3.575(2) Å for C3A(x, y, z)… N1B($-x+2, -y+1, -z+1$) and 3.597(3) Å for N1A(x, y, z)… C4A($-x+2, -y+1, -z+1$). Close distances are also found between phenyl groups of adjacent molecules with distances of 3.320(4) Å for C3A(x, y, z)… C3A($-x+2, -y+1, -z+1$) and 3.329(4) Å for C7B(x, y, z)… C7B($-x+1, -y+1, -z+1$). The largely overlapped core moieties and hence chain moieties stack alternately, leading to a smectic-like layer structure. The molecular long axes tilt with respect to the normal of the layer plane with a tilt angle of about 45°.

4. Discussion

4.1. *Comparison of nCB homologues*

The crystal structures of nCB compounds ($n \geqslant 7$) are divided into two classes. As was already mentioned [10, 15], the crystals of 8CB and 10CB have a very similar packing mode, where closely arranged CN groups are lined up in an infinite chain; those of 9CB and 11CB are also very similar to each other, with CN and phenyl groups close to each other. The packing mode of 7CB belongs to the latter type. However, the crystal structure of 6CB belongs to neither of these packing modes. Thus, it is concluded that the crystal structures of nCB ($n \geqslant 7$) show a distinct odd–event effect.

For lower homologues, the crystal packing modes cannot be grouped simply as for the longer homologues. Nevertheless, an odd–even effect is clearly shown by comparing the crystal structures in terms of intermolecular distances from a CN group, as shown in table 4. 2CB has two crystalline polymorphs, both of which have layer structures with closely arranged CN groups. 4CB also has an interaction between CN groups; on the other hand, 3CB and 5CB show no specific interactions between CN groups. The crystal of 3CB

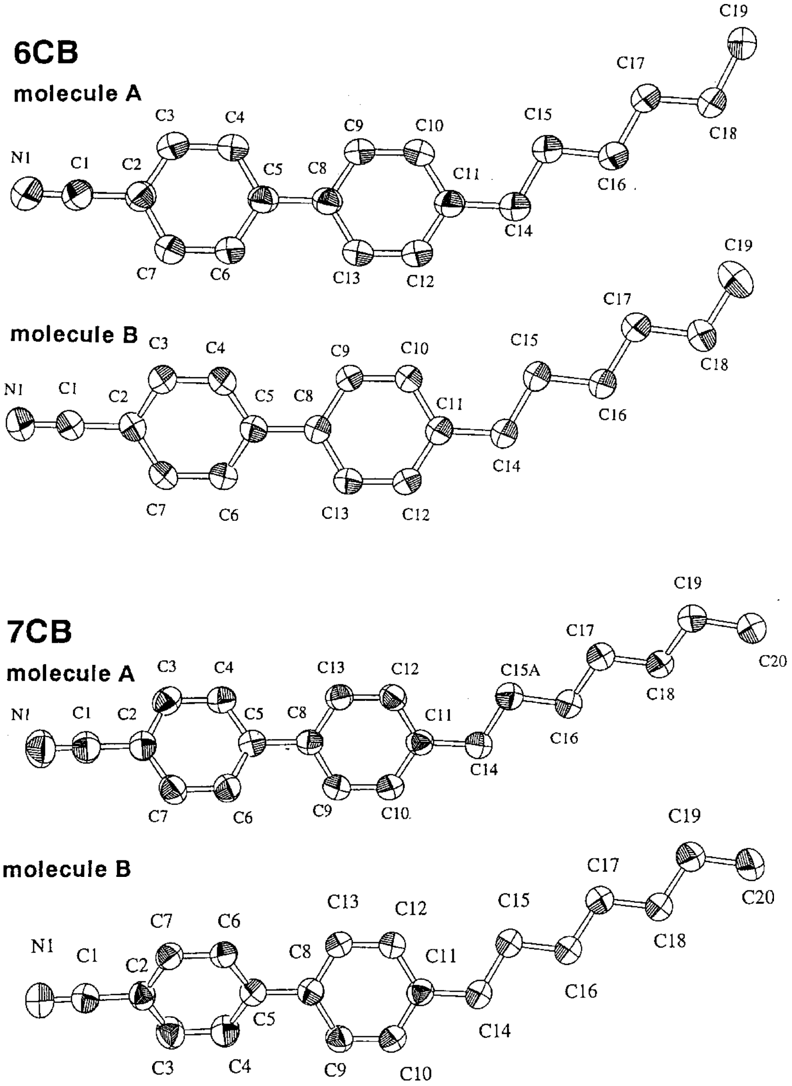

Figure 1. Structures of molecules A and B of 6CB and molecules A and B of 7CB with 50% probability displacement ellipsoids. Hydrogen atoms are omitted for clarity.

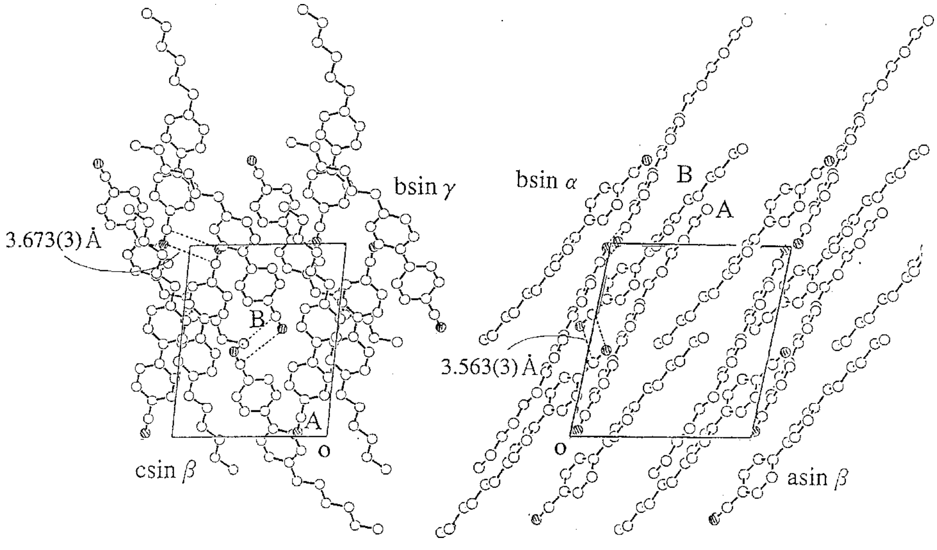

Figure 2. Crystal structure of 6CB viewed along the *a* (left) and *c* axes (right). Nitrogen atoms are denoted by hatched circles.

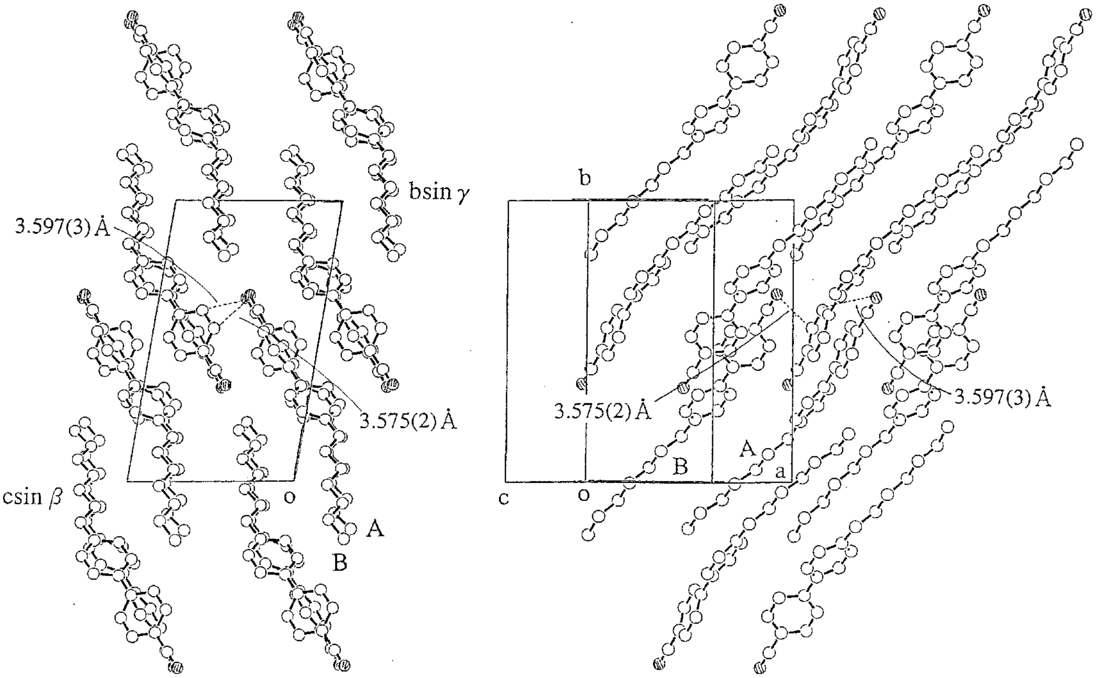

Figure 3. Crystal structure of 7CB viewed along the *a* axis (left), and along a direction skewed from the *c* and *a* axes (right). Nitrogen atoms are denoted by hatched circles.

Table 4. Interatomic distances ($<$ 3.6 Å) from the N atom of the CN group to the corresponding C atoms, for the *n*CB series. Atomic numbering for all homologues is renumbered to be analogous to that shown in figure 1.

Compound	CN–CN N(CN)…C(CN)	CN–phenyl N(CN)…C(phenyl)	CN–chain N(CN)…C(chain)	Ref.
2CB-I	3.347, 3.566	3.440; N…C(7)		[11]
2CB-II	3.430, 3.467	3.425; N…C(7)		[11]
3CB		3.573; N…C(13)		[12]
4CB	3.448	3.489; N…C(3) 3.545; N…C(12)		[13]
5CB			3.565; N…C(17) 3.577; N…C(18)	[14]
6CB	3.563	3.482; N(B)…C(13A) 3.500; N(A)…C(6B)		this work
7CB		3.575; N(B)…C(3A) 3.597; N(A)…C(4A)		this work
8CB	3.283, 3.336	3.342; N…C(7) 3.492, 3.531; N…C(3)		[15]
9CB		3.586; N(A)…C(7B)		[16]
10CB	3.279, 3.427	3.446; N…C(3) 3.515, 3.534; N…C(7) 3.546; N…C(6)	3.556; N…C(15) 3.568; N…C(16)	[17]
11CB		3.573; N(A)…C(3B)		[18]

has largely overlapped core regions as for the longer odd-members, while 5CB has a unique structure with largely bent molecules. The crystal of 6CB shows longer CN…CN distances than other even-members, as mentioned above. Thus, the *n*CB series shows an odd–even effect in terms of CN–CN or CN–phenyl interactions in all crystal structures except for 5CB and 6CB. The odd–even effect in the packing modes for higher homologues ($n \geqslant 7$) is regarded as a specific case of the CN–CN or CN–phenyl interactions. It should be pointed out that the exceptional members, 5CB and 6CB, show the lowest melting points.

4.2. *Comparison of the nCB and nOCB series*

The odd–even effects found in the crystal structures of the *n*CB series are in contrast to the features of those of the *n*OCB series. Table 5 summarizes the arrangements around a CN group for both series. There are three types of arrangements of the CN–CN interactions: clusters (dimer or tetramer), one-dimensional infinite chains and two-dimensional infinite networks, as schematically shown in figure 4. The crystal structures of *n*OCB compounds in respect to the arrangements of the CN group, are as follows. CN and phenyl groups are closely arranged in crystals of 1OCB and 2OCB, while an infinite stacking (one-dimensional infinite chains) of CN groups is found in the 3OCB crystal [5]. In the crystal of 4OCB, however, there are no close distances between CN–CN or CN–phenyl groups comparable to those of 1OCB, 2OCB and 3OCB [5]. In 5OCB, an infinite stacking of CN groups is again found [6]. In the 6OCB crystal, CN groups are closely arranged between two neighbouring molecules [7], while in the needle crystals of 7OCB [7] and 8OCB [9] dimers formed by CN–CN interaction are further arranged to form a tetramer. In the parallelepiped crystal of 8OCB [9], close distances are found between CN and phenyl groups. As mentioned in §1, the square-plate crystal form, which has a distinct smectic-like bilayer structure with two-dimensional infinite networks of closely arranged CN groups [8, 10], appears in common for higher homologues of *n*OCB ($n = 7$–$10, 12$) [10]. These results show that crystals of *n*OCB compounds are controlled more dominantly by CN–CN interaction than those of *n*CB compounds, which are influenced by the numbers of alkyl chains, odd or even.

5. Conclusions

Crystal structures of 6CB and 7CB have been determined, enabling us to compare the crystal structures of the homologous series of *n*CB and *n*OCB compounds. Distinct odd–even effects due to the alkyl chains, CN–CN

Table 5. Types of arrangements of CN groups in the *n*CB and *n*OCB series.

CN–CN				
Cluster	1-D chain	2-D network	CN–phenyl	Other
4CB	2CB (I, II) 8CB 10CB		3CB 7CB 9CB 11CB	5CB 6CB
6OCB 7OCB(needle) 8OCB(needle)	3OCB 5OCB	7OCB(sq-plate) 8OCB(sq-plate) 9OCB(sq-plate) 10OCB(sq-plate) 12OCB(sq-plate)	1OCB 2OCB 8OCB(parallelepiped)	4OCB

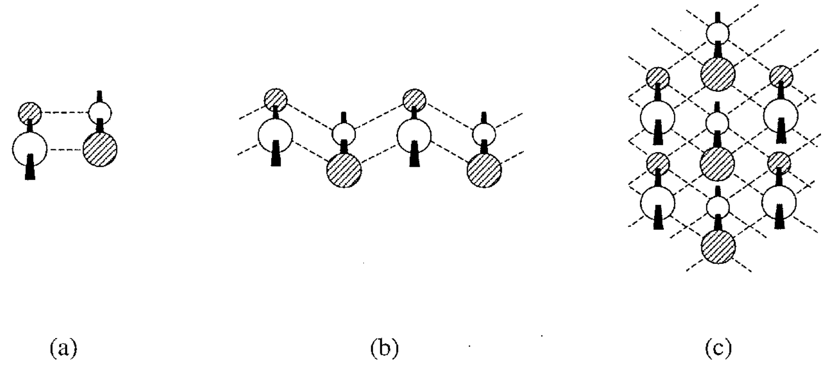

Figure 4. Schematic diagrams of CN–CN interactions: (*a*) a cluster, (*b*) a one-dimensional chain, and (*c*) a two-dimensional network. Nitrogen atoms are shown by hatched circles. Close C…N distances are shown by dashed lines.

or CN–phenyl interactions in the crystal structures (except for 5CB and 6CB), and more specifically the packing modes for higher homologues ($n \geqslant 7$), are observed for the crystals of the nCB series. The crystal structures of the nOCB series are controlled more dominantly by CN–CN interactions.

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