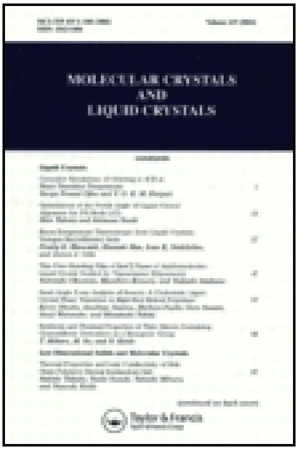

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The Crystal and Molecular Structures of Four Homologous, Mesogenic trans,trans-4,4′-dialkyl-(1α,1′-bicyclohexyl)-4ß-carbonitril (CCN's)

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The Crystal and Molecular Structures of Four Homologous, Mesogenic *trans,trans*-4,4′-dialkyl-(1α,1′-bicyclohexyl)-4β-carbonitril (CCN's)

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The crystal and molecular structures of four homologous ($R'(CN)—C_6H_9—C_6H_{10}—R$, CCN's) were determined using single crystal x-ray diffraction data. In all four structures the cyano groups occupy axial positions whereas the alkyl groups occupy equatorial ones. The cyclohexane rings are approximately perpendicular to each other in CCN33 ($R{=}R'{=}C_3H_7$), in CCN35 ($R{=}C_3H_7$, $R'{=}C_5H_{11}$) and in CCN38 ($R{=}C_3H_7$, $R'{=}C_8H_{17}$) leading to a room filling of the free space produced by the cyano groups. More than that, the hydrogen-hydrogen contacts between the cyclohexane rings are minimal in such an arrangement. However, in CCN46 ($R{=}C_4H_9$, $R'{=}C_6H_{13}$) the molecules contain nearly coplanar bicyclohexyl moieties. These and some other structural features are discussed with regard to the question of the extent to which the crystalline state can be interpreted as a precursor of liquid crystalline states.

Keywords: crystalline state, molecular conformation, CCH's, CCN's

INTRODUCTION

The 4,4′-disubstituted bicyclohexyl group has been found to be a good element in technically-relevant liquid crystalline substances. The *trans*-4′-alkyl-trans-4-(1,1′-bicyclohexyl)-carbonitril (CCH's) are well known examples for such compounds.[1,2] Recently, compounds with liquid crystalline properties were prepared[3,4] and investigated,[5] having, instead of a 4α-carbonitrile group, a 4β-carbonitrile group

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(CCN's). These compounds possess very interesting liquid crystalline properties, especially in smectic phases. The existence of the particularly interesting smectic phases gives rise to a search for characteristic structural elements in the crystalline state. The conformative arrangement of the substituents at the cyclohexyl group as well as the geometry of the bicyclohexyl moiety, is of principal interest, since investigations on several groups of mesogenic compounds have shown that the molecular subunits prefer characteristic arrangements to each other.[6-13] They are the result of intramolecular and intermolecular effects.

We report now on the structural properties of four members of the CCN group; a preliminary structural report was given elsewhere.[13] Also some results on the liquid crystalline properties will be presented and discussed.

EXPERIMENTAL

Crystal data

Crystals suitable for x-ray diffraction measurements were obtained by recrystallization from methanol (CCN33, CCN38, CCN46) and acetone (CCN35). The data collections were carried out using a STOE-STADI-4 four-circle diffractometer (CCN33, CCN35, CCN46) and a STOE-SIEMENS-AED-2 four-circle diffractometer (CCN38). The crystal data are listed in Table I.

Structure determination and refinement

The structures of the four compounds were solved by direct methods using the program MULTAN-80[14] (CCN35, CCN38, CCN46) and SHELX-76[15] (CCN33) after performing Lorentz and polarization corrections. The refinements were carried out using the program SHELX-76.

The best E-map of CCN33 depicted the whole molecule. Refinement with anisotropic thermal parameters for non-H atoms and hydrogen atoms in geometrically idealized positions (C—H = 1.080 Å) during the refinement cycles of the s.o.f. converged at an R value of 0.1441. A difference map revealed distinctly, that the ring II (Figure 7) with the atom C(8)——C(13) is disordered. Nearly perpendicular to this ring in its original position, a second one appeared in the form of chair-like arranged-difference map peaks. The further refinement was modified in the following way: With different site occupation factors, by restricted refinement cycles, the occupation ratio between the two rings was estimated, which was found to be about 0.7:0.3.

To avoid strong correlations the temperature factors were kept constant (U_{iso} = 0.08 Å^2). Subsequently the parameters of the two cyclohexane rings were refined anisotropically with a bond length constraint of 1.540(5) Å for all ring bonds as well as for the distances C(5)—C(8) and C(11)—C(14). The refinement converged at R = 0.0717. The low temperature factors indicate a static disorder. A final difference map was essentially featureless.

The three other structures were defined with anisotropic temperature factors for non-H atoms and hydrogen atoms in fixed positions (C—H = 1.080 Å). The

TABLE I

Basic crystal data and experimental details

	CCN33	CCN35	CCN38	CCN46
Molecular formula	$C_{19}H_{33}N$	$C_{21}H_{37}N$	$C_{24}H_{43}N$	$C_{23}H_{41}N$
Formula weight (g · mol^{-1})	275.48	303.54	345.62	331.59
Space group (no. in int. tables)	Pbca (61)	$P2_1/c$ (14)	$P2_1/c$ (14)	$P2_1/c$ (14)
a (Å)	6.740(1)	16.053(5)	16.832(4)	6.027(2)
b (Å)	15.168(3)	6.735(2)	6.642(2)	9.436(2)
c (Å)	35.742(8)	19.928(5)	24.235(6)	38.857(8)
β (°)	–	112.58(1)	119.84(1)	92.113(5)
V (Å^3)	3653.98	1989.39	2350.20	2208.32
Number of strong reflections used for lattice parameter refinement	46	48	58	48
Z	8	4	4	4
D_X (g · cm^{-3})	1.002	1.013	0.977	0.997
μ[a] (cm^{-1})	3.58	0.29	0.27	3.53
Number of reflections measured	6045	3709	3188	6336
Number of independent reflections	2652	2287	3064	3139
Merging *R*	0.0300	0.0256	0.0430	0.0402
Number of unobserved reflections[b]	307	321	1488	127
$R(R_w$ with $w = 1/\sigma^2(F_o)$)	0.0717 (0.0720)	0.0706 (0.0611)	0.1164 (0.1034)	0.0683 (0.0744)

[a] Cu-K_α (λ = 1.54178 Å, graphite monochromated) in case of CCN33 and CCN46, range $3° \leq 2\vartheta \leq 115°$.
Mo-K_α (λ = 0.71069 Å, graphite monochromated) in case of CCN35 and CCN38, range $3° \leq 2\vartheta \leq 45°$.

[b] Using $F_o < 3\sigma(F_o)$ in case of CCN33 and CCN38 and $F_o < 2\sigma(F_o)$ in case of CCN35 and CCN46.

refinements converged at the *R* values given in Table I. The comparatively small number of significant reflections in the case of CCN38 [1488 having $F_o < 3\sigma(F_o)$] resulted in an only moderate *R* value.

Fractional coordinates and thermal parameters (U_{eq}) for all non-hydrogen atoms are listed in Table II. Essentially normal C—C and C—N distances for CCN33, CCN35 and CCN46 permit us to dispense with a complete listing of all distances and angles. Selected bond distances and the N_1—C_1—C_2 angles as well as some mean bond distances are given in Table III.†

Description of the structures

Figure 1 shows a schematic representation of the central part of the molecule, which is the same for all four compounds. The Roman numbers define the molecular subunits used in Table IV, in which the angles between the best planes through these subunits are presented. As an example of the molecular structures of the compounds with a twisted arrangement (see below) a plot of the CCN35 molecule

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†Hydrogen atom coordinates, all distances and angles, and F_o–F_c listings are available from the authors on request.

TABLE II

Positional and thermal parameters

$$\left(U_{eq} = \frac{10^3}{3}\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* (a_i a_j)/\text{Å}^2\right)$$

with e.s.d.'s (not for U_{eq}) for CCN33 (1), CCN35 (2), CCN38 (3) and CCN46 (4)

		x	y	z	U_{eq}
N(1)	1	0.0642(4)	0.2402(2)	0.3148(1)	127
	2	0.1524(2)	0.3445(4)	0.0890(2)	92
	3	0.7209(6)	0.3165(12)	0.3373(4)	117
	4	0.7403(4)	0.2183(2)	0.3787(1)	100
C(1)	1	0.2332(4)	0.2382(2)	0.3161(1)	82
	2	0.1523(2)	0.5126(5)	0.0904(2)	66
	3	0.7214(6)	0.4856(17)	0.3375(4)	84
	4	0.6273(3)	0.1215(2)	0.3804(1)	69
C(2)	1	0.4515(3)	0.2338(1)	0.3179(1)	66
	2	0.1503(2)	0.7347(4)	0.0900(2)	62
	3	0.7187(7)	0.7124(12)	0.3340(5)	82
	4	0.4832(3)	−0.0038(2)	0.3824(1)	62
C(3)	1	0.5141(4)	0.2177(2)	0.3585(1)	70
	2	0.2476(2)	0.8131(4)	0.1166(2)	71
	3	0.6241(6)	0.7790(12)	0.2807(4)	84
	4	0.5661(3)	−0.1155(2)	0.3571(1)	69
C(4)	1	0.4639(4)	0.2940(1)	0.3844(1)	72
	2	0.2962(2)	0.7574(4)	0.0668(2)	70
	3	0.5474(6)	0.7267(12)	0.2941(4)	86
	4	0.5423(3)	−0.0696(2)	0.3196(1)	66
C(5)	1	0.5552(4)	0.3804(1)	0.3715(1)	72
	2	0.2443(2)	0.8286(4)	−0.0111(2)	66
	3	0.5635(8)	0.8165(13)	0.3558(5)	98
	4	0.3030(3)	−0.0299(2)	0.3088(1)	60
C(6)	1	0.4864(4)	0.3986(2)	0.3314(1)	80
	2	0.1490(2)	0.7478(4)	−0.0381(2)	71
	3	0.6555(7)	0.7443(15)	0.4103(4)	100
	4	0.2212(3)	0.0835(2)	0.3335(1)	68
C(7)	1	0.5355(4)	0.3230(2)	0.3048(1)	78
	2	0.0993(2)	0.8026(4)	0.0110(2)	68
	3	0.7358(6)	0.7929(14)	0.3985(4)	100
	4	0.2446(3)	0.0385(3)	0.3712(1)	72
C(8)	1[a]	0.5287(6)	0.4525(3)	0.4015(1)	63
	1[b]	0.4676(26)	0.4787(8)	0.3921(4)	98
	2	0.2921(2)	0.7853(4)	−0.0635(2)	73
	3	0.4758(9)	0.7802(17)	0.3632(6)	129
	4	0.2796(3)	0.0180(2)	0.2708(1)	58
C(9)	1[a]	0.6844(5)	0.5258(2)	0.3971(1)	72
	1[b]	0.5625(20)	0.4589(6)	0.4310(3)	115
	2	0.3319(2)	0.5788(4)	−0.0563(2)	81
	3	0.4638(8)	0.9348(16)	0.3992(6)	144
	4	0.3863(3)	−0.0851(2)	0.2458(1)	69
C(10)	1[a]	0.6630(6)	0.5961(3)	0.4277(1)	74
	1[b]	0.4863(21)	0.5366(5)	0.4550(3)	131
	2	0.3738(2)	0.5410(5)	−0.1122(2)	91
	3	0.3782(8)	0.9047(17)	0.4065(5)	127
	4	0.3566(3)	−0.0372(2)	0.2083(1)	75
C(11)	1[a]	0.4537(6)	0.6359(6)	0.4279(1)	68
	1[b]	0.5634(22)	0.6247(7)	0.4396(3)	89
	2	0.4461(2)	0.6912(5)	−0.1070(2)	75

TABLE II

(*continued*)

		x	y	z	U_{eq}
	3	0.3730(10)	0.6983(18)	0.4276(7)	152
	4	0.1155(3)	−0.0164(2)	0.1969(1)	62
C(12)	1[a]	0.2996(5)	0.5630(2)	0.4321(1)	75
	1[b]	0.4778(15)	0.6338(5)	0.4000(3)	91
	2	0.4068(2)	0.8986(4)	−0.1145(2)	78
	3	0.3851(9)	0.5472(19)	0.3910(7)	180
	4	0.0080(3)	0.0864(2)	0.2219(1)	68
C(13)	1[a]	0.3178(5)	0.4926(2)	0.4015(1)	72
	1[b]	0.5501(20)	0.5556(5)	0.3761(3)	106
	2	0.3643(2)	0.9372(4)	−0.0586(2)	79
	3	0.4714(7)	0.5762(15)	0.3844(5)	111
	4	0.0365(3)	0.0405(2)	0.2594(1)	67
C(14)	1	0.4360(5)	0.7055(2)	0.4590(1)	99
	2	0.4870(2)	0.6474(5)	−0.1634(2)	80
	3	0.2786(7)	0.6651(15)	0.4277(5)	122
	4	0.0932(4)	0.0331(2)	0.1595(1)	73
C(15)	1	0.5484(5)	0.7902(2)	0.4528(1)	93
	2	0.5690(2)	0.7649(5)	−0.1575(2)	79
	3	0.2617(8)	0.7841(17)	0.4690(6)	148
	4	−0.1325(4)	0.0115(2)	0.1423(1)	75
C(16)	1	0.4834(5)	0.8638(2)	0.4787(1)	107
	2	0.6094(2)	0.6978(5)	−0.2113(2)	90
	3	0.1846(7)	0.7270(17)	0.4776(5)	127
	4	−0.1452(4)	0.0553(3)	0.1049(1)	88
C(17)	4	−0.3619(5)	0.0212(3)	0.0864(1)	106
C(18)	1	0.5231(4)	0.1592(2)	0.2919(1)	76
	2	0.1059(2)	0.8068(4)	0.1415(2)	72
	3	0.7991(6)	0.7864(12)	0.3232(4)	89
	4	0.4924(3)	−0.0572(2)	0.4198(1)	75
C(19)	1	0.4423(4)	0.0677(2)	0.3008(1)	94
	2	0.0119(2)	0.7281(4)	0.1276(2)	73
	3	0.7936(7)	0.7074(14)	0.2619(5)	104
	4	0.7201(4)	−0.1057(3)	0.4334(1)	82
C(20)	1	0.5219(5)	−0.0037(2)	0.2754(1)	108
	2	−0.0240(2)	0.8047(5)	0.1829(2)	76
	3	0.8711(6)	0.7926(14)	0.2536(4)	95
	4	0.7232(4)	−0.1538(3)	0.4704(1)	90
C(21)	2	−0.1177(2)	0.7332(5)	0.1705(2)	82
	3	0.8719(6)	0.7137(13)	0.1961(5)	102
	4	0.9517(5)	−0.2110(3)	0.4826(1)	96
C(22)	2	−0.1533(3)	0.8109(5)	0.2260(2)	101
	3	0.9451(6)	0.7985(15)	0.1848(5)	107
	4	0.9649(6)	−0.2606(4)	0.5189(1)	118
C(23)	3	0.9469(6)	0.7173(14)	0.1275(4)	103
	4	1.1892(6)	−0.3213(4)	0.5296(1)	135
C(24)	3	1.0214(7)	0.8053(16)	0.1172(5)	121
C(25)	3	1.0190(7)	0.7341(20)	0.0583(5)	152

[a] Site occupation factor 0.7.

[b] Site occupation factor 0.3.

TABLE III

Selected bond distances [Å] and angles [°] and mean bond distances [Å] for distinct groups (see Figure 1)

	CCN33	CCN35	CCN38	CCN46
C(1)—N	1.141(3)	1.133(4)	1.123(10)	1.142(3)
C(1)—C(2)	1.474(3)	1.496(4)	1.508(12)	1.471(3)
C(2)—C(18)	1.540(3)	1.536(4)	1.578(11)[c]	1.538(3)
$\overline{C-C}$, ring I[a]	1.528(7)	1.529(8)	1.529(14)	1.531(7)
C(5)—C(8)	1.543(4)[b]	1.544(4)	1.591(12)[c]	1.545(3)
$\overline{C-C}$, ring II[a]	1.534(5)[b]	1.521(7)	1.482(52)[c]	1.527(6)
C(11)—C(14)	1.538(4)[b]	1.516(4)	1.604(13)[c]	1.528(3)
$\overline{C-C}$, groups III[a]	1.510(4)	1.509(4)	1.438(12)[c]	1.507(3)
$\overline{C-C}$, groups IV[a]	1.518(4)	1.515(5)	1.508(16)	1.513(17)
N(1)—C(1)—C(2)	178.9(0.3)	178.3(0.4)	177.0(1.2)	179.5(0.2)

[a] Standard deviations of the mean values.

[b] Relates to the positions with s.o.f. 0.7.

[c] Data are somewhat anormal in order of the high thermal motion especially of groups II and III, respectively.

is depicted in Figure 2, whereas Figure 3 shows a plot of the coplanar arranged CCN46 molecule. It shows, acting for all the four compounds, that the cyano groups occupy axial positions whereas both the alkyl groups occupy equatorial ones. The latter are arranged in an all-*trans*-configurated fashion.

The N—C_1 bond distances and the angles N—C_1—C_2 are normal compared with the data given for CCH3 and CCH5.[6] Also all carbon–carbon bond distances for CCN33, CCN35 and CCN46 are normal (Table III), as well as the bond angles. Some distances for CCN38 are markedly deviating (Table III), especially those in which atoms of groups II and III are involved. This is related to the high thermal motion of the cyclohexyl group II and the alkyl group III (Table II) and the somewhat poor quality of the x-ray data leading to $R = 0.1164$ (Table I).

Table IV reveals immediately the principal difference in the molecular structures of three members of the CCN series to those of the CCH series.[6] While in CCH3, CCH5 and CCH7 an approximately coplanar arrangement of the cyclohexane rings within the bicyclohexyl subunits was observed, three CCN's show a completely

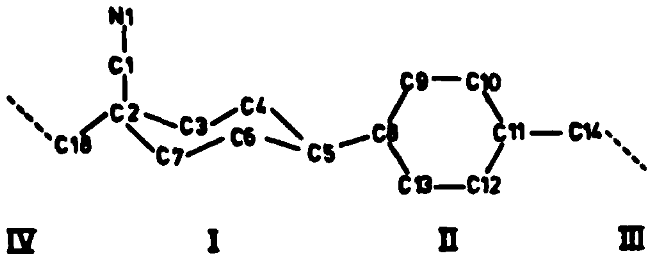


FIGURE 1 Schematic view of the molecule and numbering of the subunits.

TABLE IV

Dihedral angles [°] between best planes defined in Figure 1

	I/II	II/III	I/IV
CCN33	77.3[a]	37.4[a]	33.2
	8.4[b]	46.9[b]	33.2
CCN35	81.6	35.4	33.5
CCN38	81.9	31.3	34.4
CCN46	7.3	49.7	23.6

[a] Using the atoms C(9), C(10), C(12), and C(13) with the site occupation factor 0.7 for the plane II.

[b] Site occupation factor 0.3.

different conformation. The two cyclohexane rings in CCN33, CCN35 and CCN38 are nearly perpendicular to each other. In CCN33 ca. 30% of the molecules deviate from this geometry leading to a mixture of molecules with "twisted-" and "coplanar" character. Only CCN46 crystallizes in a "coplanar" geometry (Figure 3). To answer the question, what is the reason for the principal differences, we have to consider the possibilities of a molecule arranging itself as stably as possible in the crystalline state, which will be influenced by two important factors: intramolecular constraints arising from the geometrical characteristics of the chemical bonds, and packing effects, which mainly influence the arrangement of flexible molecular parts.

An interesting feature are the calculated densities by room temperature, shown below, for compounds which are, in some sense, comparable (see Table I and Reference 6)

$C_{18}H_{31}N$ (CCH5) = 1.033 g · cm^{-3} Ref. 6

$C_{19}H_{33}N$ (CCN33) = 1.002 g · cm^{-3} (this work)

$C_{20}H_{35}N$ (CCH7) = 1.017 g · cm^{-3} Ref. 6

$C_{21}H_{37}N$ (CCN35) = 1.013 g · cm^{-3} (this work)

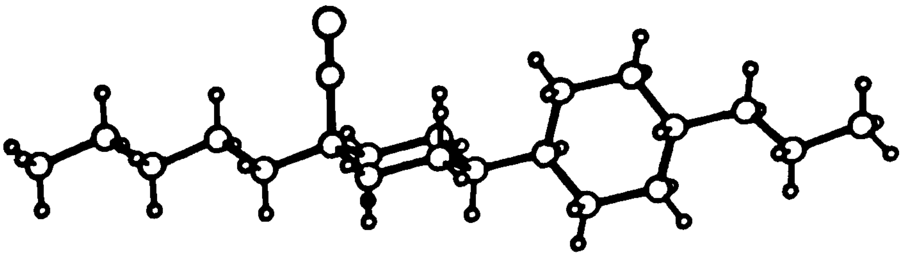


FIGURE 2 CCN35 molecule (twisted arrangement).

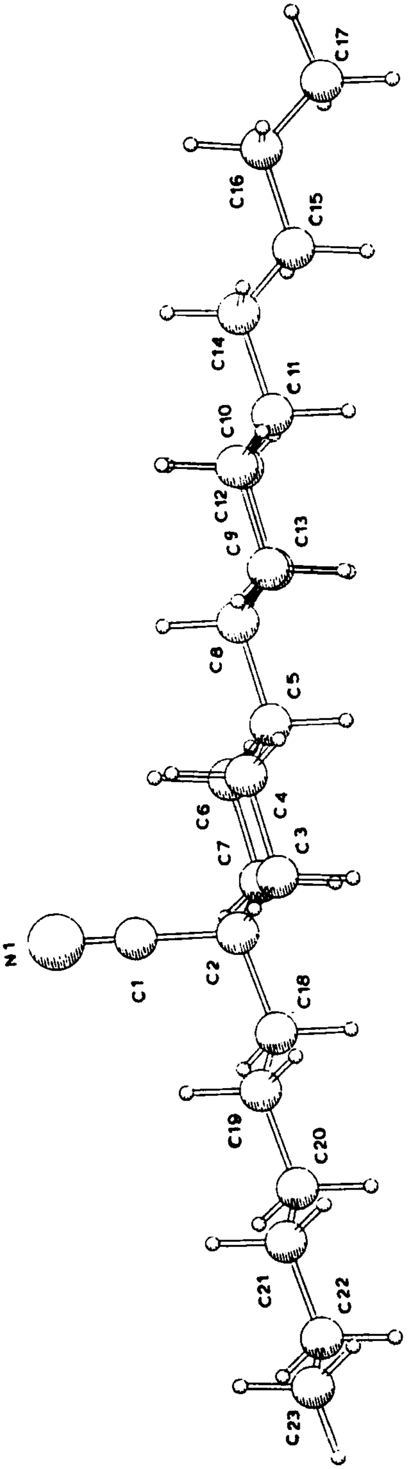


FIGURE 3 CCN46 molecule (coplanar arrangement).

It follows that the densities for the CCN series are smaller than the densities for the CCH series.

If one looks at the molecule schematically depicted in Figure 1, one can see that an axial cyano group increases the local requirements of the cyanocyclohexyl group compared with an equatorially-substituted cyclohexane ring. Assuming a primitive cylinder model that starts from the condition that the place available perpendicular to the longest molecular axis is approximately constant for the whole molecule, one will find that in a CCN molecule the cyano group increases the volume distinctly. Contrary to the CCH's, where no axial substituents are present, the cyano group automatically increases the free space also for the second cyclohexane ring. Since the cyano group prevents an overall flat structure of the molecules, a coplanar arrangement of the cyclohexane rings in the case of the CCN's will not lead to the same effective packing in the crystalline state as in the case of the CCH's.

Table V shows the two shortest H···H distances between H-atoms of the cyclohexane rings in all structurally investigated CCN's and CCH's, which would change by twisting one ring. One can see that a coplanar arrangement produces H···H distances always shorter than 2.2 Å while no distance smaller than this value is observed in twisted configurated molecules. A measure of 2.2 Å is approximately twice the van der Waals radius of hydrogen.

Contacts of H···H between neighboring phenyl rings were variously discussed with regard to their influence on conformational details. In cases of biphenyl molecules without substituents in ortho-positions, dihedral angles between 0° and 50° are observed[7,11,13] in the crystalline state. This shows that sometimes packing effects overcompensate the H···H repulsions. Theoretical calculations reveal an energy barrier of about 8 kJ mol^{-1} at 0° relating to an arrangement having an angle of about 40°.[16] Higher dihedral angles lead to loss of conjugation between the rings,

TABLE V

The two shortest H···H distances [Å] in the molecules of the CCN-series and of the CCH-series. (Only those atoms are taken into account, which would change their distances by twisting a cyclohexane ring.)

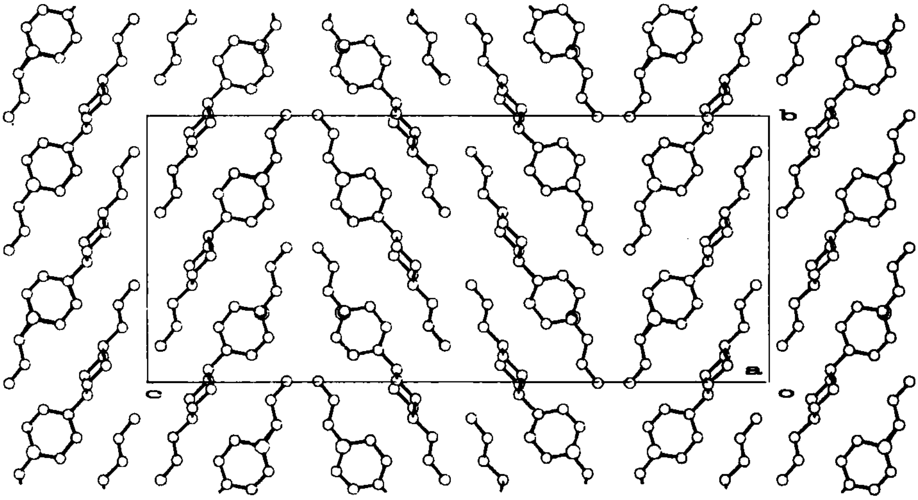
CCN33	2.23[a] 2.24[a]
CCN35	2.21 2.29
CCN38	2.22 2.25
CCN46	2.07 2.07
CCH3	2.11[b] 2.12[b]
CCH5	2.11[b] 2.15[b]
CCH7	2.05[b] 2.11[b]

[a] Twisted-form.

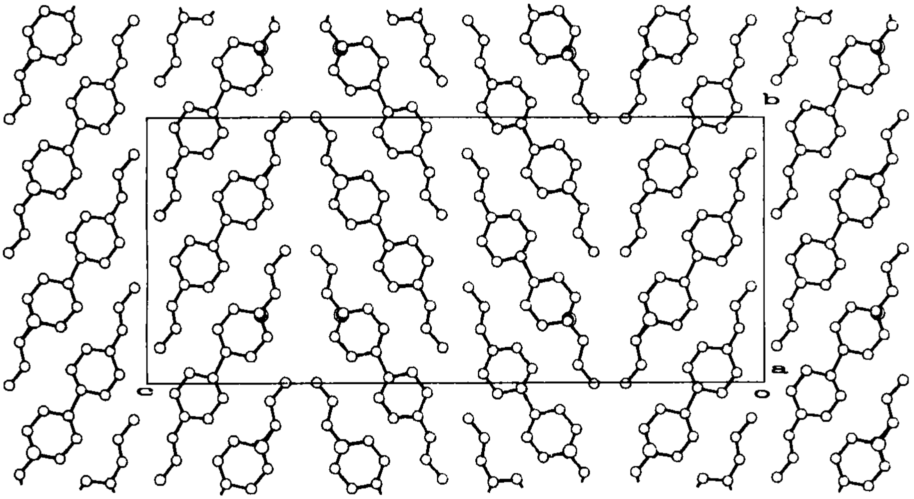
[b] Calculated from the data, given in Reference 6.

but there is no analogy here to the CCH's/CCN's. We suppose from geometrical consideration that the energy barrier in the cyclohexylcyclohexane moieties is smaller than in biphenyl moieties.

The dihedral angle between the cyclohexyl groups and the alkyl chains recently has been found to be in a preferred range also (Table IV). Values of 30–40° have been found for a few compounds containing this structural element.[7] The CCN's confirm that such an arrangement is a very favorable one.



(right)



(left)

FIGURE 4 CCN33, view along [100]. Left: coplanar arrangement; right: twisted arrangement.

Crystal packing

A very short *a* axis and an extremely long *c* axis are characteristic of the CCN33 lattice. The molecules are arranged (Figure 4) in a herring-bone pattern with an angle of about 30° between the molecular long axis and [010]. The molecules form sheets parallel to [100] with $x \approx 0$ or 1/2. The cyano groups are parallel to [100]. According to their axial position no short cyano–cyano contacts, as observed in the CCH's,[6] are possible.

Figures 5 and 6 present plots of the molecular structure of CCN35. Although compounds CCN35 and CCN38 (Figure 7) are not isostructural, they show several similarities which should be discussed. The same space group and similar lattice

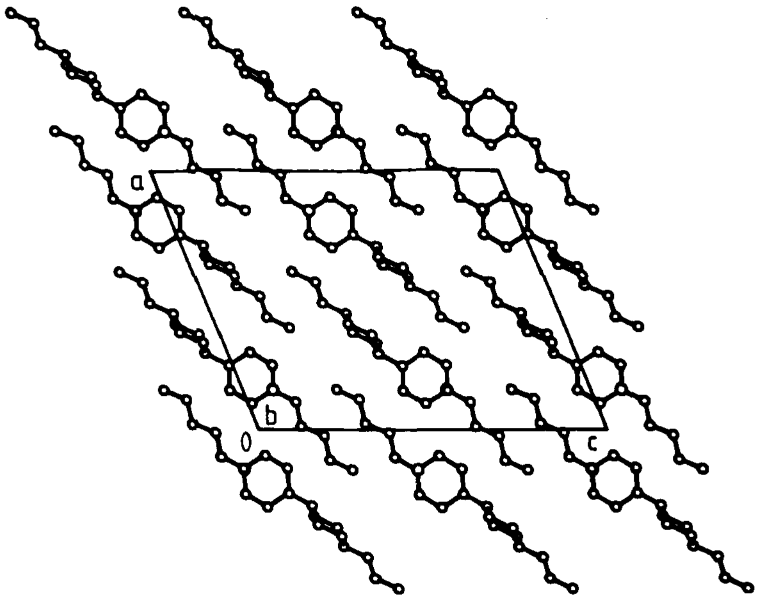


FIGURE 5 CCN35, along [010].

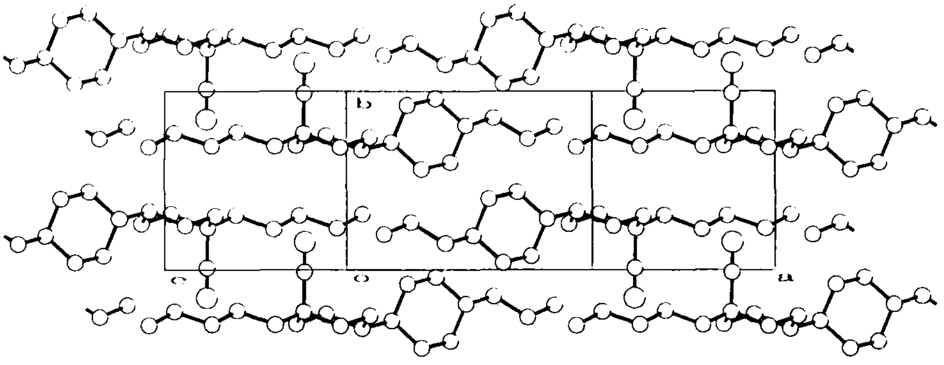


FIGURE 6 CCN35, along [001], *z* varied from 0.25 to 0.75.

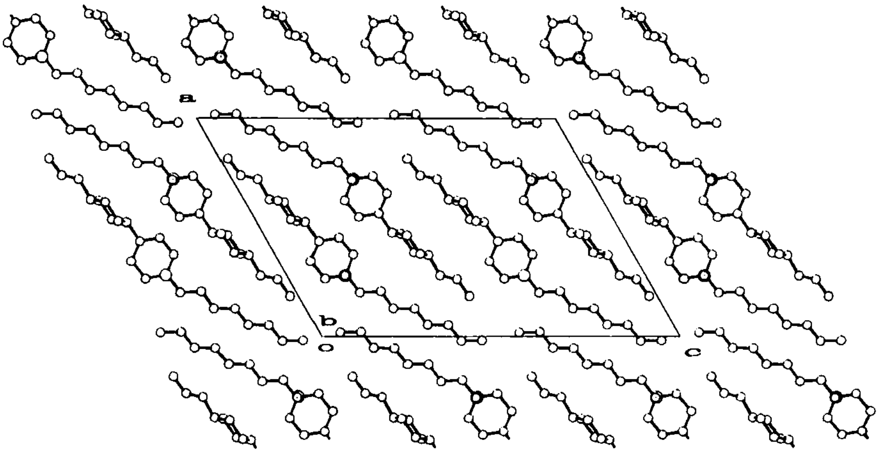


FIGURE 7 CCN38, along [010].

constants, especially the b̲ values, as well as the similar arrangement of the molecules in sheets with $y \approx 1/4$ and 3/4 are noticeable. The molecular long axes are parallel to [201] leading to a parallel arrangement of the cyano groups to [010]. Figures 5 and 7 show also a similar arrangement of the propylbicyclohexyl subunits within both structures.

A very short *a* axis and a very long *c* axis characterize the structure of CCN46 (Figure 8). The flat molecular bicyclohexane skeletons are arranged in sheets perpendicular to [010] with $y \sim 0$ and 1/2. The molecular long axes lie parallel to [301].

A common characteristic of all four structures is one very short axis. In cases of CCN33, CCN35 and CCN38 sheets of the molecules are perpendicular to this axis.

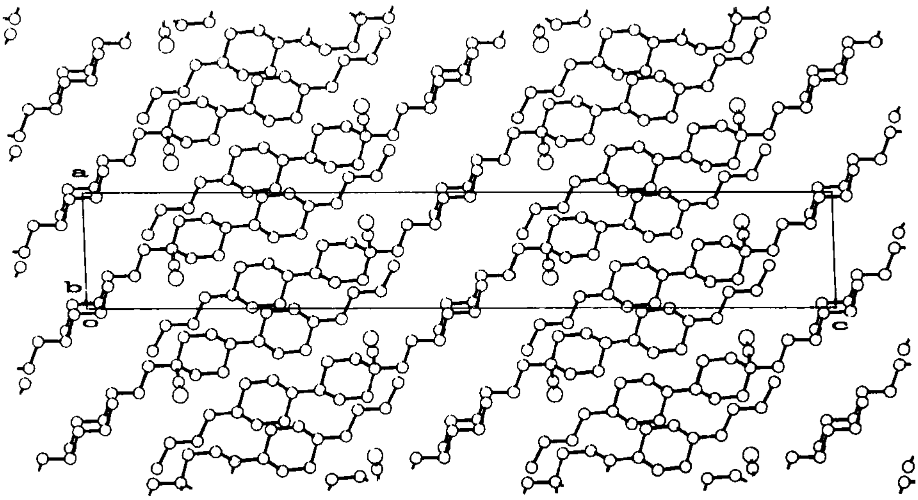


FIGURE 8 CCN46, along [010] (not all atoms in the cell are presented).

TABLE VI

Comparison of solid state molecular length and fluctuation wavelength/layer thickness in the mesophase [Å][a]

Compound	Solid state	Mesophase	Phase	Reference
CCN33	17.18			this work
CCN35	19.69	17.1	N	this work
CCN38	23.04	20.9	N	this work
CCN46	22.10	19.6	N	this work
CCH3	15.13	27.3	S_B	18
CCH5	17.52	27.2	N	18
CCH7	20.18	31	N	18

[a] Comparison of solid state molecular length includes the covalence radii of H with 0.3 Å.

Within all four structures no cyano–cyano contacts exist. A strict antiparallel arrangement of all cyano dipoles is observed in CCN33, CCN35, CCN38, a slight deviation from parallelism exists in CCN46. A similar arrangement of the cyano group as observed for compounds with cyanophenyl units[11,17] and 4α-cyanocyclohexyl units,[6] respectively, where dimeric and infinite aggregations via cyano–cyano interactions were observed, is not possible here.

Table VI shows a comparison of the calculated molecular lengths in the crystalline state with those obtained from x-ray measurements in the mesophase.

One can see immediately, that the CCN compounds give comparable values for the single crystal data and the liquid crystalline ones. The CCH compounds, however, give values for the mesophases which give rise to assume dimeric units.[18]

Acknowledgments

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