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### Electric Permittivities and Elastic Constants of the Cyano Bi-Cyclohexanes (CCH)

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# ELECTRIC PERMITTIVITIES AND ELASTIC CONSTANTS OF THE CYANO BI-CYCLOHEXANES (CCH)

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
(Submitted for publication 20 May 1981)

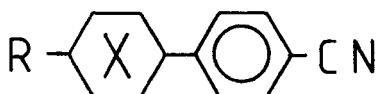
## ABSTRACT


Measurements of the electric permittivities and the splay and bend elastic constants of the cyano bi-cyclohexanes (CCH) are reported as a function of temperature. Comparison of the ratio of the bend to splay constants with that of analogous compounds containing phenyl rings shows unexpected trends, and attention is drawn to the possible relevance of recent novel structures of CCH determined by X-rays.

## INTRODUCTION

The electric permittivities and elastic constants of nematic liquid crystals are important quantities on at least two counts. They are used to test models of the ordered liquid crystal state. Secondly, they determine the response of electro-optic display devices to an applied electric field, and therefore form an important criterion for assessing the usefulness in devices of new liquid crystal materials.

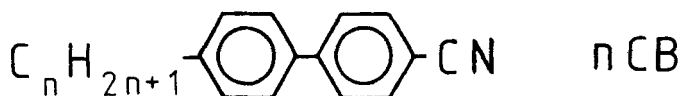
Recent studies have looked at the effects of substituting various rings  into the structure<sup>(1,2)</sup>



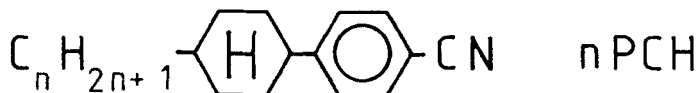
In particular the ratio of the bend to splay elastic constant ( $k_{33}/k_{11}$ ) was found to increase when the phenyl ring in position  was substituted by a trans-1, 4-disubstituted cyclohexane ring. This letter examines the effect of the replacement of the phenyl ring adjacent to the cyano group by a trans-1, 4-disubstituted cyclohexane ring.

#### MATERIALS

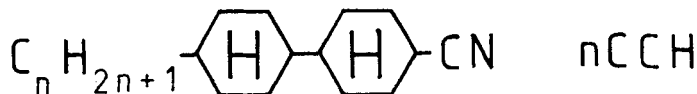
The 4'-n-alkylbiphenyl-4-carbonitriles<sup>(3)</sup>



the 4-trans-(4'-n-alkyl)-cyclohexylbenzonitriles<sup>(4)</sup>



and the trans, trans-4'-n-alkylbicyclohexyl-4-carbonitriles<sup>(5)</sup>



form three series of stable nematic compounds with a progressive replacement of the phenyl rings by trans-1, 4-disubstituted cyclohexane rings. The transition temperatures of the homologues used are shown in Table 1.

Material	$T_{KN}(^{\circ}C)$	$T_{NI}(^{\circ}C)$
5CB	24	35.3
7CB	30	42.3
3PCH	43	45.5
5PCH	30	54.7
7PCH	30	56.8
3CCH <sup>1</sup>	58	80.0
5CCH <sup>2</sup>	62	85.2
7CCH	71	82.1

TABLE 1 Melting points ( $T_{KN}$ ) and clearing points ( $T_{NI}$ ) of the materials.

1.  $T_{SN} = 57^{\circ}C$ ; 2.  $T_{SN} = 52^{\circ}C$ .

#### EXPERIMENTAL TECHNIQUE

The perpendicular ( $\epsilon_{\perp}$ ) and parallel ( $\epsilon_{\parallel}$ ) components of the electric permittivity and the splay ( $k_{11}$ ) and bend ( $k_{33}$ ) elastic constants were found by analysing the capacitance voltage curves of a zero tilt parallel aligned layer<sup>(6)</sup>. An HP4274A was used to measure the capacitance at 1 kHz and a Datron 1041 monitored the voltage via a high impedance instrumentation amplifier. All functions including the control of temperature to within  $0.1^{\circ}C$  were directed by an HP9825 desktop computer.

The low voltage data gave  $\epsilon_{\perp}$  directly, and an estimate of  $\epsilon_{\parallel}$  was obtained from the high voltage data using a  $V^{-1}$  extrapolation<sup>(7)</sup>. A three parameter non-linear least squares fitting programme<sup>(8)</sup> was used to determine  $(k_{33}-k_{11})/k_{11}$ ,  $V_c$  (threshold voltage), and  $(\epsilon_{\parallel}-\epsilon_{\perp})/\epsilon_{\perp}$ , where

$$V_c^2 = \frac{\pi^2 k_{11}}{\epsilon_o(\epsilon_{\parallel}-\epsilon_{\perp})}$$

## RESULTS AND DISCUSSION

The electric permittivities of the CCH homologues are illustrated in Figure 1, and  $\bar{\epsilon} = (\epsilon_{\parallel} + 2\epsilon_{\perp})/3$  is seen to be

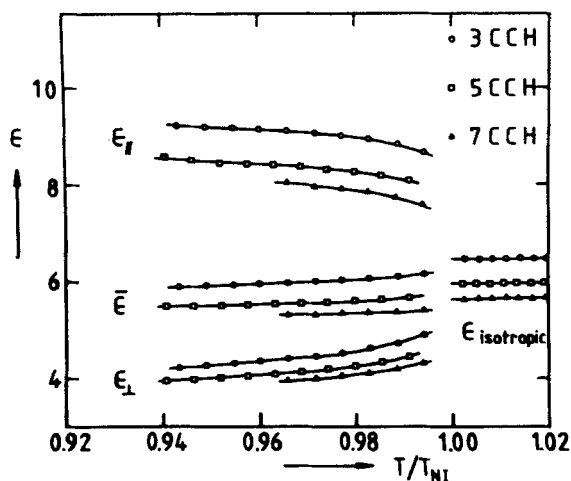


FIGURE 1. The Electric Permittivities of CCH.

virtually independent of temperature and discontinuous with  $\epsilon(\text{isotropic})$  at  $T_{\text{NI}}$ . These two factors are indicative of the strong anti-parallel local ordering of molecules found in cyano systems<sup>(9)</sup>. The fractional discontinuity at  $T_{\text{NI}}$  in CCH is similar to that observed in CB and PCH, this is somewhat surprising as one might have anticipated that the more polar CB and PCH would show a larger discontinuity. The electric permittivities of CB<sup>(10,11,12,13)</sup> and PCH<sup>(13)</sup> and the permittivity anisotropy of 7CCH<sup>(13)</sup> have already been reported.

The splay elastic constants  $k_{11}$  of the CCH homologues are shown in Figure 2 and are similar in magnitude to the values already known for CB<sup>(1,14,15,16,17)</sup> and PCH<sup>(1,18)</sup>. The ratio of bend/splay elastic constants  $k_{33}/k_{11}$  is shown for all three series of compounds in Figures 3 ( $n=3$ ), 4 ( $n=5$ ), and 5 ( $n=7$ ). The replacement of a phenyl ring in

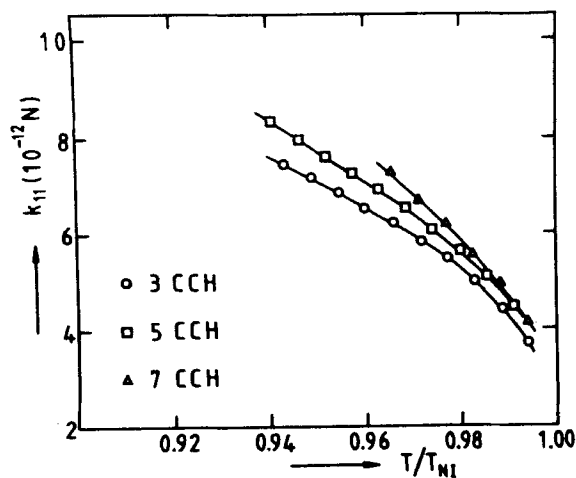


FIGURE 2. Splay Elastic Constant ( $k_{11}$ ) of CCH.

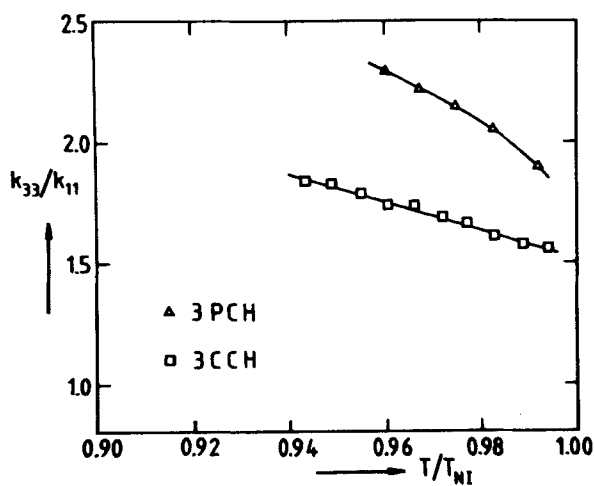


FIGURE 3. Ratio Bend/Splay ( $k_{33}/k_{11}$ ) of 3PCH and 3CCH.

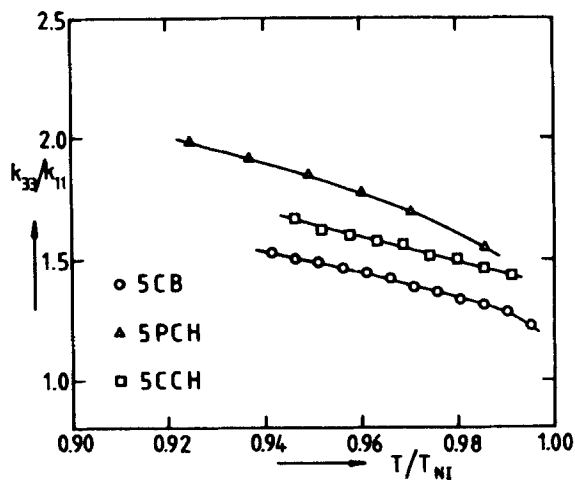


FIGURE 4. Ratio Bend/Splay ( $k_{33}/k_{11}$ ) of 5CB, 5PCH and 5CCH.

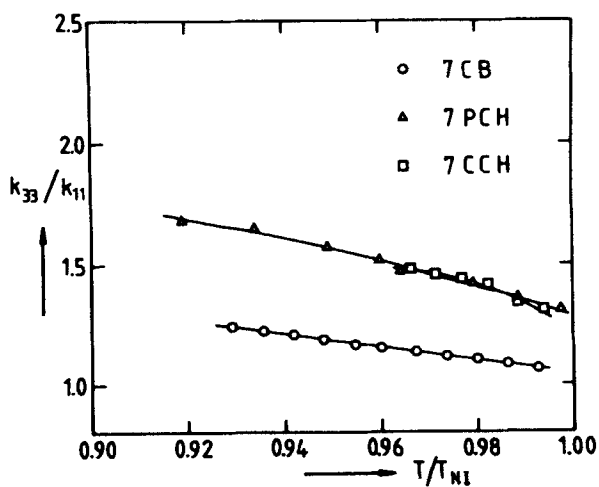


FIGURE 5. Ratio Bend/Splay ( $k_{33}/k_{11}$ ) of 7CB, 7PCH and 7CCH.



CB by a single trans cyclohexane ring to form PCH increases the ratio  $k_{33}/k_{11}$  in accordance with previous observations<sup>(1,2)</sup>. However, the replacement of the second phenyl ring to form 3CCH and 5CCH decreases  $k_{33}/k_{11}$  towards the CB values, whereas 7CCH and 7 PCH have similar values.

The anti-parallel local ordering in CCH compounds has recently been found by X-ray measurements to correspond to overlap of only the cyano groups<sup>(19)</sup>, quite different to the core overlap found in CB and PCH. This different local order must affect the elastic constant ratios, and may well explain the unexpected observations in the ratio  $k_{33}/k_{11}$  of the CCH compounds.

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