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INVITED ARTICLE

Determination of the translational order parameter for smectic liquid crystals using small-angle neutron scattering

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A simple method to determine the translational order parameter of a smectic liquid crystal is presented. It is based on a measurement of the absolute intensity of the first-order layer reflection from an unaligned (powder) sample using small-angle neutron scattering. The Lorentz factor and molecular form factor are used to derive the order parameter from the intensity. The method is demonstrated for 4-octyl-4'-cyanobiphenyl (8CB), using two different isotopomers which give a consistent translational order parameter value of 0.5 in the smectic A phase.

Keywords: smectic; translational order parameter; small-angle neutron scattering

1. Introduction

A key quantity in liquid crystal science is the orientational order parameter. It is the parameter that distinguishes the nematic phase from an isotropic liquid and it is ubiquitous in the liquid crystal literature. It is measured by experiments such as nuclear magnetic resonance (NMR) imaging [1, 2], it governs properties such as the magnetic and electric anisotropy and it is predicted by theories of the nematic–isotropic transition such as the Maier–Saupe molecular field theory [3–5].

The translational order parameter distinguishes the smectic A phase from a nematic. It is defined as $\tau = \langle \cos 2\pi\delta/d \rangle$ where δ is the displacement of a molecule from its ideal position, centred in the smectic layer, d is the layer thickness and the angle brackets indicate an average over all the molecules in the phase. Strictly this is the dominant member of a series of translational order parameters defined by $\tau_n = \langle \cos 2n\pi\delta/d \rangle$, where n is a positive integer. The translational order parameter defines the amplitude of the one-dimensional density wave in the smectic A phase and characterises how well molecules are confined to a smectic layer. It is the main output of theories of the nematic–smectic transition such as the McMillan theory [6]. It is, therefore, surprising that its value for different materials is rarely reported [7–12]. In this paper we discuss the difficulties in measuring the translational order parameter and outline a simple method for determining it in smectic liquid crystals. Our motivation was to determine values of the translational order parameter for the bulk smectic A phase that could be compared with the values determined in surface-induced smectic layers in nematic phases that have been reported elsewhere [13–15].

Diffraction is sensitive to the position of atoms and molecules so is clearly the most promising method for measuring τ. In his original work [16], McMillan pointed out that τ is proportional to the intensity of the first-order Bragg reflection from the smectic layers:

$$\tau = k\sqrt{I_{001}}.$$

Therefore, determination of τ should be simple if I_{001} is measured and k is known. Unfortunately, there are two difficulties. Firstly, it has not been common to measure X-ray scattering intensities as absolute cross sections until the last decade. This is because the standard samples for intensity measurement have tended to be weak and so rather inconvenient to use. Some of the first measurements were, therefore, in arbitrary units and a quantity proportional to the order parameter was determined [16].

The classical method [17] used to determine τ avoids the need to measure the absolute cross section because it uses the intensity ratio of the first- to second-order diffraction peaks. It suffers from several drawbacks which limit its application: the second-order peak may be too weak to observe above the background [18, 19]; it requires a molecular form factor calculation which is difficult to carry out realistically for X-ray scattering; and it also assumes a Gaussian distribution of displacements about the layer centre. Hence, it has not been widely adopted for routine measurements.

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An ingenious method [20] has recently been suggested that makes a Haller-like extrapolation of the intensity to absolute zero. Since $\tau = 1$ at absolute zero, the extrapolated value of $\sqrt{I_{001}}$ may be used to determine the value k. This method assumes that k is independent of temperature and it requires the smectic range to be wide enough to be able to extrapolate reliably.

Another approach has been to link the order parameter to the correlation distance of the smectic layers [21, 22]. The latter can be determined from the width of the layer reflection so the absolute cross section is not needed. However, the order parameter is only linked to the correlation distance for an assumed model of the disorder. So, while this method is useful for a qualitative comparison of similar materials (e.g. side chain liquid crystal polymers), it should be regarded as rather indirect.

In recent years it has become more common to measure absolute X-ray cross sections by comparing the scattered intensity with that from a standard [23] and so this is no longer a difficulty. For small-angle neutron scattering, the normal practice over several decades has been to measure absolute cross sections by comparing the sample scattering with that from water [24, 25]. Water has a large incoherent cross section so this method is easy and convenient for reactor-based small-angle neutron scattering (SANS) instruments. On pulsed sources, a secondary standard consisting of a block copolymer with deuteriated and hydrogenous blocks is often used. Thus, with both X-rays and neutron small-angle scattering, it is now possible to determine the absolute cross section corresponding to the layer reflections.

The second difficulty is to find a reliable value for k. In this work, diffraction from an unaligned (powder) rather than a monodomain sample has been used because it is much simpler to set up the SANS measurement for a powder and it is not always easy to prepare a perfect monodomain. In Section 2, it is shown that for a powder sample the constant, k, depends on the number density of molecules in the liquid crystal and the molecular form factor. This is not trivial because there is a distribution of molecular conformations and orientations for typical mesogenic molecules. For simplicity, we have chosen a single conformer and orientation. This would introduce a major systematic error into the calculation for X-rays. X-rays are scattered by electron density and the main contrast in a smectic layer results from the lower density regions around the tips of the alkyl chains. This is very sensitive to the choice of conformer and how the conformer fits into the layer. For neutrons, the systematic error can be much less if the molecules are chosen to have a high scattering length moiety and a low scattering length moiety. Hydrogen has a negative scattering length ($b_H = -3.74 \times 10^{-15}$ m) while carbon and deuterium have positive scattering lengths ($b_C = 6.64 \times 10^{-15}$ m, $b_D = 6.67 \times 10^{-15}$ m). The smectic layer is formed by partial segregation of the aliphatic parts (empirical formula CH_2, giving negative scattering length density) and the aromatic parts (empirical formula CH, giving positive scattering length density). Thus the scattering contrast arises between the aliphatic and aromatic strata and their separation is not greatly influenced by the choice of orientation and conformation, given that a pair of molecules has to fit within a smectic layer. If the aromatic part of the molecule is deuteriated (empirical formula CD) its scattering length density is even higher giving greater contrast. Thus, in Section 5, the molecular form factors for some typical conformations and different orientations are presented to establish that, for neutron scattering, they are rather insensitive to these parameters. The values have then been used to calculate the translational order parameter in the smectic A phase of 4-octyl-4'-cyanobiphenyl (8CB) as a demonstration of the method.

2. Theoretical background

The intensity of the Bragg reflection from a single crystal with perfect order is usually characterised by the differential cross section $\left(\frac{d\sigma}{d\Omega}\right)$. It has the dimensions of area per unit solid angle. Standard diffraction theory [26] may be used to show that a Bragg peak is a Dirac delta function that is positioned at a scattering vector **Q** equal to the reciprocal lattice vector, **G**:

$$\left(\frac{d\sigma}{d\Omega}\right) = A\delta(\mathbf{Q} - \mathbf{G}). \tag{1}$$

The magnitude of the scattering vector is determined by the scattering angle, 2θ, and the wavelength, λ of the radiation:

$$Q = 4\pi \sin\theta/\lambda. \tag{2}$$

The strength of the peak, A, depends on four factors: the number of unit cells in the crystal, N; the structure factor of a unit cell, $F(\mathbf{Q})$; the polarisation factor, P; and the volume of a unit cell of the reciprocal lattice, υ^*:

$$A = N|F(\mathbf{Q})|^2 P\upsilon^*. \tag{3}$$

Only neutron scattering is considered here so we can assume that the polarisation factor is unity. This would not be so for transverse waves such as X-rays. For a powder sample, with a uniform distribution of crystallite orientations, the intensity per crystal is obtained by averaging over all angles between the scattering vector and the reciprocal lattice vector. This converts the argument of the delta function from a vector to a scalar and introduces two further factors,

$$\left\langle \frac{d\sigma}{d\Omega} \right\rangle = \frac{1}{4\pi G^2 \cos\theta} mA\delta(Q-G), \tag{4}$$

where θ is half the scattering angle. The first factor is known as the Lorentz factor [27] for powder diffraction although only the angular dependency is generally used. The cosine results from the angle at which the reciprocal lattice point sweeps through the Ewald sphere but for the small-angle scattering discussed here, it may be omitted. The second factor, m, is the multiplicity of the Bragg peak.

In the small-angle scattering technique, the intensity is usually measured as the differential cross-section per unit volume of the sample which has the dimension of inverse length. Thus the intensity measured, $I(Q)$, is obtained by multiplying by the number of crystals per unit volume, $\left(\frac{N_{cr}}{V}\right)$:

$$\begin{aligned} I(Q) &= \left\langle \frac{d\sigma}{d\Omega} \right\rangle \left(\frac{N_{cr}}{V}\right) \\ &= \frac{1}{4\pi G^2} mN|F(Q)|^2 \upsilon^* \delta(Q-G)\left(\frac{N_{cr}}{V}\right). \end{aligned} \tag{5}$$

If there is no empty space between the crystals (as is the case in a polydomain smectic phase) the number of crystals per unit volume may be calculated from the bulk density of the material, ρ, and the molar mass of the atoms in a unit cell, W:

$$\left(\frac{N_{cr}}{V}\right) = \frac{\rho N_A}{WN}, \tag{6}$$

where N_A is the Avogadro constant. Dividing by the number of unit cells per crystal, N, converts from cells per unit volume to crystals per unit volume.

The volume of the unit cell of the reciprocal lattice may also be calculated from the bulk density, ρ, and the molar mass of the atoms in a unit cell, W:

$$\upsilon^* = \frac{8\pi^3}{\upsilon} = 8\pi^3\left(\frac{\rho N_A}{W}\right). \tag{7}$$

Substituting for $\left(\frac{N_{cr}}{V}\right)$ and υ^*in Equation (5) gives the following equation for the intensity:

$$I(Q) = \frac{1}{G^2} m\, 2\pi^2 |F(Q)|^2\, \delta(Q-G)\left(\frac{\rho N_A}{W}\right)^2. \tag{8}$$

It is important to note that it does not contain the number of unit cells per crystal, N, which would be difficult to determine, and all the other factors are accessible experimentally.

The case of the first-order layer reflections from a polydomain smectic A sample is now considered. The multiplicity m is 2 because there are only two layer reflections (indexed 001 and 00$\bar{1}$). The structure factor only needs to comprise a summation over the z-coordinates of the atoms because these reciprocal lattice points have no components perpendicular to the layer normal. However, for a smectic phase, all the unit cells are not identical. The structure factor must take account of the facts that the unit cell is an entire layer and that all the layers are not identical because of the partial orientational and translational order. In this work we have sought to circumvent this difficulty by using a simplified model which captures the important features of the structure factor for the purposes of determining the translational order parameter. The simplified model assumes that the orientational order is high and the conformation of every molecule is effectively the same. The centre of gravity of the molecules are displaced from their central position in the layer by a distance δ so the structure factor of a particular cell may be written as a product of a molecular form factor, $M(\mathbf{Q})$, which is defined by the molecular conformation and a phase factor. The Dirac delta function in Equation (8) means that we need only consider the structure factor and molecular form factor on at $\mathbf{Q} = (0, 0, Q_z)$ where the z-component of $\mathbf{Q}$ is parallel to the layer normal. That is,

$$F(\mathrm{Q_z}) = M(Q_z)\exp(iQ_z\delta). \tag{9}$$

Since the smectic phase is non-polar, two molecules must be included in the molecular form factor calculation. A pair of molecules, pointing in opposite directions, ensures that the layer structure is not polar. Thus the W in Equation (8) refers to the mass of a pair of molecules and the molecular form factor is a summation over the atoms in such a pair:

$$M(Q_z) = \sum_j b_j \exp(iQ_z z_j), \tag{10}$$

where j extends over all the atoms in a pair, and b_j is the scattering length and z_j is the position of atom j. If the molecular conformation is the same in every layer and displacements in different layers are not correlated, the intensity is determined by the structure factor, at $Q_z = G$, averaged over all values of the displacement δ which has an even distribution function. This gives

$$I \propto \langle F(G) \rangle^2, \tag{11}$$

$$\begin{aligned}\langle F\rangle &= |M(G)|\langle\cos G\delta\rangle = |M(G)|\left\langle\cos\frac{2\pi\delta}{d}\right\rangle\\ &= |M(G)|\tau, \end{aligned}\qquad (12)$$

where $\tau = \left\langle\cos\frac{2\pi\delta}{d}\right\rangle$. The translational order parameter, τ, has a value of one if all the centres of gravity of all the pairs of molecules are confined to the central plane of the smectic layers and a value of zero if they are displaced by any distance with equal probability as expected in a simple, non-cybotactic, nematic phase.

So for a powder sample of a smectic phase, the integrated intensity of the layer reflection is related to the scattering vector ($G = 2\pi/d$), the molecular form factor of a representative pair of molecules at this scattering vector, $M(G)$, their molecular mass, W, the density of the material, ρ, and the smectic order parameter, τ. It is:

$$I_{001} = \frac{1}{G^2}4\pi^2|M(G)|^2\tau^2\left(\frac{\rho N_A}{W}\right)^2. \qquad (13)$$

Hence the order parameter may be determined using

$$\tau = \frac{1}{d}\frac{1}{|M(G)|}\left(\frac{W}{\rho N_A}\right)\sqrt{I_{001}}. \qquad (14)$$

The values of $M(G)$ have been calculated as described in Section 5. The intensities have been measured using the method described in Section 3 and are presented in Section 4. The resulting translational order parameters have been calculated using Equation (14) and are also presented in Section 5.

3. Experimental method

The SANS measurements reported here were made using the LOQ instrument at the ISIS neutron source [28, 29]. The scattered neutrons are registered by a two-dimensional detector. Since the source is pulsed, a white beam is used and the different wavelengths are identified by their time of flight from source to detector. The data are corrected for their transmission and the empty cell background then regrouped into intensity *vs.* Q profiles and scaled to the intensity from standard samples. This was done using the Colette program [30] and the output was the scattering cross section per unit volume of the sample. The resolution of the LOQ instrument is effectively constant in the Q range of interest at 6% FWHM. The uncertainties this introduces on the peak position, shape and integrated peak intensity are therefore negligible.

The samples were contained in fused silica cells with a 2 mm path length for the neutron beam. The beam dimensions were defined by an 8 mm aperture and so the illuminated volume was precisely defined. The samples were prepared by rapid cooling from the isotropic phase by soaking the outside of the cell with acetone and vibrating the sample with a laboratory mixer. The method demonstrated a reasonably isotropic powder. Figure 1(a) shows a typical diffraction pattern from the layer reflections of 8CB in its smectic A phase. It can be seen that the powder is reasonably isotropic but not perfect. These data were then regrouped to give a mean intensity *vs.* Q curve (such as that in Figure 1(b)) which effectively takes the mean of all data at the same $|Q|$ and to some extent compensates for any preferred alignment of the layers.

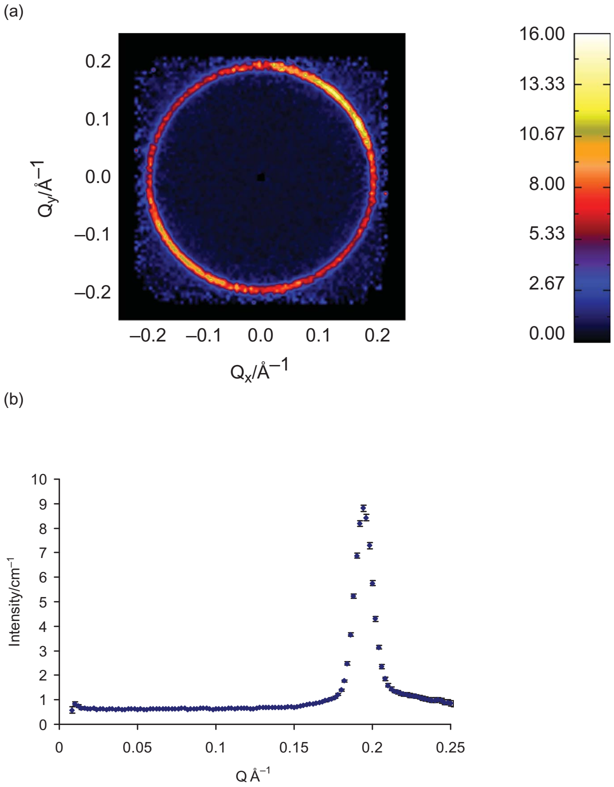


Figure 1. SANS from core-D 8CB measured at 32°C. (a) The intensity, in units of cm^{-1}, as a function of Q_x and Q_y and (b) regrouped to give the mean intensity as a function of Q.

For this exploration of the method, we used three different isotropic versions of 8CB: the normal all hydrogenous material (all-H), one with the aromatic core deuteriated (core-D) and a perdeuteriated version (all-D).

4. Results

The integrated intensity of the layer reflections was calculated by integrating the peaks around $Q = 0.2$ Å^{-1} and subtracting the incoherent background interpolated

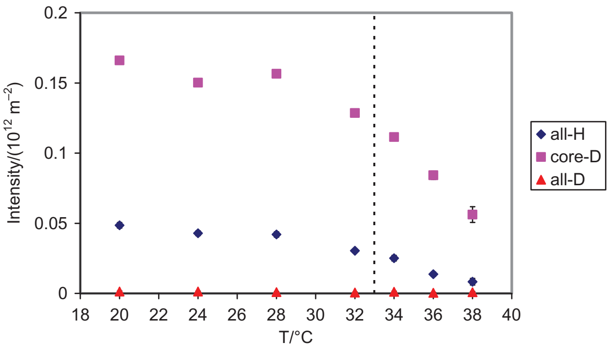


Figure 2. Integrated neutron scattering intensity from three differently deuteriated versions of 8CB. The vertical dashed line marks the smectic A-to-nematic transition temperature.

from either side. Figure 2 shows the integrated intensities from the three isotopomers as a function of temperature. The intensity from the all-D version is very much weaker than for the other two because its scattering length density is relatively uniform, with no contrasting substrata in the layer. The molecular form factor for SANS from this molecule will be similar to the X-ray case because it will depend in an unpredictable way on lower density regions around the tips of the tails. We have not attempted to deduce a translational order parameter from these data. The scattering from the core-D and all-H are much stronger as expected from layers with a high scattering length (aromatic) substratum between two aliphatic substrata. These intensities have been used to deduce values of the translational order parameter.

5. Analysis

The molecular form factor of the all-H and core-D molecules were calculated for pairs of molecules within a smectic layer of thickness 31.5 Å. The atomic coordinates were generated using Cerius^2® software. The molecules were initially oriented with their principal axes of inertia tilted by 10° to the layer normals. Their extremal atoms were located at a van der Waals radius from the layer boundary as shown in Figure 3. This gave a fair estimate of the molecular form factor. Values were calculated for five conformers of 8CB and these are shown in Table 1. Table 2 shows that there is rather little effect of the choice of conformer on the molecular form factor so in the following analysis, conformer 4 was used as a typical case.

The effect of varying the tilt of the molecules and shifting them towards or away from the layer centre was also explored. Figure 4 shows the values for conformer 4 as a function of shift and tilt. It can be seen that there is very little variation ($<$10%) for tilts up to 20° and shifts of ±2 Å. It would, therefore, be quite possible to estimate the order parameter to an accuracy of 10% using Equation (14) and picking a molecular form factor for zero shift and 10° tilt.

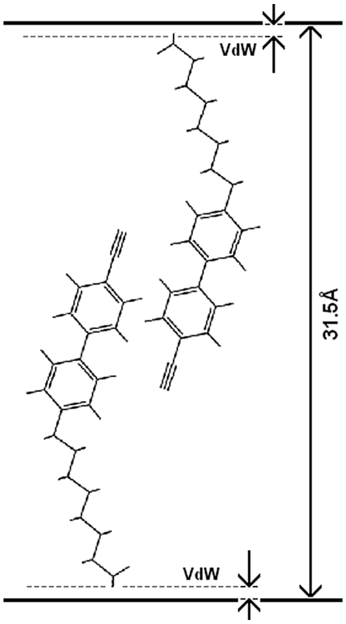
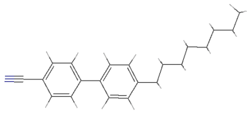
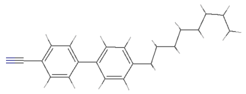
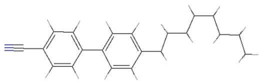
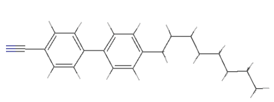
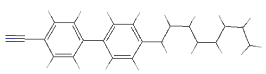


Figure 3. Two 8CB molecules in a smectic A layer. They were initially placed at a van der Waals radius from the limit of the layer. The effects of changing their tilt and shifting them in and out were explored.

The following procedure was followed to find a consistent value for the order parameter from both sets of intensity data. The order parameters from each isotopic version were calculated as a function of the assumed shift and tilt of the molecules, using Equation (14). The value used for the layer spacing, d, was 31.5 Å; the relative molar mass of the all-H version was calculated to be $W = 299.5$ Daltons and its density, ρ, was taken to be 0.99 g cm^{-3} [31, 32]. The ratio W/ρ (the molar volume) was assumed to be the same for the core-D version. The resulting order parameters were similar as is shown in Figure 5. The (shift, tilt) values that make the τ values equal are marked with a line. The lines indicate that consistent values of τ are obtained if a small degree of interdigitation between molecules in adjacent layers is assumed. Following the line in both diagrams (Figures 5(a) and (b)) show a remarkably slight variation in τ for (shift, tilt) of (–2.0 Å, 0°) to (–3.0 Å, 20°). We selected the molecular form factors for (–2.5 Å, 10°) and used them to determine the order parameter as a function of temperature. The values of 1.37×10^{-26} m^2 and 5.75×10^{-26} m^2 for the all-H and core-D respectively are slightly lower than the range found for (0 Å, 10°) in Table 2. The experimental error at each temperature was estimated from the counting error in the intensity and the variation in

Table 1. Conformers of the 8CB molecule.

Conformer number	Conformer
1	
2	
3	
4	
5	

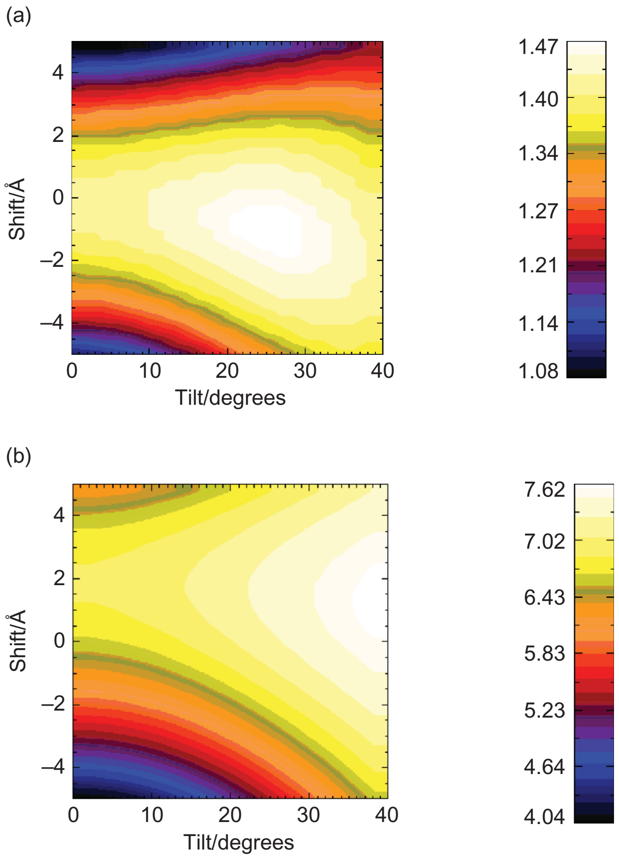


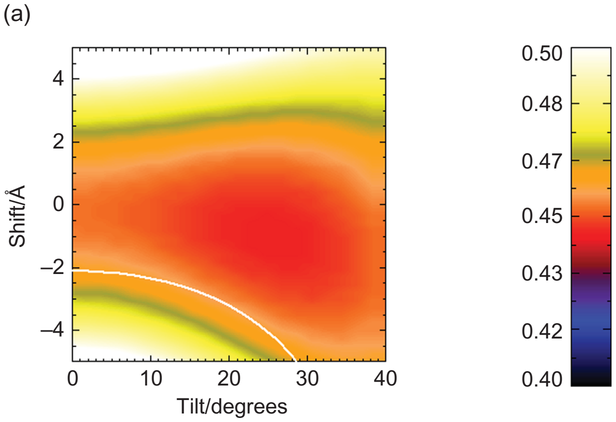
Figure 4. Molecular form factor squared for 8CB in units of 10^{-26} m^2 (a) from the all-H version and (b) from the core-D version of conformer 4.

the molecular form factor for a generous range of shift and tilt (–2.5 to 2.5 Å and 5 to 15°). Since the pairs of τ values for each temperature agreed within experimental error, the weighted average was taken and is shown in Figure 6. The figure shows that the translational order parameter decreases gradually with increasing temperature in the smectic phase.

In the nematic phase, this method gives a non-zero value because of the smectic A-like short-range order in 8CB. The main change on transforming from the smectic A to the nematic phase is a broadening of the peaks due to the finite range of correlation. The broadening does not influence the integrated intensity of the layer reflections and so values for the translational order parameter can be calculated. However, the translational order parameter of a nematic phase is zero, by definition, and these values only reflect the amplitude of the local density wave in the nematic. It can be seen in Figure 6 that the amplitude of the density wave changes very little at the transition from the smectic phase and begins to decrease with temperature in the nematic phase.

Table 2. Squared molecular form factors calculated for a shift of 0 Å and a tilt of 10° for different conformers (see Table 1).

	All-H		Core-D	
Conformer number	$\|M\|^2 10^{-26}$ m^2	% Deviation from average	$\|M\|^2 10^{-26}$ m^2	% Deviation from average
1	1.47	2.89	6.61	3.42
2	1.43	0.57	6.34	0.79
3	1.38	3.05	6.01	6.34
4	1.43	0.61	6.72	4.94
5	1.41	1.21	6.26	2.03



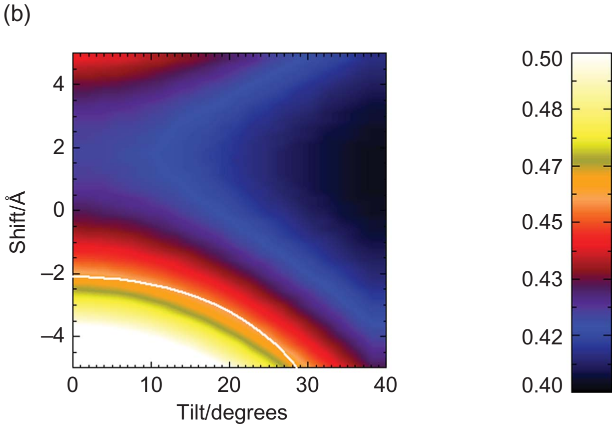


Figure 5. Order parameter, τ, for 8CB calculated from (a) the all-H version and (b) the core-D version of conformer 4. The line shows the combinations of shift and tilt for which τ is the same from both isotopomers.

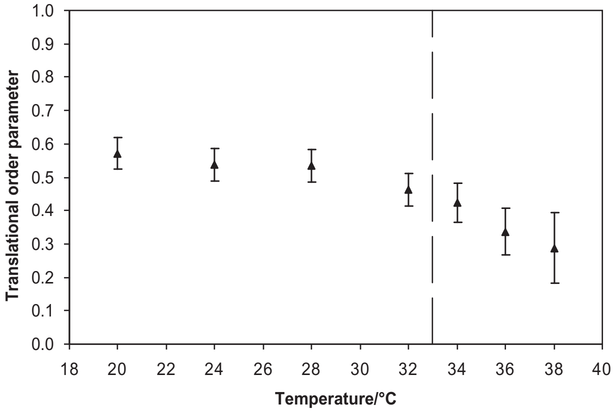


Figure 6. Translational order parameter determined for 8CB using the molecular form factor values for conformer 4 with a tilt of 10° and a shift of −2.5 Å. The weighted average has been taken of the all-H and core-D values. The vertical dashed line marks the smectic A-to-nematic transition temperature.

6. Discussion and conclusion

The value of $\tau = 0.46 \pm 0.05$ to 0.57 ± 0.05 in the smectic A phase may be compared with the results obtained by Leadbetter *et al.* [31]. They compared the relative intensities from differently deuteriated versions of 8CB to establish the overlapping cores dimer model and in the case of core-D 8CB they were able to measure first- and second-order reflections so the order parameter could be deduced [19]. In fact, they quoted the root mean square displacement of the molecules, $\sigma = 6.5$ Å. The corresponding order parameter can be evaluated from

$$\tau = \frac{1}{\sqrt{2\pi}\sigma} \int_{-d/2}^{d/2} \cos\left(\frac{2\pi z}{d}\right) \exp\left(\frac{-z^2}{2\sigma^2}\right) dz \qquad (15)$$

provided $\sigma << d$. Thus, their order parameter value is estimated to be 0.44, which is slightly lower than the values found in this work, but within experimental error near the transition to the nematic phase.

The value of τ for 8CB obtained from the Haller extrapolation method [20] is in the range 0.64 to 0.74. This appears to be significantly higher than the other values and suggests that the extrapolated value of the intensity may be too low.

The method described in this paper does give a robust estimate of the order parameter in 8CB. The main experimental uncertainty is in the effect of the preferred orientation in the powder. In future, alternative methods for producing a perfectly random powder will be explored. The actual scattering experiment is very simple to perform given the availability of SANS instrumentation that is able to measure intensity, routinely, on an absolute scale. The choice of molecules that form smectics with substrata of different scattering length density is the main requirement. This is not difficult to achieve. The formation of smectic phases is often driven by the tendency for aliphatic and aromatic regions of the molecules to microphase segregate. Since aliphatic regions will have a lower scattering length density than aromatic regions, the required strata form automatically. The contrast between the strata can also be enhanced by deuteriation of the aromatic moieties. For most molecules there will be scope for optimisation of the sensitivity to the translational order parameter by selective deuteriation. The aim would be to produce a labelled molecule so that the deuteriated sites form a stratum of about half the thickness of a perfectly ordered layer. The analysis is expected to work more simply for a SmA_1 phase rather than a SmA_d phase since there would be less ambiguity about the relative positions of the two molecules. The method should be widely applicable.

The method is offered as a simple way to measure the dominant translational order parameter in smectic liquid crystals. The choice of a single conformer is clearly a severe simplification that has been made so that the method is tractable for routine measurements. A more laborious but rigorous approach would be to compare the intensity calculated from an atomistic simulation with the experimental values [33]. A parameter controlling the segregation of aliphatic and aromatic parts could then be adjusted until agreement was reached and then the translational order parameter could be calculated.

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