A molecular model for the smectic B phase. The stabilized molecular rotor

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A molecular model for the smectic B phase
The stabilized molecular rotor

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Transition temperatures and smectic B mesophase ranges are examined for a number of homologous series, and some general rules are proposed that relate the smectic B phase behaviour to molecular structure. A mechanical model is developed for the crystal and hexatic smectic B phases, based on the dynamics of rigid or elastic rotors, which suggests two possible types of behaviour. It is found that such predicted behaviour is observed for particular series, but in general the smectic B phase characteristics of homologous series may be between the limits established for the model.

1. Introduction

A major objective for much liquid crystal research has been to relate the observation of particular liquid crystal phases to the structure of constituent molecules. While some progress has been made in the the prediction of nematic, smectic A and smectic C mesophases, the incidence of smectic B phases for particular molecular structures is still difficult to rationalize [1]. For most homologous series of mesogens, extending the length of a terminal n-alkyl or alkoxy chain increases the tendency to form smectic rather than nematic phases, and beyond a particular chain length the nematic properties are extinguished and the compounds are purely smectic. This behaviour is very general for S_A and S_C phases, but the appearance of S_B phases in a homologous series is much less regular. For example, p-n-alkoxybenzylidene-p-aminobenzoic acid ethyl esters [2] and 2-(4′-n-alkoxyphenyl)-5-(4-n-alkoxyphenyl)pyrazines [3] show smectic B phases for only a few members of those homologous series. Other examples are n-alkyl-4′-octyloxybiphenyl-4-carboxylates [4] and n-alkyl 4′-n-hexyloxybiphenyl-4-carboxylates [5]: smectic B phases only appear for the first members of the homologous series of the former, while they occur for most members of the latter series, but with very short temperature ranges. Clearly the relationship between the formation of smectic B phases and molecular structure is a very subtle matter.

In this paper we examine some homologous series of mesogens exhibiting smectic B phases. We propose some general rules which relate the persistence of smectic B phases to the molecular structures, and these rules are examined for both crystal smectic B and hexatic smectic B phases. The appearance and persistence of a smectic B phase is strongly related to the core structure, and for a particular homologous series, there is an optimum total chain length. The rules appear to apply generally for crystal smectic B phases, and to a lesser extent for hexatic B phases. In order to explain the relationship between the formation of smectic B phases and mesogenic structures, we propose a

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molecular model for the smectic B phase consisting of a restricted core rotor pivoted between layers by terminal substituents. A classical rotor model has previously been used [6] to explain molecular dynamics in rotator phases of molecular crystals.

2. Smectic B phase stability and molecular structure

The upper transition temperature of a smectic B phase provides a measure of its relative stability based on the internal energy of the phase, but the relative persistence of smectic B phases, defined as the difference between the high transition temperature of the phase and the melting temperature of the crystal to S_B phase (i.e. $T_{S_B} - T_{CRYST}$ $= \Delta T_{S_B}$) is also of interest. In attempting to make molecular structure correlations, the first problem is the critical dependence of smectic B phase persistence on the terminal alkyl chains. For molecules containing ester or thioester linkages, the total length of alkyl chain necessary to stabilize the smectic B phase increases in the following order of core structures:
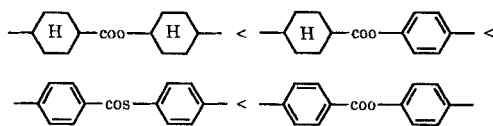
However, if the mesogens are without an ester or thioester core it is more difficult to identify any relationship between the nature of the core and the optimum total chain length necessary to maximize the tendency for smectic B phase formation. Since our proposed model for smectic B phases is a dynamic one, it is natural to attempt a correlation between phase behaviour and principal moments of inertia. A survey of literature results on the transition temperatures of various series of smectic B forming mesogens has revealed two limiting types of relationship between molecular structure and transition temperatures, which are illustrated in figure 1. In this figure the upper transition temperature T_{S_B} is plotted against the principal moment of inertia about the short axis for two selected groups of mesogens. There is a remarkable difference in behaviour between the two groups, yet we find that our proposed rotor model can predict both limiting types of behaviour. In reality, we believe that the observed behaviour of many smectic B forming series will be between these two limits. For the purposes of our model we classify S_B mesogenic molecules as either (i) elastic rotors or (ii) rigid rotors having an essentially rigid core. The precise definition of those two types will be given in the following section in the context of the mechanical rotor model, but it is more difficult to make a connection between actual molecular structures and rotor types. In this paper we give examples of the two types of behaviour, but our present understanding of the model is insufficient to allow us to categorize mesogens as rigid or elastic rotors: we can only identify the observed behaviour as conforming to one or other of the rotor types, or having features of both.

A survey of many other homologous series having S_B phases [7] confirms the following general observations concerning the occurrence of such phases:

(i)   The appearance and persistence of a S_B phase is strongly related to the core structure, and a proper core structure is a necessary condition for the formation of smectic B phases. It appears that the two types of molecular structures behave differently as far as the persistence of the S_B phases.

(ii) In a particular homologous series, there is an optimum total chain length for the maximum persistence, which in many cases corresponds to equal length alkyl chains at each end of the molecule.
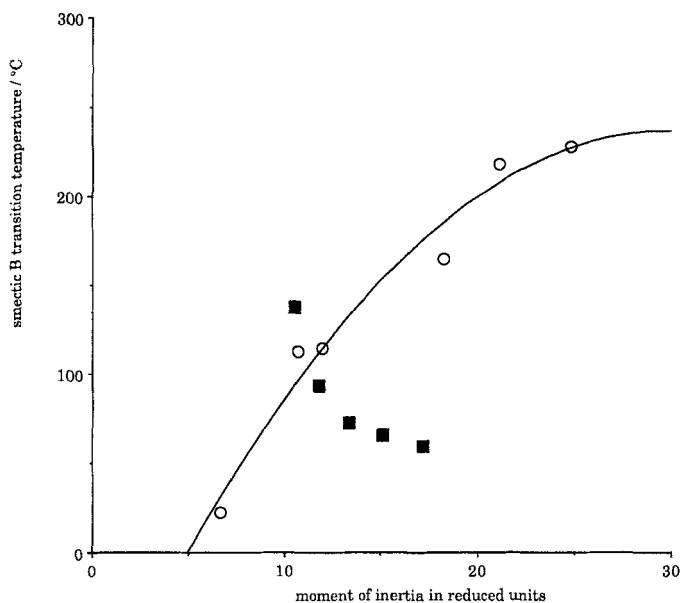
Figure 1. Smectic B transition temperature as a function of moment of inertia. ○, Cyclohexane-containing mesogens (see figure 2 for structures), ■, *n*-alkyl 4′-*n*-hexyloxybiphenyl-4-carboxylates (see figure 4 for structures).

3. The stabilized molecular rotor in a hexagonal array

The generally accepted model for the smectic B phase consists of hexagonal arrays of molecules which are rotating rapidly about their long axes. However, since the unit cell dimension of the hexagonal net is less than the width of the molecules, the rotation of molecules must be cooperative [8]. Also it has been shown [9, 10] that for a number of smectic B phases exhibited by the *N*-(4′-*n*-alkoxybenzylidene)-4-*n*-alkylanilines (*n*O.*m*s), the layers are arranged such that molecules in one particular layer are located in the interstices of adjacent layers. In order to maintain this inter-layer and intra-layer structure, the rotational axis of each molecule has to fit between the rotational axes for molecules in neighbouring layers. Thus the core should ideally be of uniaxial symmetry, with a symmetrical mass distribution around the rotor axis, while the terminal substituents will help to stabilize the molecular rotation within a layer. Examples of high core symmetry molecules with strong S_B persistence are 4′-(4-*n*-pentylcyclohexyl)-4′-(4-*n*-propylcyclohexyl)biphenyl [11], for which $\Delta T_{S_B} = 174°C$, and 4,4-diheptylter-cyclohexane [12] for which $\Delta T_{S_B} = 175°C$. A large moment of inertia about the rotation axis might be expected to stabilize the hexagonal packing within the layers and a clear example of this is provided by the comparison between 4-trifluoromethyl-*N*-(4-*n*-heptyloxybenzylidene)aniline [13] and its non-fluorinated equivalent [14]: the former has a large $\Delta T_{S_B} = 45·5°C$, while the latter only has a monotropic S_B phase.

The influence of terminal substituents on S_B phase stability is a rather subtle problem. We have already identified the importance of terminal alkyl or alkoxy chain length as well as the importance of the moment of inertia of the terminal substituent. The terminal substituents contribute to the S_B phase persistence both as the termination of the inertial axes of the molecular rotors, and as part of the bearing for the rotating axes of the rotors in the neighbouring layers. Before discussing a molecular

basis for the contribution of the terminal substituent to the S_B phase persistence, it is necessary to introduce a more quantitative model for the molecular rotors in the S_B phases.

4. Mechanics of a rotor and application to mesogenic molecules

The mechanics of a rotor and bearing are well established [15], and the essential dynamics of such systems can be described in terms of a simple cylindrical rotor. A rotor may have an eccentricity ε, which is the distance between the centre of the mass (G) and the rotation axis (see figure A 1 in the Appendix). In molecular terms this results for structures where the packing constraints in adjacent layers force the rotation axis not to pass through the centre of mass of the molecule. The centrifugal force $F = \varepsilon m \omega^2$ on G should be balanced by forces F and F' at the bearing, and so for a rigid rotor, the forces on the bearings increase quadratically with angular velocity (ω). For very rapid rotation, a rigid rotor may become catastrophically unstable either through breaking of the axis or destruction of the bearing. The situation is quite different for an elastic rotor, since there is an additional force from the elastic deformation of the rotor due to the rotation. As shown in the Appendix, the centre of the axis (S) executes a forced harmonic oscillation in the plane perpendicular to the line joining the centres of the bearings, and the elastic deformation of the axis ρ is given by

$$\rho = \varepsilon \eta^2 / (1 - \eta^2) \tag{1}$$

where, $\eta = \omega/\omega_n$, $\omega_n = (k/m)^{1/2}$, k is the bend elastic constant and m is the mass of the rotor. From equation (1), the amplitude is a function of the parameter ε as well as the rotational frequency of the rotor. In the limit $\eta \to 1$ (or $\omega \to \omega_n$), the amplitude of the forced oscillation goes to infinity. This represents a critical rotational state, and $\omega = \omega_n$ is the critical angular velocity (see figure A 2 in the Appendix). In the next section of this paper, the critical rotational state will be related to the catastrophe in the molecular rotation in the smectic B phase, which results in a thermal phase transition between the S_B phase and related high temperature phases such as smectic A and smectic C phases.

To apply the mechanical rotor model to mesophases, we adopt a single particle model such that intermolecular interactions and correlations are reduced to an effective potential acting on a single rotor. It is necessary to introduce concepts of internal and external damping which account respectively for internal energy transfer between rotational and vibrational modes and the effects of specific short range intermolecular forces. Damping by the environment will always attenuate the oscillations of the rotor (see equations (A 8) and (A 9)), and help to stabilize the rotation. For angular velocities below critical, internal damping will also reduce the amplitude of the forced oscillation of the rotor, but if the critical velocity has been exceeded then internal damping may enhance the unstable oscillation of the rotor axis.

4.1. The rigid molecular rotor

Within our mechanical model, the upper limit for the stability of the rigid rotor is independent of the parameters k and m: the stability is determined only by the stability of the bearings. The upper limit of the stability of the smectic B phase should depend on some molecular mechanism which destroys the cooperative rotation within the layer. In figure 2 for rigid molecular rotors, a linear relationship is identified between the upper S_B phase transition temperature T_{S_B} and the fourth power of the molecular length. These molecules have linear directly-coupled polycyclic structures; consideration of lath-like molecules such as terphenyls is deferred until § 5.
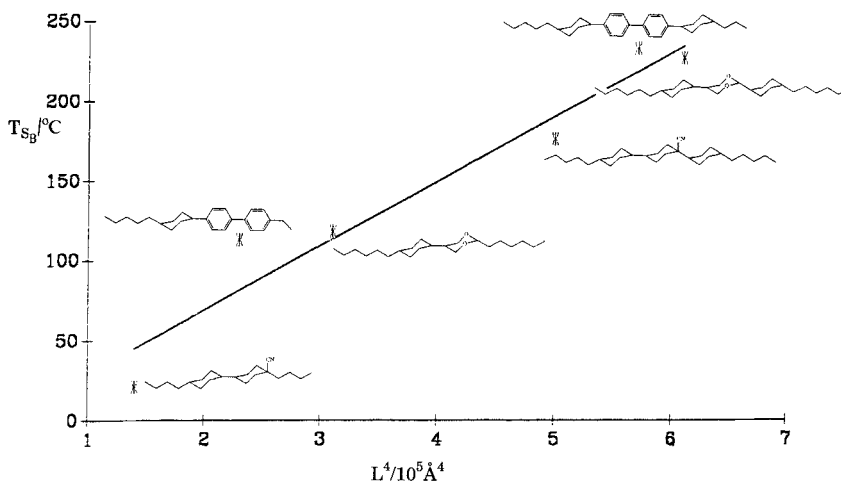
Figure 2. Smectic B transition temperatures as a function of the fourth power of the molecular length.

The correlation noted above may be explained in the following way. Disruption of the S_B phase occurs when the coupled libration of the rigid core and the vibration of the terminal chains exceeds some critical frequency (see figure 3). We further assert that the critical librational frequency is proportional to the length of the molecule, justified as follows. For a given temperature the rotational energy is proportional to $k_B T$, and if this temperature corresponds to the critical frequency ω_c, then the critical librational energy will be proportional to $\frac{1}{2} I \omega_c^2$. Since for a rigid rod of length L and mass m, the moment of inertia is $I = \frac{1}{24} m L^2$, the critical librational energy becomes proportional to $L^2 \omega_c^2$. Doubling the length of a molecule while keeping the mass constant, will halve the librational frequency ($\omega' = \frac{1}{2}\omega_c$), assuming that the temperature is the same, and the libration of the core is no longer critical. The original critical frequency ω_c is only a function of the termination of the rotor, and for the librational frequency of the elongated molecule to match this, it must be doubled.

On the basis of this model, the disruption of the S_B phase due to critical librational motion should happen at a temperature given by

$$k_B T_c = \text{const.}\, I \omega_c^2 + E_{\text{vib}}, \qquad (2)$$

where, k_B is Boltzmann's constant, I is the moment of inertia, and E_{vib} is the internal vibrational energy. Since ω_c is proportional to L, we obtain the experimentally observed result

$$T_c = aL^4 + b. \qquad (3)$$

Thus we conclude that the phase behaviour of some types of smectic B mesogenic molecules can be described by a rigid rotor model, and the transition to a higher temperature disordered phase is modelled by a catastrophic divergence of coupled motion of the librational motion of the molecule and the vibrational motion of the terminal chains which are anchored on the interstitial holes of the neighbouring layers.

4.2. Molecular elastic rotor

As we have described in the Appendix, the elastic rotor has the following characteristics:

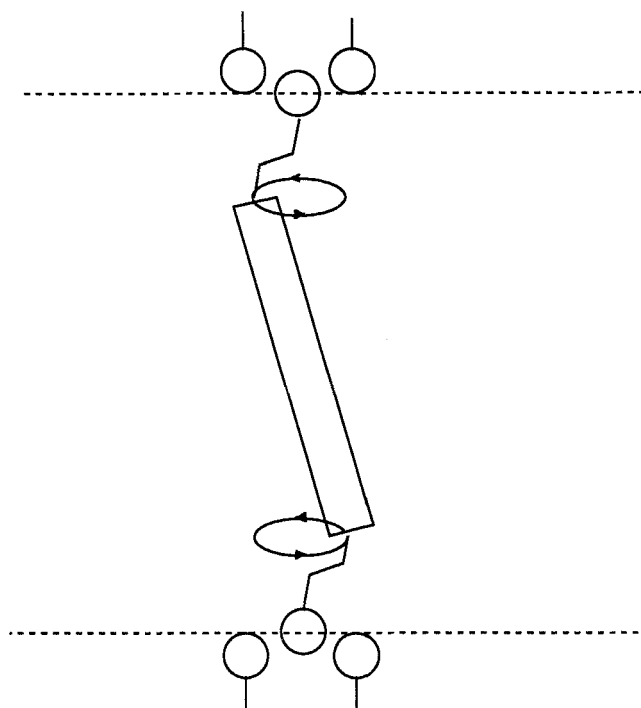$$\omega_n = (k/m)^{1/2} \qquad (4)$$

Figure 3.   Motion of a rigid rotor molecule: at critical frequency, core libration couples with chain vibration.

and

$$k = 48\gamma I'/(L^3), \tag{5}$$

where γ is Young's modulus, and I' is now the moment of inertia around the long axis. The simplest elastic rotor model for the S_B phase and its transition to a disordered phase is a system composed of the elastic rotor with rigid bearings. This simple model predicts that a catastrophe of rotational motion of the elastic rotor occurs when the rotational frequency equals the frequency of the forced oscillation of the axis in the plane perpendicular to the undisturbed rotation axis, i.e.

$$\omega_c = \omega_n. \tag{6}$$

Assuming again that the upper phase transition temperature is proportional to the critical rotational energy, and noting that the moment of inertia about the long axis is independent of molecular length, we find that for the elastic rotors

$$T_{S_B} = aL^{-3} + b. \tag{7}$$

The smectic B transition temperatures for the n-alkyl 4'-n-hexyloxybiphenyl-4-carboxylates are plotted as a function of molecular length in figure 4, and are in accordance with equation (7). The deviation observed for the homologues with longer terminal chains may be due to a reduction in the effective terminal chain length because of contributions from $gauche$ conformers.

   An important feature of the dynamics of molecular elastic rotors is internal damping associated with the flexible units in the core. Our model for internal damping is analogous to the Voigt model for polymer rheology. We propose that rotational to
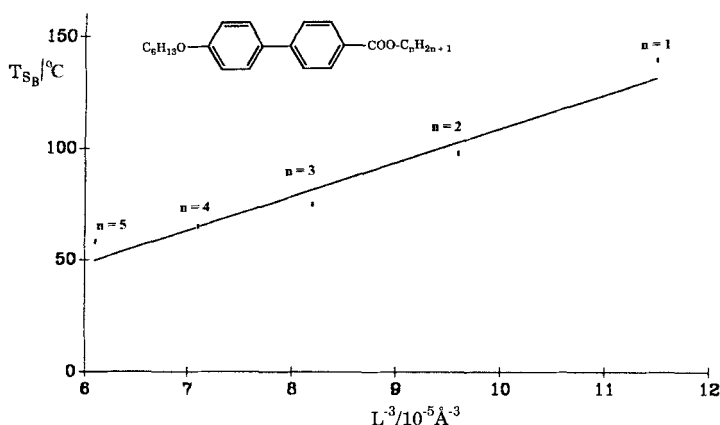
Figure 4.   Smectic B transition temperatures for *n*-alkyl 4'-*n*-hexyloxybiphenyl-4-carboxylates as a function of the inverse cube of the molecular length.

vibrational energy transfer, and subsequent vibrational relaxation through interaction with the environment provides a mechanism for internal damping of molecular rotation. Therefore molecules with linking ester or thioester groups may be able to undergo internal energy transfer which results in damping of molecular rotations in S_B phases. From equation (2), we can write

$$k_B(T_c - T_0) = \tfrac{1}{2} I \omega_c^2$$
$$= \frac{24 I'^2 \gamma}{L^3}, \qquad (8)$$

where the temperature range of the S_B phase is $(T_c - T_0)$, and $\omega_c = \omega_n \gg \omega_0$ are the corresponding rotational frequencies. It has been assumed that over relatively narrow temperature ranges $E_{vib} = E'_{vib}$. Equation (8) predicts that for an internally damped molecular rotor, the S_B phase persistence is proportional to L^{-3} (where L is the molecular length). In figure 5, we present results for molecules consisting of two rings linked by ester or thioester groups, and their S_B persistence $(T_c - T_0)$ varies with molecular length as predicted. For the series of *n*-alkyl 4'-*n*-hexyloxybiphenyl-4-carboxylates (see figure 4), it seems that homologues with shorter chains ($n < 5$) show a similar behaviour, but for longer chain homologues the coupling between the terminal chain vibration and molecular rotation may be less efficient.

5.   Molecular structure and the incidence of crystal smectic and hexatic smectic B phases

In this section we will summarize the experimental observations concerning the appearance of crystal smectic B and hexatic smectic B phases, and then consider the application of the mechanical rotor model to these phases. There are still relatively few results available on the characterization of hexatic and crystal smectic B phases for different homologous series [16], and so the molecular structural features responsible for the incidence of one or other of these phases have not been identified. From the limited number of materials that have been studied, we can conclude that the general rules (i) and (ii) noted earlier apply to crystal smectic B phases, but they are not obviously applicable to hexatic B phases. For example many members of the
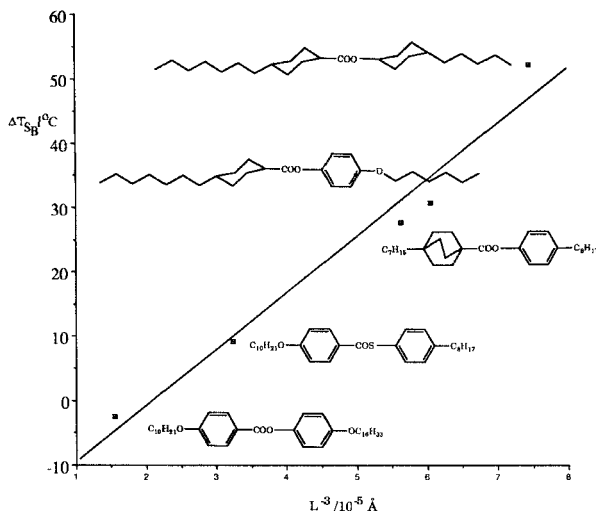
Figure 5. Smectic B persistence as a function of the inverse cube of the molecular length.

homologous series of 4-n-alkoxyphenyl 4'-n-octyloxybiphenyl-4-carboxylates [9] and 4-halophenyl 4'-octyloxybiphenyl-4-carboxylates [4] form hexatic B phases over short ranges of temperature, apparently independent of their chain length. Members of the homologous series of 4-propionyl-4'-n-alkanoyloxyazobenzenes [17] exhibit both crystal smectic and hexatic smectic B phases: the crystal B phase has its largest persistence for an alkyl chain length of $n = 6$ and disappears for $n = 8$, while hexatic B phases appear with similar persistence for homologues from $n = 5$ to $n = 8$ [17]. From this it can be inferred that for the appearance of a crystal B phase, the nature of the terminal chain is important, but is of less significance in determining the formation of hexatic B phases. This observation is in accord with the accepted understanding that in the crystal smectic B phase there are strong inter-layer correlations, which are absent in the corresponding hexatic phases [9]. Thus it is reasonable that the proposed general rules should be valid for the crystal B phases and less applicable to hexatic B phases.

In the previous section we proposed a mechanical model which could explain the variation of crystal smectic B phase transition temperatures with molecular length. Rule (i) refers to the importance of core structure, although it has different consequences for rigid and elastic molecular rotors. Rule (ii) may be explained if we assume that terminal chains act as rotor axes for the molecules. In order to suppress the crystal B phase, the molecular rotor should be elastic, and since the upper S_B transition temperature T_c depends on L^{-3}, longer molecules will tend to lose the crystal smectic B phase. Perhaps most importantly, interaction of the rotor with its neighbours (external damping) effectively suppresses the mechanical vibration of the rotor as described in the Appendix and hence stabilizes both smectic B phases. Reducing external attenuation, for example, replacing a bulky cyclohexane by a benzene ring, can result in the destabilization of the crystal smectic B and the appearance of a hexatic smectic B phase. In fact, most hexatic B phases are formed from substituted phenyl benzoates or alkyl biphenyl-carboxylates, so the ester linkage seems to be important for the existence of these phases.

One of the characteristics of the hexatic smectic B phases is their short mesophase temperature ranges. We will now propose a mechanical model for the hexatic smectic B

phase, which can explain the short mesophase range as well as providing an explanation for the reduced interlayer correlation. The basis for the model is the biaxial elastic rotor, having different elastic constants along two directions perpendicular to the local rotational axis. By analogy with the cylindrical rotor, two critical frequencies may now be defined corresponding to the two elastic constants $\omega_\zeta = (k_\zeta/m)^{1/2}$ and $\omega_\psi = (k_\psi/m)^{1/2}$. From the mechanical analysis of the biaxial rotor given in the Appendix, the differential equations of the motion have two solutions. The homogeneous solution corresponds to the free vibration of the rotor, while the other inhomogeneous solution describes an unbalanced forced oscillation. In this forced oscillation, the axis rotates while the rotor has a fixed bend, and there exist two critical angular velocities ω_ζ and ω_ψ. The correspondence of the hexatic smectic B phase to this mechanical model is that it represents the state between two critical frequencies (ω_ζ and ω_ψ) where the instability of the free oscillation results in decoupling of the terminal axes from their bearings; in other words the hexatic smectic B phase looses its inter-layer correlations. One of the origins for the instability of the free oscillation is the mechanical biaxiality of the molecular rotor as explained in the Appendix. Another source of the instability could be internal damping, especially when external damping due to molecular interactions are weak. Summarizing the conclusions of this biaxial model, we propose that for rotational frequencies (or equivalent temperatures) below ω_ζ the rotor is stable and conforms to a crystal smectic B phase or plastic crystal, while at higher temperatures ($\omega > \omega_\psi$) no unstable solutions can exist, and the corresponding phase is a disordered smectic (A or C). Between these limits the hexatic smectic B phase can exist in which the axes of coupled rotating molecules are no longer fixed by adjacent layers.

6. Conclusions

In this paper we have proposed a model for smectic B phases based on the idea that the molecules act as dynamically stabilized rotors within the layers. Concepts of internal and external damping have been applied to identify those features of the molecular structure which are responsible for the incidence of crystal smectic B or hexatic smectic B phases. It is concluded that the internal damping of biaxial elastic rotors strongly affects the dynamical stability of the rotors and this explains why, in the hexatic B phase, the long range hexagonal order within the layers of molecules is relatively small, and inter-layer interactions are minimized. Small changes of the temperature or pressure can disrupt the delicate balance of the external and internal damping, so the stability of the phase is limited. We have noted two empirical rules which apply to the dependence of smectic B phase stability on the structure of the constituent molecules. The importance of both the core structure and the nature of the terminal substituents has been identified, and the basis for the rules is discussed in the context of the molecular rotor model. It is proposed that crystal smectic B phases are stabilized by the terminal alkyl chains which can rotate in the interstices of the adjacent layers. The behaviour of such a system is explained by analogy with the dynamical model of a rotor and bearing. The properties of the rotor which influence its behaviour are whether it is rigid or elastic, and its principal moments of inertia. These mechanical concepts seem to apply at the molecular level and can account for some characteristics of smectic B phases; they may be applicable to other phases and phase transitions.

A. Appendix

Dynamics of an elastic rotor

In figure A 1 (b) an elastic rotor with a bent axis is illustrated; the original point O coincides with the centre of the rotor $S(y, z)$ when the axis has no bend; G is the centre of gravity, and the equation of the motion is:

and

$$
\left.
\begin{aligned}
m\frac{d^2 z_G}{dt^2} &= -kz \\[2em]
m\frac{d^2 y_G}{dt^2} &= -ky
\end{aligned}
\right\}
\tag{A 1}
$$

where $z_G = z + \varepsilon \cos \phi$, $y_G = y + \varepsilon \sin \phi$, and ε is the displacement of G from the rotation axis. For the point S, we have following inhomogeneous differential equations

and

$$
\left.
\begin{aligned}
\frac{d^2 z}{dt^2} + \omega_n^2 z &= \varepsilon\left(\frac{d\phi}{dt}\right)^2 \cos\phi + \varepsilon\frac{d^2\phi}{dt^2}\sin\phi \\[2em]
\frac{d^2 y}{dt^2} + \omega_n^2 y &= \varepsilon\left(\frac{d\phi}{dt}\right)^2 \sin\phi - \varepsilon\frac{d^2\phi}{dt^2}\cos\phi,
\end{aligned}
\right\}
\tag{A 2}
$$

where $\omega_n = (k/m)^{1/2}$, k is the stiffness for the bending of the rotor's axis and m is the mass of the rotor. To solve these differential equations under the condition of a stationary state reduces to solving the following equations

and

$$
\left.
\begin{aligned}
\frac{d^2 z}{dt^2} + \omega_n^2 z &= \varepsilon\omega^2 \cos(\omega t + \beta) \\[2em]
\frac{d^2 y}{dt^2} + \omega_n^2 y &= \varepsilon\omega^2 \sin(\omega t + \beta).
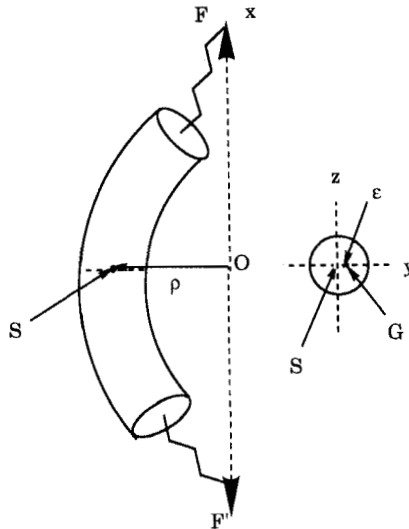\end{aligned}
\right\}
\tag{A 3}
$$

Figure A 1.   The elastic rotor: S is the centre of the rotor axis, G is the off-centre centre of gravity, F and F′ are the forces on the bearings, ε is the eccentricity of the rotor and ρ is the rotation-induced deformation of the rotation axis.

The solution of the above equations is given by a superposition of the general solution (z_1, y_1) for the homogeneous equations of equation (A 3) (i.e. setting the right hand sides equal to zero) and the particular solution (z_2, y_2) for the inhomogeneous equations as written. The general homogeneous solution is

and

$$
\left.
\begin{aligned}
z_1 &= a_{z0} \cos(\omega_n t + \delta_z) \\[2mm]
y_1 &= a_{y0} \sin(\omega_n t + \delta_y).
\end{aligned}
\right\}
\qquad (A\,4)
$$

This corresponds to free oscillation (vibration) of the rotor, while the inhomogenous solution is as follows:

and

$$
\left.
\begin{aligned}
z_2 &= \varepsilon \frac{\eta^2}{(1-\eta^2)} \cos(\omega t + \beta) \\[2mm]
y_2 &= \varepsilon \frac{\eta^2}{(1-\eta^2)} \sin(\omega t + \beta),
\end{aligned}
\right\}
\qquad (A\,5)
$$

where, $\eta = \omega/\omega_n$. This describes the motion of the centre of the axis S, which is a forced oscillation, the amplitude of which is proportional to the eccentricity ε, and is also a function of the rotational velocity of the axis ω. When $\eta \to 1$ ($\omega \to \omega_n$), the amplitude of the forced oscillation diverges to infinity and this is the critical rotational state for the elastic rotor (see figure A 2).
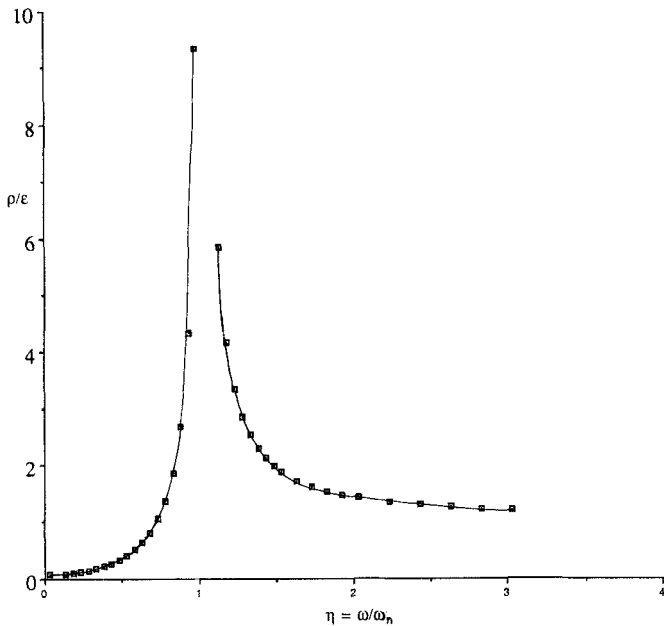

Figure A 2.   The elastic rotor: the displacement of the rotor axis as function of frequency.

The elastic rotor with external and internal damping

External damping

The rotor interacting with its environment generally feels frictional forces, for example due to local viscosity. To introduce these damping effects into the dynamics, extra terms linear in the velocity components are added to the left-hand sides of equation (A 3) giving:

$$m\frac{d^2z}{dt^2} + c_{ex}\frac{dz}{dt} + kz = m\varepsilon\omega^2\cos(\omega t + \beta)$$

and

$$m\frac{d^2y}{dt^2} + c_{ex}\frac{dy}{dt} + ky = m\varepsilon\omega^2\sin(\omega t + \beta),$$

$$(A\,6)$$

where c_{ex} is the proportionality constant for the external damping. The general solution of the above equation is quite similar in form to that for equation (A 3), i.e. the homogeneous solution; $r_1 = z_1 + iy_1$ plus the inhomogeneous solution $r_2 = z_2 + iy_2$. There is little interest in the homogenous solution (free oscillation) because it decays with time, i.e. it is overdamped. The particular solution which expresses the stationary motion after the damping of the free oscillation is

$$r_2 = \rho \exp i(\omega t + \beta),\qquad (A\,7)$$

with

$$\rho = \varepsilon \frac{\eta^2}{\{(1-\eta^2)+i2D_{ex}\eta\}},\qquad (A\,8)$$

where, $D_{ex} = c_{ex}/2m\omega_n$. In the stationary state, the orbital of the centre of the axis S is a circle of radius

$$|\rho| = \varepsilon \frac{\eta^2}{\{(1-\eta^2)^2 + 4D_{ex}^2\eta^2\}^{1/2}}.\qquad (A\,9)$$

The characteristics of the elastic rotor with external damping is that even at the critical frequency (ω_n), the displacement of the centre of the axis, i.e. the bending of the rotor axis, is limited to a maximum value of $\varepsilon(2D_{ex})^{-1}$.

Internal attenuation

For a macroscopic rotor with internal damping, the energy loss does not depend on the absolute velocity dz/dt, dy/dt of the centre of the axis S, but rather is proportional to the relative velocity $d\zeta/dt$, $d\psi/dt$ where ζ and ψ are the coordinates of the centre of the axis in a rotating frame. The equation of the motion is as follows:

$$\frac{d^2\zeta}{dt^2} - 2\omega\frac{d\zeta}{dt} + (c_i/m)\frac{d\zeta}{dt} + (\omega_n^2 - \omega^2) = \varepsilon\omega^2\cos\beta$$

and

$$\frac{d^2\psi}{dt^2} + 2\omega\frac{d\psi}{dt} + (c_i/m)\frac{d\psi}{dt} + (\omega_n^2 - \omega^2) = \varepsilon\omega^2\sin\beta,$$

$$(A\,10)$$

where c_i is the coefficient of internal damping. The important conclusion from this is that the homogeneous solution diverges to infinity when $\omega \to \omega_n$.

Coexisting external and internal damping

The equations of motion for a rotor experiencing both external and internal damping can be written down and solved, but here we will refer only qualitatively to the important conclusions. External damping stabilizes the rotor for all angular velocities, even at the critical frequency ω_n. On the other hand, the internal damping can cause an instability in the region $\omega > \omega_n$. If both external and internal damping are present there can be competitive effects, and the resultant behaviour depends on the precise conditions. For the homogeneous solution, if $D_{ex} > D_i (D_i = c_i/2m\omega_n)$, internal damping cannot cause instability, but if the external damping is negligibly small, even a small internal attenuation can cause instability at and above the critical velocity.

The biaxial elastic rotor

For a mechanically biaxial rotor, the stiffness or elastic constants for the bending of the rotor axis are different for the ζ and ψ directions, and are defined as k_ζ and k_ψ respectively $(k_\zeta < k_\psi)$, the corresponding critical rotational frequencies are

$$\omega_\zeta = (k_\zeta/m)^{1/2}, \quad \omega_\psi = (k_\psi/m)^{1/2} \tag{A 11}$$

and

$$\omega_n^2 = (k_\zeta + k_\psi)/2m. \tag{A 12}$$

By introducing biaxiality, the general solution of the homogeneous equation (free oscillation) may now become unstable in the region $\omega_\zeta < \omega < \omega_\psi$. This solution corresponds to motion of the centre of the axis S along a line in the rotating coordinate system, exponentially with time. This is the significant result of the unstable solution of the homogeneous equation, and represents the coupling of a Coriolis force with biaxility.

The inhomogenous solution for the biaxial rotor corresponding to a forced oscillation is similar to the uniaxial rotor, but has two critical angular velocities defined as

$$\omega_\zeta = \omega_n(1 - \mu)$$

and $\tag{A 14}$

$$\omega_\psi = \omega_n(1 - \mu)$$

where

$$\mu = \frac{(k_\psi - k_\zeta)}{(k_\zeta + k_\psi)} \tag{A 15}$$

and the parameter μ expresses the deviation from axial symmetry. Between the two critical frequencies, the stability depends on the biaxiality and the internal damping.

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