

# **7: Definitions of Basic Terms Relating to Low-Molar-Mass and Polymer Liquid Crystals**

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## **1 PREAMBLE**

This document provides definitions of the basic terms that are widely used in the field of liquid crystals and in polymer science (See references 1-39). It is the first publication of the Commission on Macromolecular Nomenclature dealing specifically with liquid crystals.

The recommendations made, resulting from the joint effort of the IUPAC Commission IV.1 Working Party and members of the International Liquid Crystal Society, are concerned with terminology relating to low-molar-mass and liquid-crystal polymers. Since much of the terminology is common to both classes of liquid crystals, this document has not been divided into sections dealing separately with these two classes of substances. After some general definitions (Section 2), there are sections dealing successively with the structures and optical textures of liquid crystals (Sections 3 and 4), their physical characteristics (including electro-optical and magneto-optical properties) (Section 5) and finally liquid-crystal polymers (Section 6). An alphabetical index of terms and a glossary of recommended symbols are provided for the convenience of the reader.

Implied definitions, occurring in Notes to the main definitions, are indicated by using bold type for the terms so defined.

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# TERMINOLOGY

## 2 GENERAL DEFINITIONS

### 2.1 mesomorphic state

#### mesomorphous state

State of matter in which the degree of molecular order is intermediate between the perfect three-dimensional, long-range positional and orientational order found in solid crystals and the absence of long-range order found in isotropic liquids, gases and amorphous solids.

Note 1: The term mesomorphic state has a more general meaning than *liquid-crystal state*, but the two are often used as synonyms.

Note 2: The term is used to describe orientationally disordered crystals, crystals with molecules in random conformations (i.e., conformationally disordered crystals), plastic crystals and *liquid crystals*.

Note 3: A compound which can exist in a mesomorphic state is usually called a *mesomorphic compound*.

Note 4: A vitrified substance in the mesomorphic state is called a **mesomorphic glass** and is obtained, for example, by rapid quenching or by crosslinking.

### 2.2 liquid-crystal state (LC state)

#### liquid-crystalline state

*Mesomorphic state* having long-range orientational order and either partial positional order or complete positional disorder.

Note 1: In a LC state, a substance combines the properties of a liquid (e.g., flow, ability to form droplets) and a crystalline solid (e.g., anisotropy of some physical properties).

Note 2: A LC state occurs between the crystalline solid and the isotropic liquid states on varying, for example, the temperature.

#### 2.2.1 liquid-crystalline phase (LC phase)

Phase occurring over a definite temperature range within the *LC state*.

### 2.3 liquid crystal (LC)

Substance in the *LC state*.

Note: A pronounced anisotropy in the shapes and interactions of molecules, or molecular aggregates is necessary for the formation of liquid crystals.

### 2.4 mesophase

Phase occurring over a definite range of temperature, pressure or concentration within the *mesomorphic state*.

#### 2.4.1 enantiotropic mesophase

*Mesophase* that is thermodynamically stable over a definite temperature or pressure range.

Note: The range of thermal stability of an enantiotropic mesophase is limited by the melting point and the *clearing point* of an *LC* compound or by any two successive *mesophase* transitions.

#### 2.4.2 thermotropic mesophase

*Mesophase* formed by heating a solid or cooling an isotropic liquid, or by heating or cooling a thermodynamically stable *mesophase* at constant pressure.

Note 1: The adjective ‘thermotropic’ describes a change of phase with a change of temperature. ‘Thermotropic’ may also be used to qualify types of *mesophase* (e.g., thermotropic *nematic*).

Note 2: Analogous changes can also occur on varying the pressure at constant temperature in which case the *mesophase* may be termed **barotropic mesophase**.

#### **2.4.3 lyotropic mesophase**

*Mesophase* formed by dissolving an amphiphilic *mesogen* in a suitable solvent, under appropriate conditions of concentration, temperature and pressure.

Note 1: The essential feature of a lyotropic liquid crystal is the formation of molecular aggregates or micelles as a result of specific interactions involving the molecules of the *amphiphilic mesogen* and those of the solvent.

Note 2: The mesomorphic character of a lyotropic mesophase arises from the extended, ordered arrangement of the solvent-induced micelles. Hence, such mesophases should be regarded as based not on the structural arrangement of individual molecules (as in a non-amphiphilic or a *thermotropic mesophase*), but on the arrangement within multimolecular *domains*.

#### **2.4.4 amphitropic compound**

Compound that can exhibit *thermotropic* as well as *lyotropic mesophases*.

Note: Examples are potassium salts of unbranched alkanoic acids, lecithin, certain polyisocyanates, cellulose derivatives with side-chains, such as (2-hydroxypropyl)cellulose, and cyanobiphenyl derivatives of alkyl(triethyl)ammonium bromide.

#### **2.4.5 monotropic mesophase**

Metastable *mesophase* that can be formed by supercooling an isotropic liquid or an *enantiotropic mesophase* at a given pressure to a temperature below the melting point of the crystal.

Note: Monotropic *transition temperatures* are indicated by placing parentheses, (), around the values.

### **2.5 transition temperature, $T_{XY}$ , SI Unit: K**

Temperature at which the transition from *mesophase X* to *mesophase Y* occurs.

Note: *Mesophase X* should be stable at lower temperatures than phase *Y*. For example, the *nematic-isotropic* transition temperature would be denoted as  $T_{NI}$ .

### **2.6 clearing point, $T_{cl}$ or $T_i$ , SI Unit: K**

#### **clearing temperature**

#### **isotropization temperature**

Temperature at which the transition between the *mesophase* with the highest temperature range and the isotropic phase occurs.

Note: The term should only be used when the identity of the *mesophase* preceding the isotropic phase is unknown.

### **2.7 virtual transition temperature**

*Transition temperature* that cannot be measured directly, determined by extrapolation of transition lines in binary phase diagrams to 100% of that particular component.

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Note 1: A virtual *transition temperature* lies outside the temperature range over which the (meso) phase implied can be observed experimentally.

Note 2: A virtual *transition temperature* is not well defined; it will, for example, depend on the nature of the liquid-crystal components used to construct the phase diagram.

Note 3: A virtual *transition temperature* is indicated by placing square brackets, [ ], around its value.

### 2.8 transitional entropy, $\Delta_{XY}S$ , SI Unit: $J K^{-1} mol^{-1}$

Change in entropy on transition from phase X to phase Y.

Note 1: The transitional entropy reflects the change in order, both orientational and translational, at the phase transition.

Note 2: Phase X should be stable at lower temperatures than phase Y.

Note 3: Numerical values of the molar entropy of transition should be given as the dimensionless quantity  $\Delta_{XY}S/R$  where  $R$  is the gas constant.

### 2.9 divergence temperature, $T^*$ , SI Unit: K

#### pre-transitional temperature

Temperature at which the orientational correlations in an isotropic phase diverge.

Note 1: The divergence temperature is the lowest limit of metastable supercooling of the isotropic phase.

Note 2: The divergence occurs at the point where the isotropic phase would be expected to undergo a second-order transition to the liquid-crystal phase, were it not for the intervention of a first-order transition to the liquid-crystal phase.

Note 3: The divergence temperature for nematogens can be measured by using the Kerr effect or Cotton-Mouton effect or by light-scattering experiments.

Note 4:  $T^*$  occurs below the clearing temperature, usually by about 1 K in isotropic-to-nematic transitions and increases to at least 10 K for isotropic-to-smectic transitions.

### 2.10 mesogenic group

#### mesogenic unit

#### mesogenic moiety

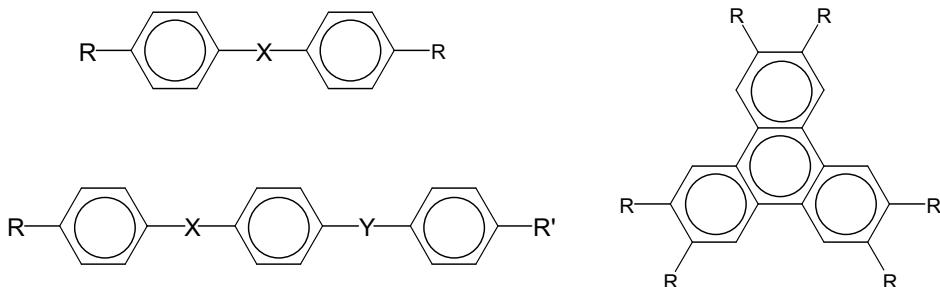
Part of a molecule or macromolecule endowed with sufficient anisotropy in both attractive and repulsive forces to contribute strongly to *LC mesophase*, or, in particular, to *LC mesophase* formation in low-molar-mass and polymeric substances.

Note 1: ‘*Mesogenic*’ is an adjective that in the present document applies to molecular moieties that are structurally compatible with the formation of *LC phases* in the molecular system in which they exist.

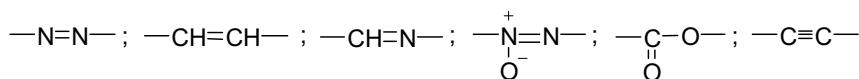
Note 2: *Mesogenic* groups occur in both low-molar-mass and polymeric compounds.

Note 3: The majority of *mesogenic* groups consist of rigid rod-like or disc-like molecular moieties.

*Examples*



Where R and R' are alkyl groups and X and Y are divalent linking units such as:



## 2.11 mesogen

**mesogenic compound**

**mesomorphic compound**

Compound that under suitable conditions of temperature, pressure and concentration can exist as a *mesophase*, or, in particular as a *LC phase*.

Note 1: When the type of *mesophase* formed is known, more precisely qualifying terminology can be used, e.g., **nematogen**, **smectogen** and **chiral nematogen**.

Note 2: When more than one type of *mesophase* can be formed, more than one qualification could apply to the same compound and then the general term mesogen should be used.

### 2.11.1 amphiphilic mesogen

*Mesogen* composed of molecules consisting of two parts of contrasting character that are hydrophilic and hydrophobic or lipophobic and lipophilic.

Note 1: Examples of amphiphilic mesogens are soaps, detergents and some block copolymers.

Note 2: Under suitable conditions of temperature and concentration, the similar parts of amphiphilic molecules cluster together to form aggregates or micelles.

### 2.11.2 non-amphiphilic mesogen

*Mesogen* that is not of the amphiphilic type.

Note 1: At one time it was thought that a non-amphiphilic molecule had to be long and rod-like for *mesophase* formation, but it has now been established that molecules of other types and shapes, for example, disc-like and banana-shaped molecules, may also form *mesophases*. (See ref. 6).

Note 2: A selection of the types of non-amphiphilic *mesogens* is given in Definitions 2.11.2.1-2.11.2.8.

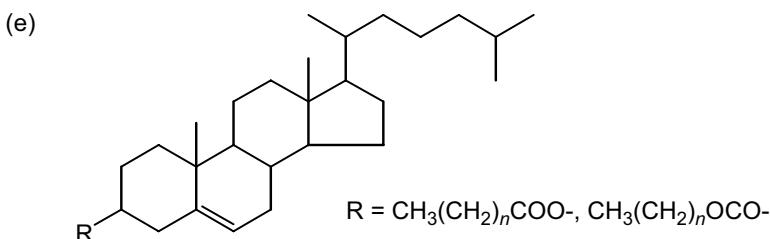
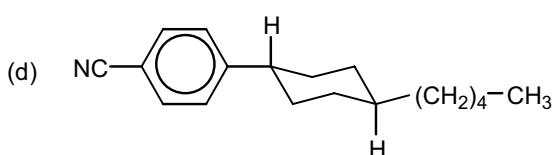
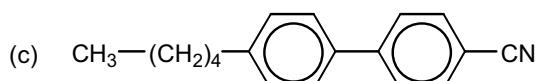
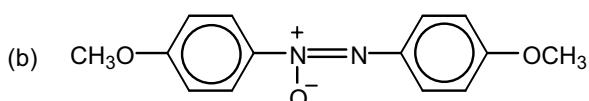
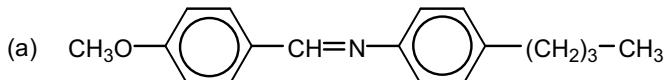
#### 2.11.2.1 calamitic mesogen

*Mesogen* composed of rod-like or lath-like molecules.

Note: Examples are:

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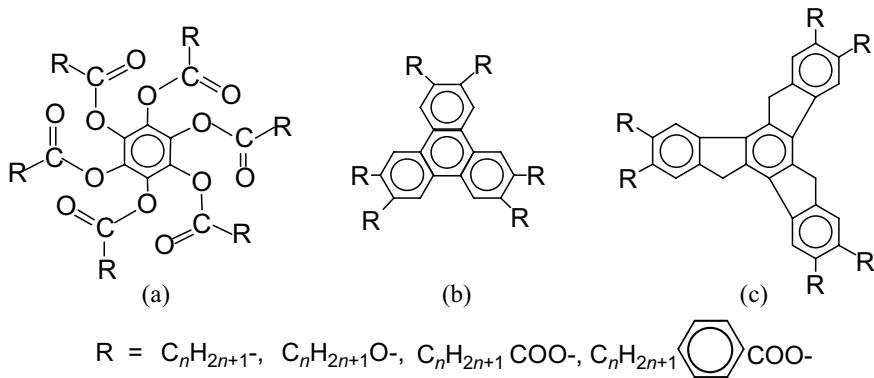
- 4-butyl-*N*-(4-methoxybenzylidene)aniline (BMBA) (a)
  - 4,4'-dimethoxyazoxybenzene (b)
  - 4'-pentylbiphenyl-4-carbonitrile (c)
  - 4-(*trans*-4-pentylcyclohexyl)benzonitrile (d)
  - cholesterol esters and esters of cholest-5-ene-3-carboxylic acid (e).



### **2.11.2.2 discotic mesogen discoid mesogen**

*Mesogen* composed of relatively flat, disc- or sheet-shaped molecules.

Note 1: Examples are: hexakis(acyloxy)benzenes (a), hexakis(acyloxy)- and hexakis(alkoxy)-triphenylenes (b), 5H,10H,15H-diindeno[1,2-*a*:1',2'-*c*]fluorene derivatives (c).



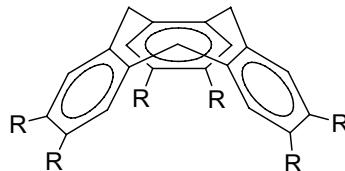
Note 2: The adjective ‘discotic’ is also employed to describe the *nematic mesophases* formed by discotic *mesogens*. The *mesophases* formed by a columnar stacking of disc-like molecules are described as *columnar mesophases*.

### 2.11.2.3 pyramidal mesogen

#### conical or cone-shaped mesogen bowlic mesogen

*Mesogen* composed of molecules containing a semi-rigid conical core.

Note: Examples are hexasubstituted 5*H*,10*H*,15*H*-tribenzo[*a,d,g*][9]annulenes.



### 2.11.2.4 sanidic mesogen

*Mesogen* composed of board-like molecules with the long-range orientational order of the phase reflecting the symmetry of the constituent molecules.

Note: See also Definition 3.4.

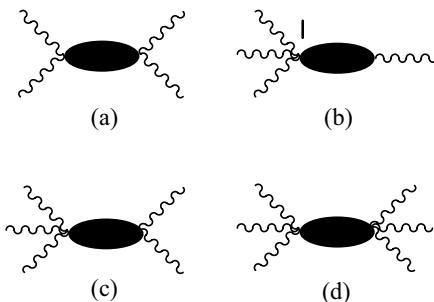
### 2.11.2.5 polycatenary mesogen

*Mesogen* composed of molecules each having an elongated rigid core with several flexible chains attached to the end(s).

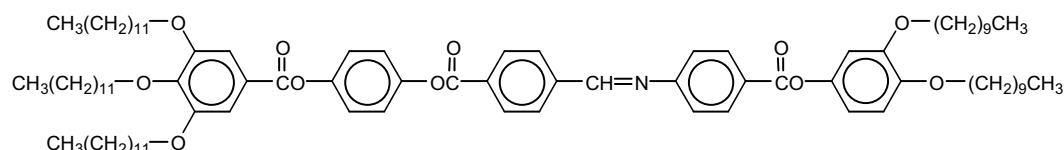
Note 1: The flexible chains are usually aliphatic.

Note 2: The numbers of flexible chains at the ends of the core can be indicated by using the term *m,n*-polycatenary *mesogen*.

Note 3: There exist several descriptive names for these *mesogens*. Examples are: (a) biforked *mesogen* (2,2-polycatenary *mesogen*), (b) hemiphasmidic *mesogen* (3,1-polycatenary *mesogen*), (c) forked hemiphasmidic *mesogen* (3,2-polycatenary *mesogen*) and (d) phasmidic *mesogen* (3,3-polycatenary *mesogen*). Examples of each type with the core represented by [REDACTED] are given together with a specific example of a forked hemiphasmidic *mesogen* (c).



a specific example is:

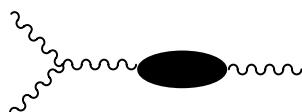


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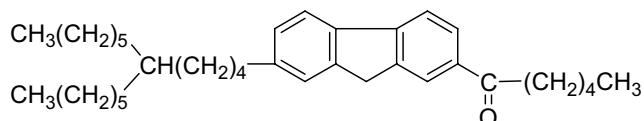
### 2.11.2.6 swallow-tailed mesogen

*Mesogen* composed of molecules each with an elongated rigid core with, at one end, a branched flexible chain, having branches of about the same length.

Note: A sketch of the structure of a swallow-tailed *mesogen* is



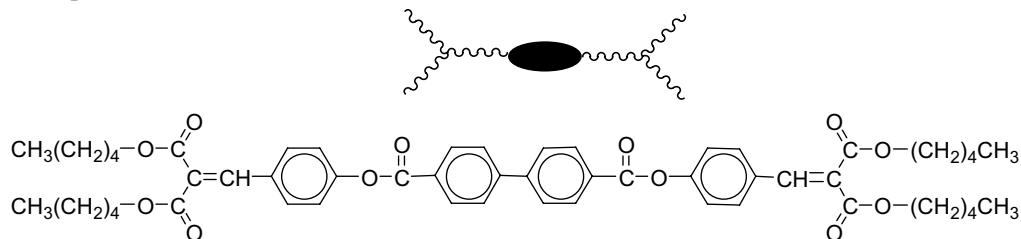
and an example is the fluorene derivative



### 2.11.2.7 bis-swallow-tailed mesogen

*Mesogen* composed of molecules each with an elongated rigid core and a branched flexible chain, with branches of about the same length, attached at each end.

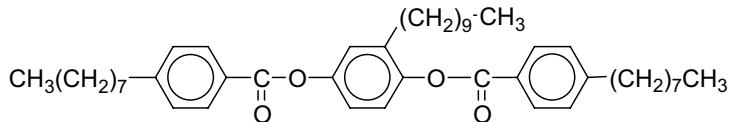
Example:



### 2.11.2.8 laterally branched mesogen

*Mesogen* composed of rod-like molecules with large lateral branches such as alkyl, alkoxy or ring-containing moieties.

Example:



### 2.11.2.9 liquid-crystal oligomer mesogenic oligomer

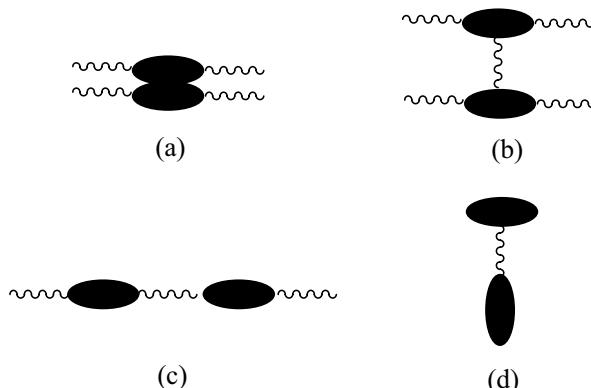
*Mesogen* constituted of molecules, each with more than one *mesogenic group*.

Note 1: The *mesogenic groups* usually have identical structures.

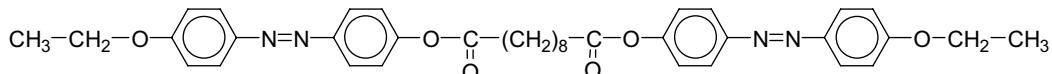
Note 2: A liquid-crystal dimer or *mesogenic dimer* is sometimes known as a twin *mesogen*. Use of the terms ‘dimesogenic compounds’ and ‘Siamese-twin *mesogen*’ for **liquid-crystal dimer** or **mesogenic dimer** is not recommended.

Note 3: Examples of *mesogenic dimers* are: (a) fused twin *mesogen*, where the *mesogenic groups* are linked rigidly by a (usually fused) ring system, (b) ligated twin *mesogen*, in

which the *mesogenic groups* are connected by a *spacer* at a central position, (c) tail-to-tail twin *mesogen*, which has a flexible *spacer* linking the two groups and (d) side-to-tail twin *mesogen*. The structures of these different types of liquid-crystal dimers are illustrated with the *mesogenic groups* represented by .



A specific example of type (c), a tail-to-tail liquid-crystal dimer, is



wherein  $-(\text{CH}_2)_8-$  is the flexible *spacer* linking the two *mesogenic groups*.

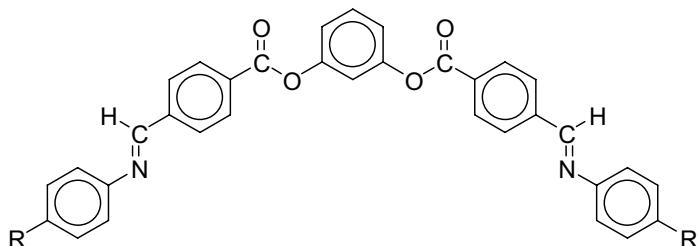
Note 4: A liquid-crystal dimer with different *mesogenic groups* linked by a *spacer* is known as an **asymmetric liquid-crystal dimer**.

Note 5: A liquid-crystal dimer with flexible hydrocarbon chains having an odd number of carbon atoms is called an **odd-membered liquid-crystal dimer**, whilst one with hydrocarbon chains having an even number of carbon atoms is called an **even-membered liquid-crystal dimer**.

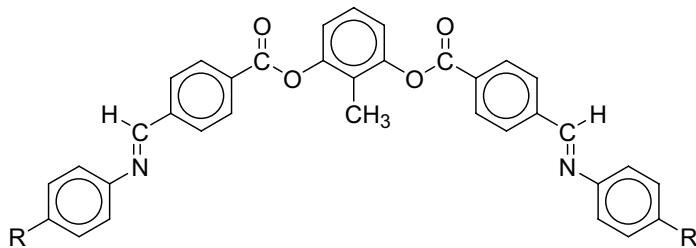
#### 2.11.2.10 banana mesogen

*Mesogen* constituted of bent or so-called banana-shaped molecules in which two *mesogenic groups* are linked through a semi-rigid group in such a way as not to be co-linear.

Note: Examples of such structures are:



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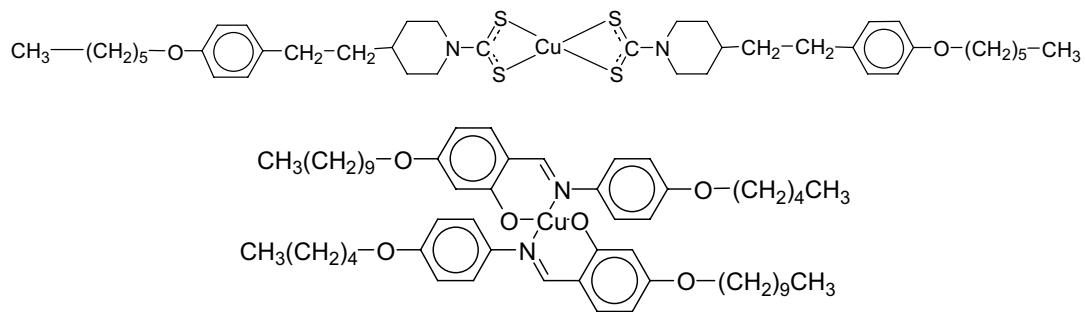
with the substituent R being an unbranched alkoxy group, ( $-O-C_nH_{2n+1}$ ).

### 2.11.3 metallomesogen

*Mesogen* composed of molecules incorporating one or more metal atoms.

Note: Metallomesogens may be either *calamitic* or *discotic mesogens*.

Examples



## 3 TYPES OF MESOPHASE

### 3.1 mesophases of calamitic mesogens

#### 3.1.1 uniaxial nematic mesophase, N or $N_u$ nematic

*Mesophase* formed by a non-chiral compound or by the racemate of a chiral compound in which the spatial distribution of the molecular centers of mass is devoid of long-range positional order and the molecules are, on average, orientationally ordered about a common axis defined as the *director* and represented by the unit vector  $\mathbf{n}$ .

Note 1: See Fig. 1 for an illustration of the molecular organization in a uniaxial nematic mesophase.

Note 2: The unit vector,  $\mathbf{n}$ , is defined in 3.1.1.1. (See also Fig. 1.)

Note 3: The direction of  $\mathbf{n}$  is usually arbitrary in space.

Note 4: The extent of the positional correlations for the molecules in a nematic phase is comparable to that of an isotropic phase although the distribution function is necessarily anisotropic.

Note 5: From a crystallographic point of view, the uniaxial nematic structure is characterised by the symbol  $D_{\infty h}$  in the Schoenflies notation ( $\infty/m\bar{m}$  in the International System).

Note 6: Since the majority of nematic phases are uniaxial, if no indication is given, a nematic phase is assumed to be uniaxial but, when there is the possibility of a biaxial as well a uniaxial nematic, a uniaxial phase should be denoted as  $N_u$ .

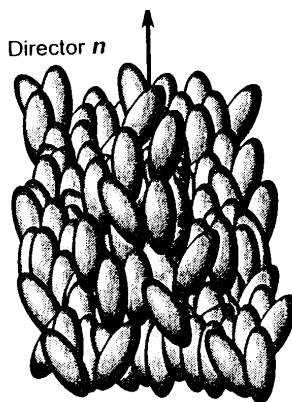
### 3.1.1.1 director, $n$

Local symmetry axis for the singlet, orientational distribution of the molecules of a *mesophase*.

Note 1: The *director* is defined as a unit vector, but directions  $+n$  and  $-n$  are arbitrary.

Note 2: In *uniaxial nematics*, formed by compounds consisting of either rod-like or disc-like molecules, the mean direction of the effective molecular symmetry axis coincides with the *director*.

Note 3: The *director* also coincides with a local symmetry axis of any directional property of the *mesophase*, such as the refractive index or magnetic susceptibility.

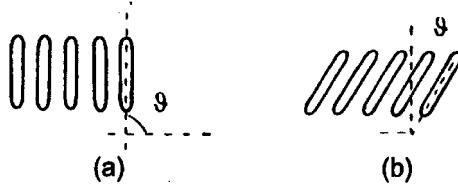


**Fig.1.** A representation of the molecular organization in a uniaxial nematic mesophase.

### 3.1.2 cybotactic groups

Assembly of molecules in a *nematic mesophase* having a short-range smectic-like array of the constituent molecules.

Note: Two types of short-range smectic-like structures are possible. One is analogous to a *smectic A mesophase* where the molecules tend to lie along a layer normal and the other is like a *smectic C mesophase* where the molecules tend to be oblique with respect to a layer normal. See Fig. 2 for illustrations of the molecular arrangements in the *smectic A* type structure and the *smectic C* type structure.



**Fig. 2.** Schematic representation of the molecules in (a) a smectic A-like local structure and (b) a smectic C-like local structure, making angle  $\theta$  with the layer normal.

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### 3.1.3 chiral nematic mesophase, N\*

**chiral nematic**  
**cholesteric mesophase**  
**cholesteric**

*Mesophase* with a helicoidal superstructure of the *director*, formed by *chiral, calamitic or discotic* molecules or by doping a *uniaxial nematic* host with chiral guest molecules in which the local *director **n*** precesses around a single axis.

See Fig. 3 for an illustration of the helicoidal molecular distribution in a chiral nematic mesophase.

Note 1: Locally, a chiral nematic mesophase is similar to a uniaxial nematic, except for the precession of the *director **n*** about the axis, Z.

Note 2: The *director* is periodic along Z with the pitch *P* of the helical structure equal to a turn of the local *director **n*** by  $2\pi$ .

Note 3: Chiral nematic mesophases exhibit Bragg scattering of circularly polarised light at a wavelength  $\lambda_R$  proportional to the pitch *P* ( $\lambda_R = \langle n \rangle P$ , where  $\langle n \rangle$  is the mean refractive index).

Note 4: The *director* precession in a chiral nematic mesophase is spontaneous and should be distinguished from an induced twisted structure produced by a mechanical twist of a *nematic mesophase* between confining surfaces.

Note 5: The term chiral nematic mesophase or chiral nematic is preferred to cholesteric mesophase or cholesteric.

### 3.1.4 blue phase, (BP)

*Mesophase* with a three-dimensional spatial distribution of helical *director* axes leading to frustrated structures with defects arranged on a lattice with cubic symmetry and lattice constants of the order of the wavelength of visible light.

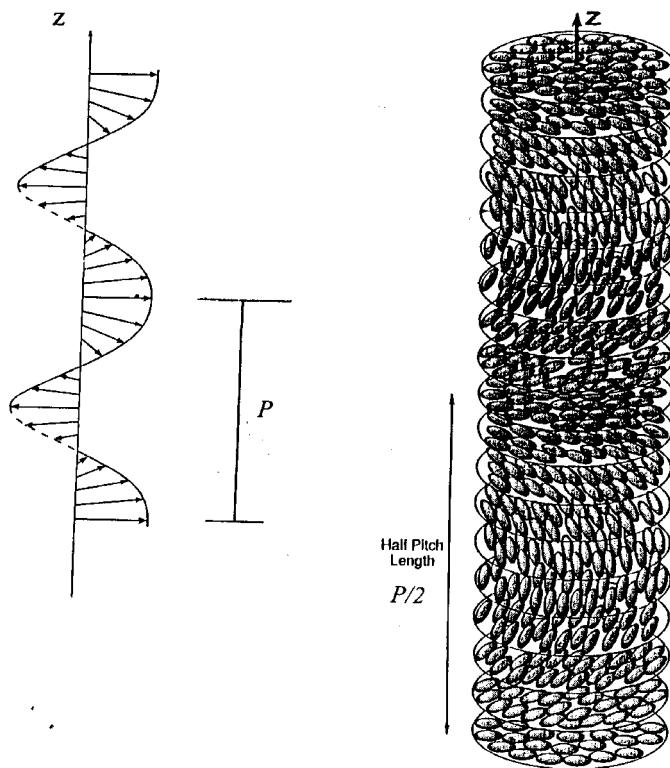
Note 1: See Fig. 4 for a possible model for a BP.

Note 2: The name ‘blue phase’ derives historically from the optical Bragg reflection of blue light but, because of larger lattice constants, BPs can reflect visible light of longer wavelengths.

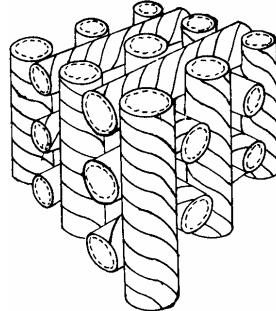
Note 3: With *chiral nematic* substances forming *chiral nematic mesophases* of short pitch (<700 nm), up to three blue phases occur in a narrow temperature range between the *chiral nematic* phase and the isotropic phase.

Note 4: A BP is optically isotropic and exhibits a Bragg reflection of circularly polarised light.

Note 5: Two BPs of different cubic symmetry (space group I 4<sub>1</sub>32 for BP I and P 4<sub>2</sub>32 for BP II) are presently known, together with a third (BPIII) of amorphous structure. Several other BPs of different cubic symmetry exist but only in the presence of external electric fields.



**Fig. 3.** Illustrating the structure of a chiral nematic mesophase.



**Fig. 4.** Illustrating a cubic lattice formed by double-twist cylinders as a possible model of a BP.

### 3.1.5 smectic mesophase, (Sm)

*Mesophase* that has the molecules arranged in layers with a well-defined layer spacing or periodicity.

Note 1: There are several types of smectic mesophases, characterised by a variety of molecular arrangements within the layers.

Note 2: Although the total number of smectic mesophases cannot be specified, the following types have been defined: SmA, SmB, SmC, SmF and SmI. The alphabetical order of suffixes merely indicates an order of discovery.

Note 3: The classification of SmD as smectic is largely a consequence of history, and should be discontinued (see Definition 3.1.9).

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Note 4: At one time, a number of *mesophases* were identified as smectic on the basis of their *optical textures*, but they are in fact soft crystals characterised by very low yield stresses. Hence, these three-dimensionally ordered phases should no longer be called smectic mesophases. They are akin to plastic crystals with some elementary long-range order and are referred to by the letters E, J, G, H, and K.

Note 5: Tilted smectic mesophases formed by chiral compounds or containing chiral mixtures are designated by the superindex <sup>\*</sup> (SmC<sup>\*</sup>, SmF<sup>\*</sup>, etc.). (See, for example, Definition 3.1.5.1.3.)

### 3.1.5.1 smectic mesophases with unstructured layers

#### 3.1.5.1.1 smectic A mesophase, (SmA)

*Smectic mesophase* involving a parallel arrangement of the molecules within layers in which the long axes of the molecules tend to be perpendicular to the layer planes and the molecular centers of mass have no long-range positional order parallel to the layer planes.

Note 1: See Fig. 5 for the molecular organization in a smectic A mesophase

Note 2: Each layer approximates to a true two-dimensional liquid. The system is optically uniaxial and the optic axis, Z, is normal to the layer planes.

Note 3: The directions +Z and -Z are interchangeable.

Note 4: The structure of a smectic A mesophase is characterised by the symbol D<sub>∞h</sub> in the Schoenflies notation ( $\infty$ , 2 in the International System).

Note 5: The *lyotropic* equivalent of a smectic A mesophase is known as a **lamellar mesophase**; where layers of amphiphilic molecules are separated by layers of solvent, normally water, or by oil in an **inverse lamellar mesophase**.

Note 6: A smectic A-phase containing a chiral molecule or dopant, can be called a chiral smectic A-phase. The recommended symbol is SmA<sup>\*</sup> wherein the (\*) indicates that the macroscopic structure of the *mesophase* is chiral.



Fig. 5. Illustrating the structure of a smectic A mesophase.

#### 3.1.5.1.2 smectic C mesophase, (SmC)

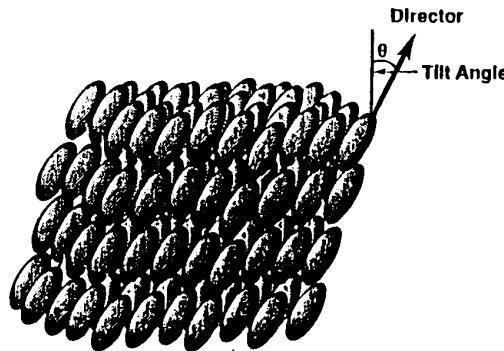
Analogue of a *smectic A mesophase* involving an approximately parallel arrangement of the molecules within layers in which the *director* is tilted with respect to the layer normal and the molecular centers-of-mass have no long-range positional order parallel to the layer planes (See Fig. 6).

Note 1: See Fig. 6 for an illustration of the molecular organization in a smectic C mesophase.

Note 2: The physical properties of a smectic C mesophase are those of a biaxial crystal.

Note 3: The smectic C structure corresponds to monoclinic symmetry characterised by the symbol  $C_{2h}$ , in the Schoenflies notation and the space group  $t\bar{2}/m$  in the International System.

Note 4: The tilt direction varies in a random manner from layer to layer in conventional smectic C *mesophases*. However it can alternate from layer to layer, as in an *antiferroelectric chiral smectic C mesophase* (see Definition 5.9, Note 7) and in the smectic C mesophase formed by certain liquid crystal dimers with an odd-number of carbon atoms in the *spacers*. The recommended symbol for this type of *mesophase* is SmCa.



**Fig. 6.** Illustrating the structure of the smectic C mesophase

### 3.1.5.1.3 chiral smectic C mesophase, (SmC<sup>\*</sup>)

*Smectic C mesophase* in which the tilt direction of the *director* in each successive layer is rotated through a certain angle relative to the preceding one so that a helical structure of a constant pitch is formed.

Note 1: See Fig. 7 for an illustration of the molecular organization in a chiral smectic C mesophase.

Note 2: The (\*) in SmC<sup>\*</sup> and analogous notations indicate, as in 3.1.5.1.2 (Note 6), that the macroscopic structure of the *mesophase* is chiral. However, it is also used simply to indicate that some of the constituent molecules are chiral even though the microscopic structure may not be.

Note 3: A SmC<sup>\*</sup> *mesophase* is formed by chiral compounds or mixtures containing chiral compounds.

Note 4: Locally, the structure of the chiral smectic C mesophase is essentially the same as that of the achiral smectic C mesophase except that there is a precession of the tilt direction about a single axis. It has the symmetry  $C_2$  in the Schoenflies notation.

Note 5: This chiral smectic C phase is also known as the *ferroelectric chiral smectic C phase*.

Note 6: The helix can be unwound by surface forces to give a surface-stabilised SmC<sup>\*</sup> which has a macroscopic polarization.

### 3.1.5.2 hexatic smectic mesophase

*Smectic mesophase* with in-plane short-range positional molecular order, weakly coupled two-dimensional layers and long-range bond orientational molecular order.

Note: There are three types of hexatic smectic mesophases: *smectic B* (SmB), *smectic F* (SmF) and *smectic I* (SmI). Here, the term ‘hexatic’ may be omitted because it is implicit for this group of *smectic mesophases*.

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### 3.1.5.2.1 smectic B mesophase, (SmB)

*Hexatic smectic mesophase* in which the *director* is perpendicular to the layers with the long-range hexagonal bond-orientational order.

Note 1: See Fig. 8 for an illustration of the molecular organization in a smectic B mesophase.

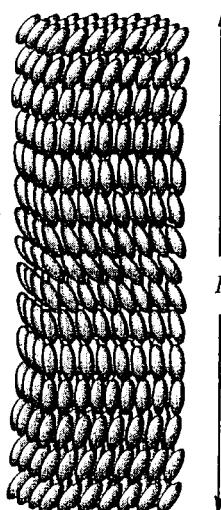
Note 2: Positional molecular order does not propagate over distances larger than a few tens of nanometers but bond orientational molecular order extends over macroscopic distances within and across layers.

Note 3: By contrast with a smectic B mesophase, a crystal B mesophase has correlations of positional order (hexagonal) in three dimensions, i.e., correlations of position occur within and between layers.

Note 4: The structure of a smectic B mesophase is characterised by a  $D_{6h}$  point group symmetry, in the Schoenflies notation, by virtue of the bond orientational order.

Note 5: A smectic B mesophase is optically uniaxial.

Note 6: A smectic B mesophase is sometimes denoted  $\text{SmB}_{\text{hex}}$ . The subscript ‘hex’ denotes the hexagonal structure of the *mesophase*.



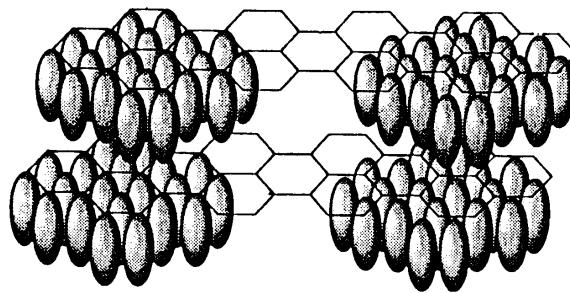
**Fig. 7.** Illustrating the structure of a chiral smectic C mesophase ( $P$  = helical pitch)

### 3.1.5.2.2 smectic F mesophase, (SmF)

*Hexatic smectic mesophase* the structure of which may be regarded as a C-centered monoclinic cell with a hexagonal packing of the molecules with the *director* tilted, with respect to the layer normals, towards the sides of the hexagons.

Note 1: See Fig. 9a for an illustration of the molecular organization in a smectic F mesophase, a tilted analogue of the *smectic B mesophase*.

Note 2: A SmF mesophase is characterised by in-plane short-range positional correlations and weak or no interlayer positional correlations.



**Fig. 8.** Illustrating the structure of a smectic B mesophase.

Note 3: Positional molecular order extends over a few tens of nanometers but the bond orientational molecular order is long-range within a layer.

Note 4: The point-group symmetry is  $C_{2h}$  ( $2/m$ ) in the Schoenflies notation, and the space group,  $t\ 2/m$  in the International System.

Note 5: The smectic F mesophase is optically biaxial.

Note 6: Chiral materials form **chiral smectic F mesophases** denoted by  $\text{SmF}^*$ .

### 3.1.5.2.3 smectic I mesophase, (SmI)

*Hexatic smectic mesophase* the structure of which may be regarded as a C-centered monoclinic cell with hexagonal packing of the molecules with the *director* tilted, with respect to the layer normals, towards the apices of the hexagons.

Note 1: See Figs. 9(a) and (b) for illustrations of the molecular organizations of *smectic F* and *I mesophases*. They are tilted analogues of the *smectic B mesophase*.

Note 2: The smectic I mesophase is optically biaxial.

Note 3: The in-plane positional correlations in a smectic I mesophase are slightly greater than in a *smectic F mesophase*.

Note 4: Chiral materials form **chiral smectic I mesophases** denoted by  $\text{SmI}^*$ .

### 3.1.5.3 crystal B, E, G, H, J and K mesophases

Soft crystals that exhibit long-range positional molecular order, with three-dimensional stacks of layers correlated with each other.

Note 1: Originally, these *mesophases* were designated as smectic, but further investigations have demonstrated their three-dimensional character.

Note 2: In the crystal B and E *mesophases*, the molecular long axes are essentially parallel to the normals to the layer planes while in the G, H, J and K *mesophases* they are tilted with respect to the layer normals.

Note 3: The E, J and K phases have herringbone organizations of the molecular short axes and so the *mesophases* are optically biaxial.

## 3.1.6 polymorphic modifications of strongly polar compounds

### 3.1.6.1 re-entrant mesophase

Lowest temperature *mesophase* of certain compounds that exhibit two or more *mesophases* of the same type, over different temperature ranges.

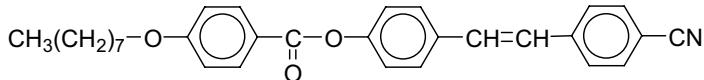
Note 1: The recommended subscript for the designation of re-entrant *mesophases* is: re.

Note 2: Re-entrant *mesophases* are most commonly observed when the molecules have strong longitudinal dipole moments (see example).

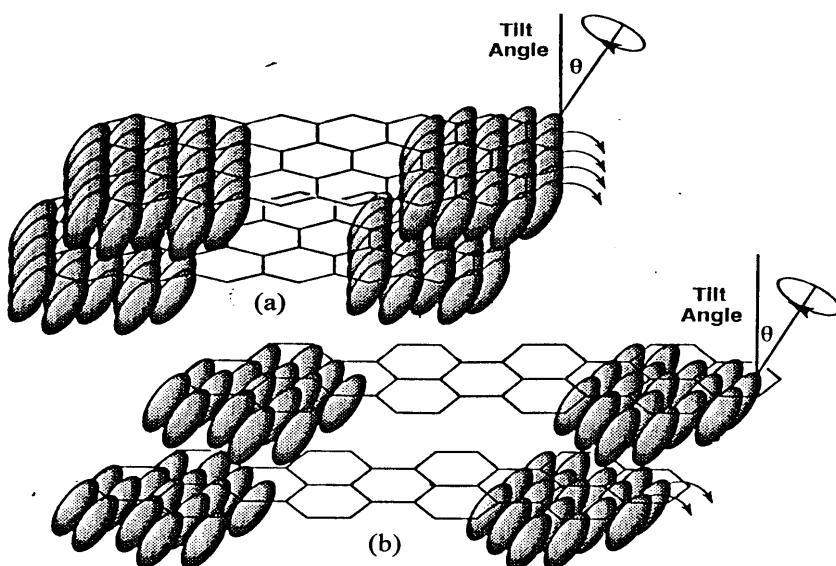
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Note 3: Sequences of re-entrant *mesophases* have also been found in binary mixtures of non-polar liquid-crystalline compounds.

*Example:* The following compound exhibits, as temperature decreases, an isotropic (I) phase, *nematic* (N), *smectic A* (SmA) re-entrant *nematic* (N<sub>re</sub>), re-entrant *smectic A* (SmA<sub>re</sub>) *mesophases* and a crystalline (Cr) phase, with transitions at the specified temperatures.



Cr 349 K SmA<sub>re</sub> 369 K N<sub>re</sub> 412 K SmA 520 K N 556 K I



**Fig. 9.** Illustrating the tilt directions of the *director* in (a) SmF and (b) SmI *mesophases* indicating, respectively, the tilt of the *director* towards the sides of the hexagons (a) and the apices of the hexagons (b).

### 3.1.6.2 smectic A<sub>1</sub> (SmA<sub>1</sub>), A<sub>2</sub> (SmA<sub>2</sub>), A<sub>d</sub> (SmA<sub>d</sub>), C<sub>1</sub> (SmC<sub>1</sub>), C<sub>2</sub> (SmC<sub>2</sub>), C<sub>d</sub> (SmC<sub>d</sub>) *mesophases*

*Smectic A* and *smectic C* *mesophases* characterised by anti-parallel (SmA<sub>2</sub>, SmA<sub>d</sub>, and SmC<sub>2</sub>, SmC<sub>d</sub>) and random (SmA<sub>1</sub> and SmC<sub>1</sub>) alignments of the molecular dipoles within the layer thickness in Fig. 10.

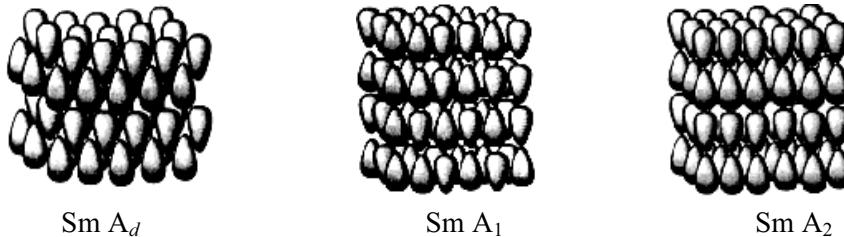
Note 1: See Figs. 10 and 11 for illustrations of the molecular arrangements in the *mesophases*.

Note 2: The subscripts 1, *d* and 2 indicate that the layer thickness is one, *d* and two times the fully-extended molecular length, with  $1 < d < 2$ .

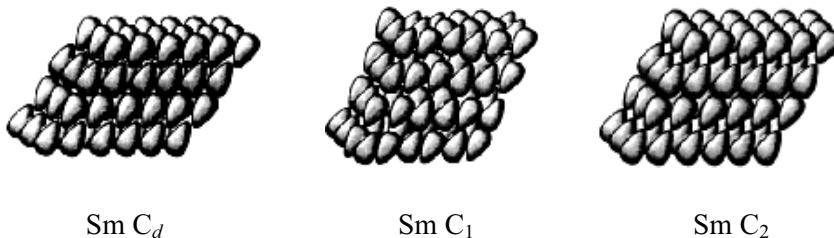
Note 3: SmA<sub>d</sub> and SmC<sub>d</sub> *mesophases* form bilayers with partial overlapping of the molecules of adjacent layers.

Note 4: SmA<sub>2</sub> and SmC<sub>2</sub> phases form bilayers with anti-parallel ordering of the molecules.

Note 5: Bilayer structures are also known for *SmB* and *crystal E mesophases*.



**Fig. 10.** Illustrating the molecular structures of SmA<sub>d</sub>, SmA<sub>1</sub>, and SmA<sub>2</sub> *mesophases*.



**Fig. 11.** Illustrating the molecular structures of SmC<sub>d</sub>, SmC<sub>1</sub>, and SmC<sub>2</sub> *mesophases*.

### 3.1.6.3 modulated smectic mesophase

*Smectic mesophase* that has a periodic in-plane density variation.

Note 1: The recommended mark to designate a modulated *smectic mesophase* is a superior tilde (~).

Note 2: See Figs 12a and 12b for illustrations of the molecular arrangements in Sm $\tilde{A}$  and Sm $\tilde{C}$  *mesophases*.

Note 3: The Sm $\tilde{A}$  *mesophase* is also known as a centered rectangular *mesophase* or anti-mesophase. The dimensional space group is *cmm* in the International System.

Note 4: The Sm $\tilde{C}$  *mesophase* is also known as an oblique or ribbon *mesophase*. The dimensional space group is *pmg* in the International System.

### 3.1.7 intercalated smectic mesophase

*Smectic mesophase* that has a spacing between layers (smectic periodicity) of approximately one half of the molecular length.

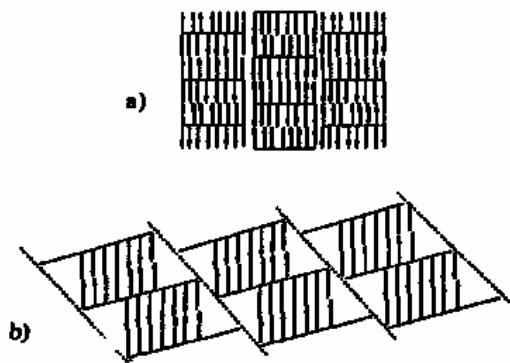
Note 1: The recommended subscript to designate an intercalated *smectic mesophase* is: c

Note 2: Intercalated *smectic mesophases* are commonly observed for liquid-crystal dimers.

Note 3: At present intercalated *smectic A* (SmA<sub>c</sub>) and *smectic C* (SmC<sub>c</sub>) as well as intercalated *crystal B* (B<sub>c</sub>), *G* (G<sub>c</sub>) and *J* (J<sub>c</sub>) *mesophases* have been observed.

Note 4: The local structure in the *nematic mesophase* of certain dimers exhibit an intercalated *smectic mesophase*.

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**Fig. 12.** Schematic drawing of the modulated smectic mesophases (a) Sm $\tilde{A}$  and (b) Sm $\tilde{C}$ .

### 3.1.8 induced mesophase

Particular *mesophase* formed by a binary mixture, the components of which do not separately form *mesophases*, with the particular *mesophase* existing above the melting points of both components.

Note 1: The formation of an induced mesophase usually results from an attractive interaction between unlike species, the strength of which exceeds the mean of the strengths of the interactions between like species.

Note 2: Examples of such interactions that have been noted are dipolar/non-polar, charge-transfer and quadrupolar.

Note 3: *Mesophases* can also be induced when the free-volume between the large, irregular molecules of one component is filled by the smaller molecules of the second component. Such *mesophases* have been called filled *smectic mesophases* although the term ‘induced’ is recommended.

Note 4: A *monotropic mesophase* can be stabilised in a mixture when, as a result of melting-point depression, a metastable *mesophase* becomes stabilised. Such a *mesophase* is distinct from an induced mesophase.

### 3.1.9 cubic mesophase, (Cub)

*Mesophase* with an overall three-dimensional order of cubic symmetry in which each micellar unit cell contains several hundred molecules in random configurations, as in a liquid.

Note 1: The *mesophase* formerly designated as *smectic D* (see Definition 3.1.5, Note 3) belongs to this class.

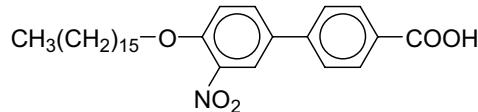
Note 2: A cubic mesophase is optically isotropic; it may be distinguished from an isotropic liquid or a homeotropic phase by the fact that the optically-black isotropic phase or homeotropic phase nucleates in the birefringent SmC phase in straight-edged squares, rhombi, hexagons and rectangles.

Note 3: A cubic mesophase may be formed by rod-like molecules with strong, specific intermolecular interactions, such as hydrogen bonding, between them. However, they are also found in *polycatenary* compounds where there are no specific, strong interactions.

Note 4: Cubic *mesophases* have long been known in thermotropic salt-like compounds and in *lyotropic* liquid-crystals.

Note 5: There are several types of *thermotropic* and *lyotropic* cubic *mesophases*, with different symmetry and miscibility properties; when the space groups of these are known, they should be included in parentheses after the term ‘Cub’.

*Example:* The following compound exhibits a crystalline phase (Cr), smectic SmC, cubic (Cub), smectic SmA mesophases, and an isotropic (I) phase, with transitions at the specified temperatures:



Cr 399.95 K SmC 444.15 K Cub 471.65 K SmA 472.15 K I

### 3.2 mesophases of disc-like mesogens

#### discotic mesophases

#### discotics

##### 3.2.1 discotic nematic mesophase, N

###### discotic nematic

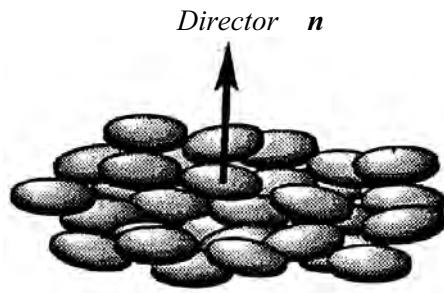
*Nematic mesophase* in which disc-shaped molecules, or the disc-shaped portions of macromolecules, tend to align with their symmetry axes parallel to each other and have a random spatial distribution of their centers of mass.

Note 1: See Fig. 13 for an illustration of the molecular arrangement in a *discotic mesophase*.

Note 2: The symmetry and structure of a *nematic mesophase* formed from disc-like molecules is identical to that formed from rod-like molecules. It is recommended therefore, that the subscript ‘D’ is removed from the symbol ‘N<sub>D</sub>’, often used to denote a *nematic* formed from disc-like molecules.

Note 3: In some cases the discotic nematic mesophase is formed by compounds that do not have molecules of discotic shape (for example, phasmidic compounds, salt-like materials and oligosaccharides).

Note 4: *Chiral discotic nematic mesophases, N<sup>\*</sup>*, also exist.



**Fig. 13.** Illustrating the organization of molecules in a discotic nematic mesophase.

##### 3.2.2 columnar mesophase, (Col)

###### columnar discotic mesophase

###### columnar discotic

*Mesophase* in which disc-shaped molecules, the disc-shaped moieties of macromolecules or wedge-shaped molecules assemble themselves in columns packed parallel on a two-dimensional lattice, but without long-range positional correlations along the columns.

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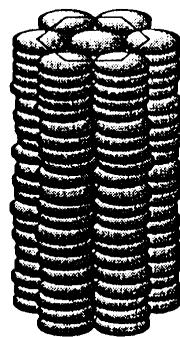
Note: Depending on the order in the molecular stacking in the columns and the two-dimensional lattice symmetry of the columnar packing, the columnar *mesophases* may be classified into three major classes: hexagonal, rectangular and oblique (see Definitions 3.2.2.1. to 3.2.2.3).

### 3.2.2.1 columnar hexagonal mesophase, ( $\text{Col}_h$ )

*Columnar mesophase* characterised by a hexagonal packing of the molecular columns.

Note 1: See Fig. 14 for an illustration of the molecular arrangement in a  $\text{Col}_h$  mesophase.

Note 2: Hexagonal *mesophases* are often denoted  $\text{Col}_{ho}$  or  $\text{Col}_{hd}$  where h stands for hexagonal and o and d refer to the range of positional correlations along the column axes: o stands for ordered and d for disordered. The use of the subscripts o and d should be discontinued. In both cases, the ordering is liquid-like, only the correlation lengths are different.



**Fig. 14.** Illustrating the molecular organization of a columnar hexagonal mesophase.

Note 3: The relevant space group of a  $\text{Col}_h$  mesophase is  $P\ 6/mmm$  (equivalent to  $P\ 6/m\ 2/m$  in the International System and point group  $D_{6h}$  in the Schoenflies notation).

Note 4: The *lyotropic* equivalent of a columnar hexagonal mesophase is known as a **hexagonal mesophase**; in it, columns of amphiphilic molecules are surrounded by the solvent, normally water, or an oil in an **inverse hexagonal mesophase**.

### 3.2.2.2 columnar rectangular mesophase, ( $\text{Col}_r$ )

*Columnar mesophase* characterised by a liquid-like molecular order along the columns, in which the columns are arranged in a rectangular packing.

Note 1: See Figs 15a–c for illustrations of molecular arrangements in columnar rectangular mesophases.

Note 2: The average orientation of the planes of the molecular discs is not necessarily normal to the column axes.

Note 3: Depending on the plane space-group symmetries, three rectangular *mesophases* are distinguished (See Fig. 15a–c).

Note 4: There also exist chiral columnar rectangular mesophases, with the molecular discs tilted periodically in the columns and with the tilt directions changing regularly down the columns.

### 3.2.2.3 columnar oblique mesophase, ( $\text{Col}_{ob}$ )

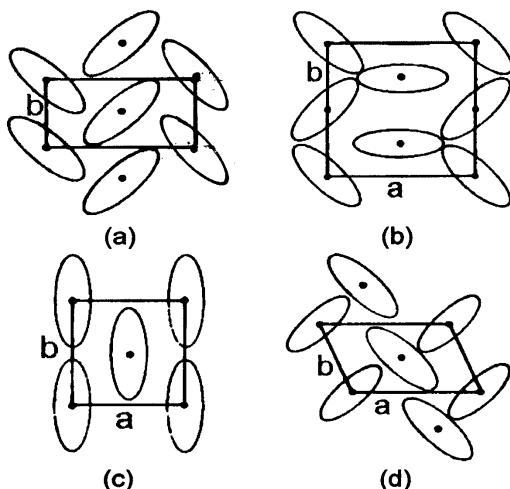
*Columnar mesophase* characterised by a liquid-like molecular order along the column, in which the columns are arranged with an oblique packing.

Note 1: See Fig. 15d for an illustration of the molecular arrangement in a columnar oblique mesophase.

Note 2: The average of the planes of the molecular discs is not necessarily normal to the columnar axes.

Note 3: The plane space-group symmetry of a  $\text{Col}_{\text{ob}}$  mesophase is  $P_1$  (see Fig. 15d).

Note 4: There also exist chiral columnar oblique mesophases, with the tilt directions of the columnar discs varying regularly along the columns.



**Fig. 15.** Plan views of the two-dimensional lattice of the columns in columnar rectangular (a) to (c) and oblique (d) mesophases. Ovals indicate the planes of the molecular discs.

Plane space group symmetries in the projection of the International System are:

(a)  $P2_1/a$ ; (b)  $P2/a$ ; (c)  $C2/m$ ; (d)  $P_1$ .

### 3.3 biaxial mesophase

*Mesophase* composed of board-like molecules in which there are long-range orderings of both the longer and the shorter molecular axes.

Note 1: The recommended subscript to designate a biaxial mesophase is: b

Note 2: A biaxial mesophase has three orthogonal *directors* denoted by the unit vectors  $l$ ,  $m$  and  $n$ .

Note 3: The tensorial properties of a biaxial mesophase have biaxial symmetry unlike the uniaxial symmetries of, for example, the *nematic* and *smectic A mesophases*.

Note 4: The biaxiality of the phase does not result from tilted structures as, for example, in a *smectic C mesophase*.

Note 5: Distinct biaxial *mesophases* are created when the molecular centers of mass are correlated within the layers. Such *mesophases* have been proposed for board-like polymers and have been called *sanidic mesophases*.

Note 6: *Sanidic* structures are analogous to the *columnar mesophases* formed by disc-like molecules.

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### 3.3.1 biaxial nematic mesophase, $N_b$

#### biaxial nematic

*Mesophase* in which the long axes of the molecules are, on average, orientationally ordered about a common *director* and one of the shorter molecular axes is ordered, on average, about a second, orthogonal *director*.

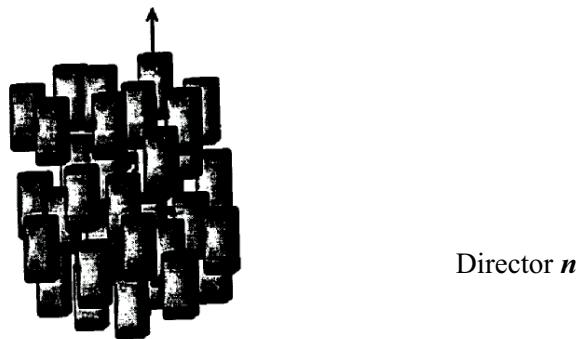
Note 1: See Fig. 16 for an illustration of the molecular arrangement in a  $N_b$  mesophase.

Note 2: From a crystallographic point of view, the biaxial *nematic* structure is characterised by the symbol  $D_{2h}$  in the Schoenflies notation ( $2/m$ ,  $m$  in International System).

Note 3: In *lyotropic* systems, biaxial nematic mesophases have been identified from the biaxial symmetry of their tensorial properties.

Note 4: The situation for *thermotropic calamitic* systems is less clear and for some compounds claimed to form a  $N_b$ , detailed investigations have found the *mesophase* to be of type  $N_u$ .

Note 5: A biaxial nematic has the same structure as a disordered *sanidic mesophase* (see Definition 3.4, Note 2); it is recommended that the latter name be discontinued and the name biaxial nematic be used.



**Fig. 16.** Schematic representation of a biaxial nematic mesophase.

### 3.3.2 biaxial smectic A mesophase, $SmA_b$

*Smectic A mesophase* composed of board-like molecules with the longer and the shorter molecular axes orientationally ordered.

Note: For a  $SmA_b$  mesophase, the molecular centers-of-mass have only short-range positional order within a layer.

### 3.4 sanidic mesophase, $\Sigma$

*Mesophase* in which *board-shaped* molecules assemble in stacks packed parallel to one another on a one- or two-dimensional lattice (see Figs. 17 and 18).

Note 1: See Figs. 17 and 18 for examples of *sanidic mesophases*.

Note 2: Short board-like shaped molecules usually form *biaxial nematic mesophases*. It is recommended that the use of the term disordered *sanidic mesophases* for such *mesophases* be discontinued (see Definition 3.3.1, Note 5).

Note 3: Rotation of the molecules around their long axes is considerably hindered.

#### 3.4.1 rectangular sanidic mesophase, $\Sigma_r$

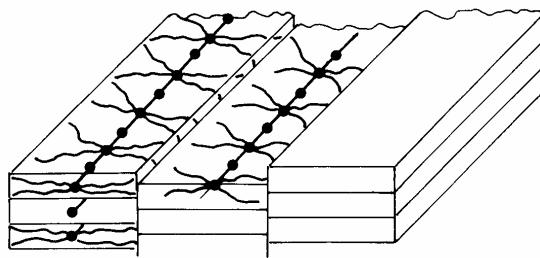
*Sanidic mesophase* in which the molecular stacks are packed regularly side-by-side with long-range order along a stack normal as well as along the long stack-axis.

Note: See Fig. 17 for an illustration of the molecular arrangement in a  $\Sigma_r$  mesophase.

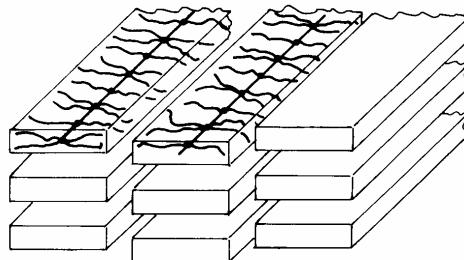
### 3.4.2 ordered sanidic mesophase, $\Sigma_o$

*Mesophase* in which the molecular stacks are packed regularly side-by-side with long-range order along a stack normal and no registration along the long stack-axis.

Note: See Fig. 18 for an illustration of the molecular arrangement in a  $\Sigma_o$  mesophase.



**Fig. 17.** Illustrating a rectangular sanidic mesophase.



**Fig. 18.** Illustrating an ordered sanidic mesophase.

### 3.5 glassy mesophase

*Mesophase* in which non-vibratory molecular motion is frozen by supercooling a *mesophase* stable at a higher temperature.

Note: The recommended subscript to designate a glassy mesophase is: g.

### 3.6 twist grain-boundary mesophase (TGB)

Defect-stabilised *mesophase* created when a *smectic A mesophase* is subjected to a twist or bend distortion.

Note 1: The twist and bend distortions can be stabilised by an array of screw or edge dislocations.

Note 2: A TGB mesophase is analogous to the Abrikosov flux-phase of certain superconductors.

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### 3.6.1 twist grain-boundary A<sup>\*</sup> mesophase (TGBA<sup>\*</sup>)

*Mesophase* with a helicoidal supramolecular structure in which blocks of molecules, with a local structure of the *smectic A* type, have their layer normals rotated with respect to each other and are separated by screw dislocations.

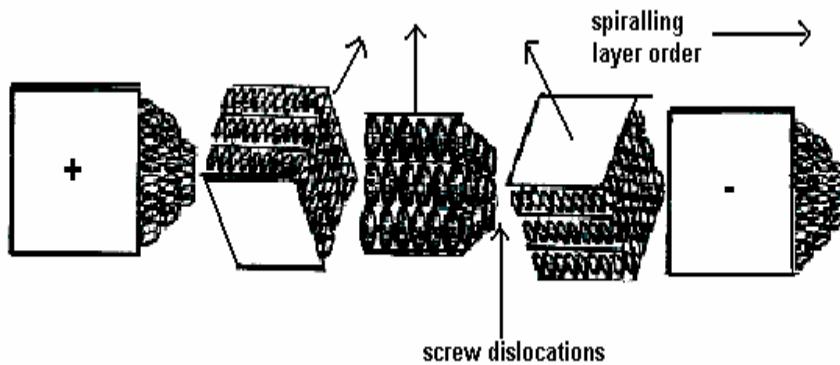
Note 1: See Fig. 19 for an illustration of the molecular arrangement of a TGBA<sup>\*</sup> mesophase.

Note 2: The TGBA<sup>\*</sup> mesophase is formed by a chiral compound or a mixture of chiral compounds.

Note 3: Two TGBA<sup>\*</sup> structures are possible; in one, the number of blocks corresponding to a rotation of the layer normal by  $2\pi$  is an integer, while in the other, it is a non-integer.

Note 4: A TGBA<sup>\*</sup> is found in a phase diagram between *smectic A* and *chiral nematic mesophases* or between a *smectic A mesophase* and an isotropic phase.

Note 5: The temperature range of existence of a TGBA<sup>\*</sup> mesophase is typically several K.



**Fig. 19.** Illustrating the structure of a TGBA<sup>\*</sup> mesophase corresponding to half of the full helical twist.

### 3.6.2 twist grain-boundary C<sup>\*</sup> mesophase (TGBC<sup>\*</sup>)

*Mesophase* of helicoidal supramolecular structure in which blocks of molecules with a local structure of the *smectic C* type, have their layer normals rotated with respect to each other and are separated by screw dislocations.

Note 1: Two forms of TGBC<sup>\*</sup> mesophase are possible: in one form the *director* within the layer is tilted and rotates coherently through the layers in a block as in a *chiral smectic C mesophase*, while in the other form the *director* within a block is simply tilted with respect to the layer normal as in a *smectic C mesophase*.

Note 2: In the case of a short pitch, when  $P$  is less than the wavelength  $\lambda$ , the macroscopic extraordinary axis for the refractive index is orthogonal to the *director*.

### 3.6.3 melted-grain-boundary mesophase (MGBC<sup>\*</sup>)

*Mesophase* with a helicoidal supramolecular structure of blocks of molecules with a local *smectic C* structure. The layer normal to the blocks rotates on a cone to create a helix-like *director* in the *smectic C*<sup>\*</sup>. The blocks are separated by plane boundaries perpendicular to the helical axis. At the boundary, the *smectic* order disappears but the *nematic* order is maintained. In the blocks the *director* rotates from one boundary to the other to allow the rotation of the blocks without any discontinuity in the thermomolecular orientation.

Note: This phase appears between the TGBA and SmC<sup>\*</sup> or N<sup>\*</sup> and SmC<sup>\*</sup> mesophases.

## 4 TEXTURES AND DEFECTS

### 4.1 domain

Region of a *mesophase* having a single *director*.

Note: See 3.1.1.1 for the definition of a *director*.

### 4.2 monodomain

Region of a uniaxial *mesophase* or a whole uniaxial *mesophase* having a single *director* or a region of a biaxial *mesophase* or a whole biaxial *mesophase* having two *directors*.

Note 1: See 3.1.1 for the definition of a *uniaxial nematic mesophase*, 5.8.1 for the definition of uniaxial *mesophase* anisotropy, and Definitions 3.3 and 5.8.2 relating to .

Note 2: For a *smectic mesophase*, the term monodomain also implies a uniform arrangement of the *smectic* layers.

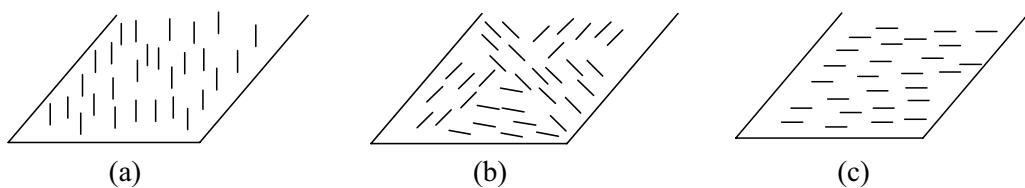
### 4.3 homeotropic alignment

Molecular alignment of which the *director* is perpendicular to a substrate surface.

Note 1: See Fig. 20a.

Note 2: When the alignment of the *director* in a homeotropic alignment deviates from the perpendicular, the alignment is said to be a **pre-tilted homeotropic alignment**; the pre-tilt angle is the deviation from 90°.

Note 3: **Surface pretilt** is the deviation angle of the *director* away from the surface. It is used to control the threshold voltage and affects viewing angles.



**Fig. 20.** Representing (a) homeotropic, (b) planar, and (c) uniform planar molecular alignments.

### 4.4 planar alignment

#### homogeneous alignment

Molecular alignment in which *directors* lie parallel to a substrate surface.

Note: See Fig. 20b.

### 4.5 uniform planar alignment

Molecular alignment in which the *director* is parallel to a substrate surface.

Note 1: See Fig. 20c.

Note 2: Sometimes a uniform planar alignment is called a ‘uniform homogeneous alignment’. The latter term is not recommended.

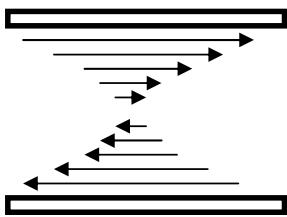
### 4.6 twist alignment

Molecular alignment for which the *director* rotates in a helical fashion when passing between two substrate surfaces having molecules in *uniform planar alignments*.

## TERMINOLOGY

Note 1: See Fig. 21. The length of a line in Fig. 21 indicates the length of a *director* projected onto the plane of the page.

Note 2: The orientation of the *directors* on the upper and lower substrate surfaces are usually mutually orthogonal and hence the *directors* undergo a 90° twist over the thickness of the liquid-crystal layer.



**Fig. 21.** Illustrating a twist alignment.

### 4.7 defect

Non-uniform molecular alignment that cannot be transformed into a uniform alignment without creating other defects.

Note 1: Dislocations and disclinations are major types of defects in liquid crystals.

Note 2: Three elementary types of defects may be distinguished in liquid crystals. They are point, line and wall defects.,

Note 3: A discontinuity in the structure (or in the mathematical function describing the structure) is considered as a singularity; in many cases a defect can be regarded as a singularity.

#### 4.7.1 dislocation

Discontinuity in a regular molecular positional arrangement.

Note: Dislocations are found mainly in solid crystals.

#### 4.7.2 disclination

*Defect* along a line in the regular orientation of *directors*.

Note 1: Disclinations are responsible for some *optical textures* seen with a polarizing microscope, such as the *schlieren texture* formed by disclination lines in nearly vertical orientations, whose projections are seen as dark points with two or four emerging dark stripes or brushes (see Definition 4.9.2).

Note 2: Disclinations are defects in molecular orientational order in contrast to dislocations that are defects in molecular positional order.

### 4.8 optical texture

Image of a liquid-crystal sample seen with a microscope, usually with crossed polarizers.

Note: An optical texture results from surface orientation of the *directors* at the boundaries of the sample and by defects formed in the sample.

## 4.9 nematic textures

### 4.9.1 nematic droplet

Spherical droplet that forms during a transition from an isotropic phase to a *nematic mesophase*. It has characteristic textures that depend on the droplet size and the *director* orientation at the nematic-isotropic interface.

Note: *Nematic* droplets display a texture characteristic of a *nematic mesophase* since they occur nowhere else.

#### 4.9.1.1 bipolar droplet texture

Texture with two point defects at the poles of a *nematic droplet*.

Note 1: A pole is the position of the extreme of a *director* in a droplet.

Note 2: The point defects are called boojums.

Note 3: A bipolar droplet texture occurs when the *director* lies in the plane of a nematic-isotropic interface.

#### 4.9.1.2 radial droplet texture

Texture with one point *defect* at the center of a *nematic droplet*.

Note 1: The point *defect* usually forms when the *director* is normal to the nematic-isotropic interface.

Note 2: The radial droplet texture shows four dark brushes located in the regions where the *director* is in the polarization plane of either the polarizer or the analyser.

### 4.9.2 schlieren texture

Texture observed for a flat sample between crossed polarizers, showing a network of black brushes connecting centers of point and line defects.

Note 1: The black brushes are also called black stripes or schlieren brushes.

Note 2: Black brushes are located in regions where the *director* lies in the plane of polarization of either the polarizer or the analyser.

Note 3: Schlieren textures observed in *nematic* samples with *planar alignment* show *defect* centers with two or four emerging brushes. Schlieren textures in *nematic* samples with tilted alignments show centers with four brushes; centers with two brushes are caused by *defect* walls.

Note 4: A thin sample of a *smectic C* phase with the layers parallel to the sample surfaces gives schlieren textures with centers that have four brushes. However, a *smectic C* phase formed by odd-membered liquid-crystal dimers (see Definition 2.11.2.9, Note 5) has schlieren textures with two or four brushes.

#### 4.9.2.1 nucleus

Center of a point or line *defect* from which black brushes originate when a liquid crystal is observed between crossed polarizers.

Note: A nucleus can indicate either the end of a *disclination* line terminating at the surface of a sample or an isolated *defect*.

#### 4.9.2.2 disclination strength, $s$

Number of rotations by  $2\pi$  of the *director* around the center of the *defect*.

$$|s| = \frac{\text{number of brushes}}{4}$$

## TERMINOLOGY

Note 1:  $s$  is positive when the brushes turn in the same direction as the polarizer and analyser when they are rotated together, and negative when they turn in the opposite direction.

Note 2:  $s$  can be an integer or half-integer since in *nematics* the *directors*  $+n$  and  $-n$  are not distinguishable.

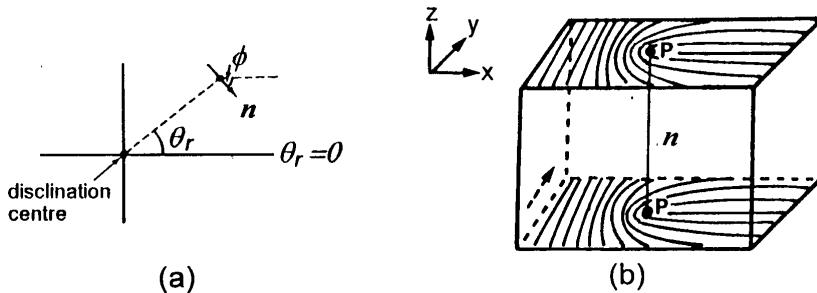
Note 3: The angular distribution  $\phi$  of the *director* around a *defect* in a *nematic* planar *texture*, in the X-Y projection, can be expressed in terms of the polar angle  $\theta_r$

$$\phi = s\theta_r + \phi_0$$

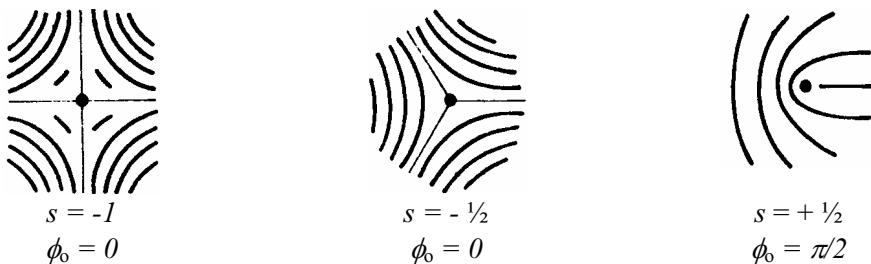
where  $\theta_r$  represents the angular polar co-ordinate of a given point with respect to the *disclination center*,  $\phi$  is the angle that the local *director* axis at that point makes with the  $\theta_r = 0$  axis and  $\phi_0$  is a constant ( $0 < \phi_0 < 2\pi$ ) (See Fig. 22).

The product  $s\theta_r$  yields the angle by which the *director* turns on a closed curve around the *disclination center*. If a complete circuit is made around the center of an  $s = \pm \frac{1}{2}$  *disclination*, the *director* rotates by  $\pi$ . For  $s = \pm 1$  a similar circuit yields a total *director* rotation of  $2\pi$ . So,  $s = \pm \frac{1}{2}$  defines a  **$\pi$ -line disclination** and  $s = \pm 1$  defines a  **$2\pi$ -line disclination**.

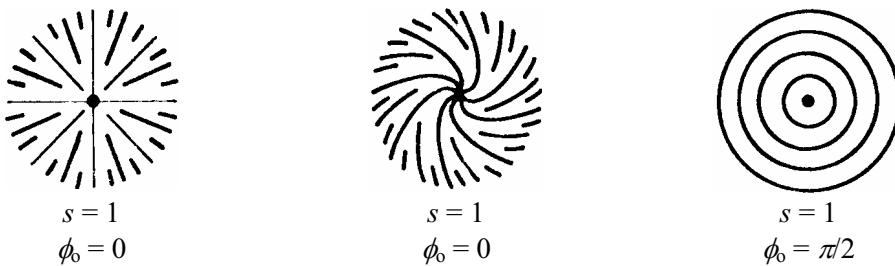
Note 4: *Director* alignments for point defects with different values of  $s$  are illustrated in Fig. 23.



**Fig. 22.** (a) Identification of the angles  $\phi$  and  $\theta_r$  used to describe a disclination. (b) Director arrangement of an  $s = \pm \frac{1}{2}$  singularity line. The end of the line attached to the sample surface appears as the point  $s = + \frac{1}{2}$  (points P). The director alignment or field does not change along the  $z$  direction. The director field has been drawn in the upper and the lower surfaces only.



cont.



**Fig. 23.** Schematic representation of the *director* alignments at disclinations with different values of  $s$  and  $\phi_0$ ;  $s = \pm \frac{1}{2}$  correspond to two-brush defects and  $s = \pm 1$  to four-brush defects.

#### 4.9.3 threaded texture

Texture with  $\pi$ -line disclinations which lie essentially parallel to the surfaces between which a sample is placed, with the ends of the lines attached to the surfaces and the other parts of the lines moving freely in the liquid crystal, appearing as thin thread-like lines.

##### 4.9.3.1 surface disclination line adhering thread

Thick, thread-like *disclination* line anchored along its length to the upper or the lower of the surfaces between which a sample is placed.

#### 4.9.4 marbled texture

Texture consisting of several areas with different *director* orientations.

Note: On observing a sample with a marbled texture between crossed polarizers, the interference colour is essentially uniform within each individual area, indicating an essentially homogeneous region.

#### 4.10 smectic textures

##### 4.10.1 bâtonnet

Droplet, usually non-spherical, of a *smectic* phase nucleating from an isotropic phase.

##### 4.10.2 focal-conic domain

*Domain* formed by deformed *smectic* layers that fold around two confocal line defects preserving equidistance of structural layers everywhere except in the vicinity of the *defect* lines.

Note 1: See Fig. 24. The confocal line defects may be an ellipse and a hyperbola or two parabolae.

Note 2: The *smectic* layers within a focal-conic domain adopt the arrangement of Dupin cyclides, since as in these figures there appear concentric circles resulting from the intersection of ellipses and hyperbolae. They also have the distinctive property of preserving an equal distance between them.

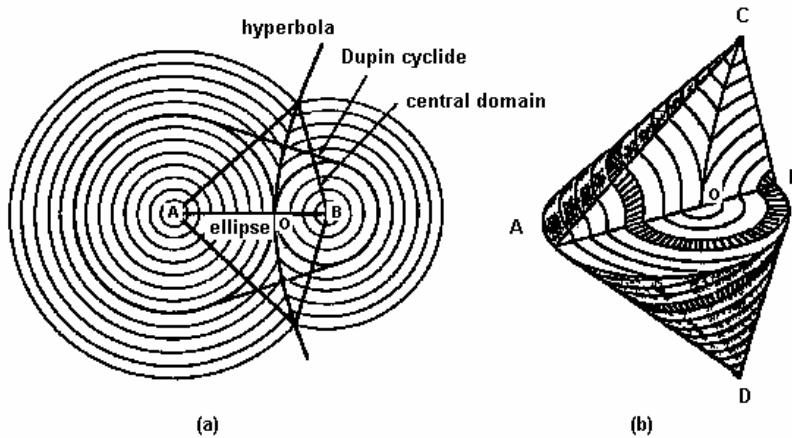
Note 3: A focal-conic domain built around an ellipse and an hyperbola is the most common type of *defect* in thermotropic *smectic A* phases. The hyperbola passes through a focus of the ellipse and the ellipse passes through the focus of the hyperbola (see Fig. 24).

Note 4: In a particular limiting case of an ellipse-hyperbola focal-conic domain, the ellipse becomes a straight line passing through the center of a circle.

## TERMINOLOGY

Note 5: A focal-conic domain built around two confocal parabolae is called a **parabolic focal-conic domain**.

Note 6: At any point inside a focal-conic domain, the *director* is oriented along the straight line drawn through the point and the two *defect* lines (ellipse and hyperbola or two parabolae or circle and straight line). See for example BD, BC and BO in Fig. 24.



**Fig. 24.** Dupin cyclide and perfect focal-conic domain construction. (a) Vertical section showing layers of the structure; thick lines indicate the ellipse, hyperbola, Dupin cyclide, and central domain. (b) Focal-conic domain showing structural layers with a representation of the arrangement of the molecules within one of them.

### 4.10.3 polygonal texture

Texture composed of *focal-conic domains* of the ellipse-hyperbola type with visible ellipses, or parts of ellipses, located at the boundary surfaces.

Note 1: See Figs. 25a and 25b.

Note 2: One branch of the hyperbola (either above or below the plane of the ellipse) is usually missing in the polygonal texture.

Note 3: Neighbouring *domains* form a family with a common apex where the hyperbolae of these *domains* join each other. This common point is located at the surface that is opposite to the surface containing the ellipses (see Fig. 26). Each family is bounded by a polygon formed by hyperbolic and elliptical axes; these are parts of *focal-conic domains* that provide a smooth variation of *smectic* layers between the *domains* of different families. These *domains* are the tetrahedra in Fig. 26.

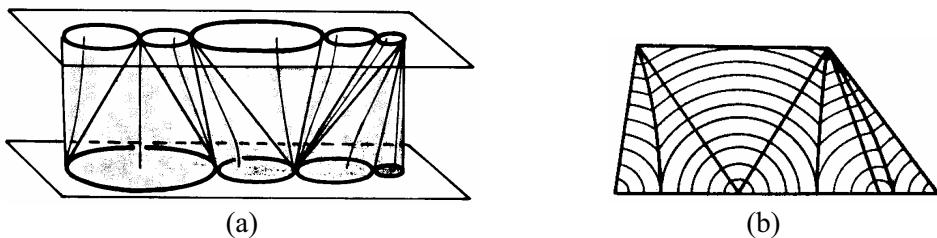
Note 4: The *smectic* layers pass continuously from one *focal-conic* to the next.

### 4.10.4 focal-conic, fan-shaped texture

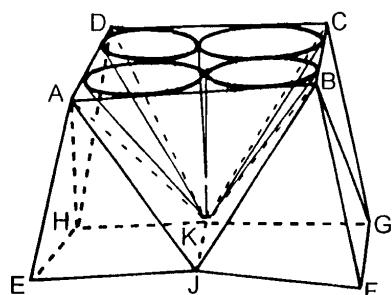
Texture formed partly by *focal-conic domains* with their hyperbolae lying in the plane of observation.

Note 1: See Fig. 27.

Note 2: The layers are aligned almost normal to the sample surfaces. The regular sets of hyperbolae are called '**boundaries of Grandjean**'; they serve as limiting surfaces between *domains* with different *director* orientations.



**Fig. 25.** Arrangement of a smectic A polygonal texture: (a) general view of the focal-conic domains filling space efficiently; (b) cross-section of the *domains* showing arrangement of the smectic layers.



**Fig. 26.** Elements of a smectic A complex polygonal texture. Upper surface: one polygon with four ellipses. Lower surface: two polygons. The whole space may be divided into three pyramids (ABCDK, AEHKJ, BFGKJ) and three tetrahedra (ABJK, ADHK, BCGK).

## 5 PHYSICAL CHARACTERISTICS OF LIQUID CRYSTALS

General Note: In this section the *director*  $\mathbf{n}$  is treated mathematically as a unit vector, with components  $n_1, n_2, n_3$  along space-fixed axes  $X_1, X_2, X_3$ .

### 5.1 order parameter, $\langle P_2 \rangle$

Parameter characterizing the long-range orientational order with reference to the *director*, with

$$\langle P_2 \rangle = (3\langle \cos^2 \beta \rangle - 1)/2$$

where  $\beta$  is the angle between the molecular symmetry axis and the *director* and  $\langle \rangle$  denotes an ensemble average.

Note 1:  $\langle P_2 \rangle$  characterises long-range molecular order.

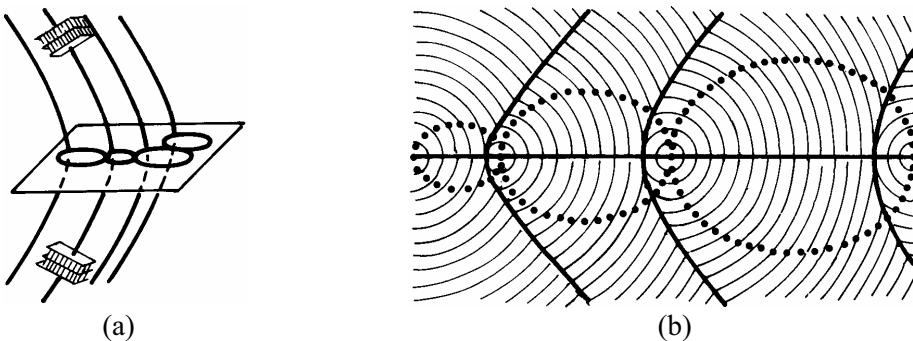
Note 2: For rod-like molecules, the order parameter of the effective molecular symmetry axis at the nematic-isotropic transition is about 0.3 and can increase to about 0.7 in the *nematic mesophase*.

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Note 3: Molecules which constitute nematogens are not strictly cylindrically symmetric and have their orientational order given by the Saupe ordering matrix which has elements  $S_{\alpha\beta} = (3<|\alpha||\beta> - \delta_{\alpha\beta})/2$ , where  $1\alpha$  and  $1\beta$  are the direction cosines between the *director* and the molecular axes  $\alpha$  and  $\beta$ ,  $\delta_{\alpha\beta}$  is the Kronecker delta and  $\alpha, \beta$  denote the molecular axes X, Y, Z.

Note 4: The constituent molecules of a *nematogen* are rarely rigid and their orientational order is strictly defined, at the second-rank level, by a Saupe ordering matrix for each rigid sub-unit.

Note 5: Even for molecules with cylindrical symmetry,  $\langle P_2 \rangle$  does not provide a complete description of the orientational order. Such a description requires the singlet orientational distribution function which can be represented as an expansion in a basis of Legendre polynomials  $P_L \cos \beta$ , with  $L$  an even integer. The expansion coefficients are proportional to the order parameters  $\langle P_L \rangle$  of the same rank. It is these order parameters which provide a complete description of the long-range orientational order.



**Fig. 27.** (a) Illustrating an arrangement of confocal ellipses and hyperbolae. The *directors* become parallel near the extremes of the hyperbolae. (b) Section showing the layer structure. The dotted ellipses in the plane of the drawing are sections perpendicular to the focal-conics.

### 5.2 distortion in liquid crystals, $a$

Deformation leading to a change in the *director*, where the distortion is described by a tensor of third rank

$$a_{3ij} = n_3 \left( \partial n_i / \partial x_j \right)$$

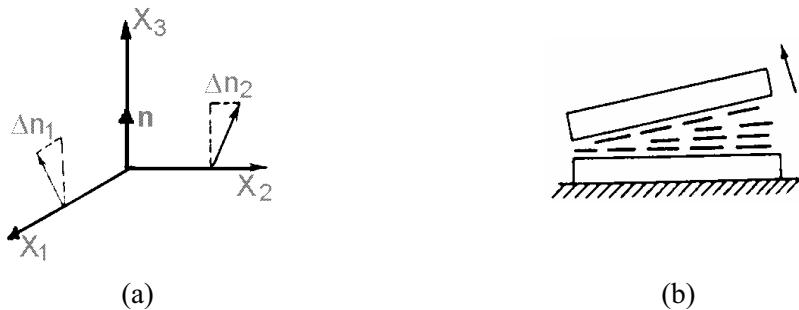
in which the initial orientation of the *director*  $n$  is chosen as the 3-axis;  $I = 1, 2$ ;  $j = 1, 2, 3$ ;  $n_3 = 1$ ,  $n_i$  is the  $i$ th component of the *director*  $n$  and  $x_j$  is a co-ordinate on axis  $X_j$ .

### 5.2.1 splay deformation, (S-deformation)

Deformation in a direction normal to the initial *director*,  $\mathbf{n}$ , characterised by  $\text{div } \mathbf{n} \neq 0$ .

Note 1: See Fig. 28 and Definition 5.3.

Note 2: A splay deformation is described by the non-zero derivatives  $n_3(\partial n_1 / \partial x_1)$  and  $n_3(\partial n_1 / \partial x_2)$ , where the symbols are defined in Definition 5.2.



**Fig. 28.** Schematic representation of a splay deformation: (a) changes in the components of the director  $\mathbf{n}$ , defining the orientational change; (b) splay deformation of an oriented layer of a nematic liquid crystal.

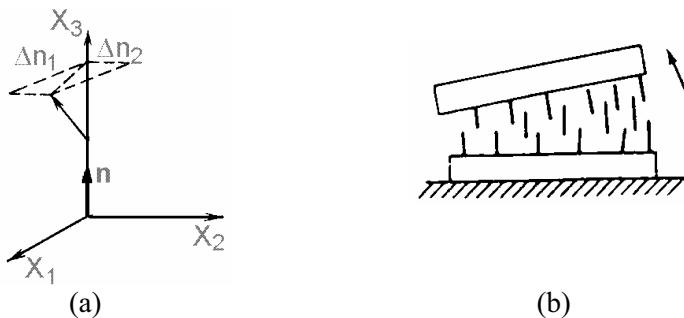
### 5.2.2 bend deformation, (B-deformation)

Deformation in the direction of the initial *director*,  $\mathbf{n}$ , characterised by  $\mathbf{n} \times \text{rot } \mathbf{n} \neq 0$ .

Note 1: See Fig. 29 and Definition 5.3.

Note 2: The degree of bending is given by the component of  $\text{rot } \mathbf{n}$  perpendicular to  $\mathbf{n}$ .

Note 3: A bend deformation is described by the non-zero derivatives  $n_3(\partial n_1 / \partial x_1)$  and  $n_3(\partial n_1 / \partial x_2)$ , where the symbols are defined in Definition 5.2.



**Fig. 29.** Schematic representation of a bend deformation: (a) changes in the components of the director,  $\mathbf{n}$  defining the orientation change; (b) bend deformation of an oriented layer of a nematic liquid crystal.

### 5.2.3 twist deformation, (T-deformation)

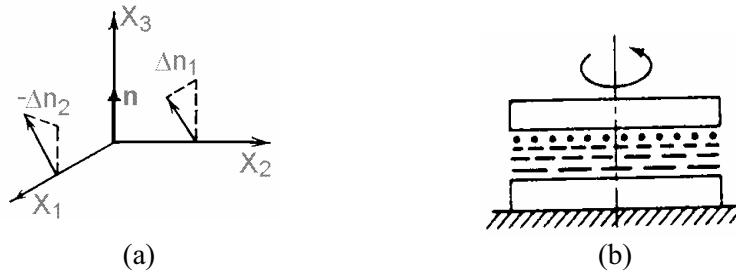
Torsional deformation of a planar-oriented layer in the direction of the initial *director*,  $\mathbf{n}$ , characterised by  $\mathbf{n} \cdot \text{rot } \mathbf{n} \neq 0$ .

Note 1: See Fig. 30 and Definition 5.3.

Note 2: The degree of twisting is given by the component of  $\text{rot } \mathbf{n}$  parallel to  $\mathbf{n}$ .

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Note 3: A twist deformation is described by the non-zero derivatives  $n_3(\partial n_1 / \partial x_1)$  and  $n_3(\partial n_1 / \partial x_1)$ , where the symbols are defined in Definition 5.2.



**Fig. 30.** Schematic representation of the twist deformation: (a) changes in the components of the director  $\mathbf{n}$ , defining the orientation change; (b) twist deformation of an oriented layer of a nematic liquid crystal.

### 5.3 elastic constants, $K_i$ where $i = 1, 2$ and $3$ , SI unit: $\text{Nm}^{-2}$ elasticity moduli

Coefficients  $K_1$ ,  $K_2$  and  $K_3$ , in the expression for the distortion-Gibbs energy density,  $g$ , of a bulk *nematic liquid crystal*; with

$$g = g_0 + 1/2[K_1 (\operatorname{div} \mathbf{n})^2 + K_2 (\mathbf{n} \times \operatorname{rot} \mathbf{n})^2 + K_3 (\mathbf{n} \times \operatorname{rot} \mathbf{n})^2],$$

where  $g_0$  is the Gibbs-energy density of the undistorted liquid crystal,  $\mathbf{n}$  is the *director*, and  $K_1$ ,  $K_2$ , and  $K_3$  are the elastic constants for splay, twist, and bend deformations, respectively.

Note 1: In the equation for  $g$ , the term  $g_0$  is usually equal to zero because the undistorted state of *nematics* is the state of uniform alignment. However, for *chiral nematics*, a non-zero value of  $g_0$  allows for the intrinsic twist in the structure. In order to describe  $g$  for *smectic* phases, an additional term must be added, due to the partially solid-like character of the *smectic* state and arising from positional molecular deformations.

Note 2: In low molar mass *nematics* composed of rod-like molecules, the bend constant  $K_3$  is the largest while the twist constant  $K_2$  is the smallest. Typical values of  $K_1$  are  $10^{-11} - 10^{-12} \text{ N m}^{-2}$ .

Note 3: The names of Oseen, Zocher, and Frank are associated with the development of the theory for the elastic behaviour of *nematics* and so the elastic constants may also be described as the **Oseen-Zocher-Frank constants**, although the term **Frank constants** is frequently used.

### 5.4 Leslie-Ericksen coefficients, $\alpha_i$ , $i = 1, 2, 3, 4, 5$ and $6$ , SI unit: $\text{Pa s}$

Six viscosity coefficients required for a description of the dynamics of an incompressible, *nematic liquid crystal*.

Note 1: Assuming Onsager's reciprocal relations for irreversible processes,

$$\alpha_2 + \alpha_3 = \alpha_6 - \alpha_5$$

and the number of independent coefficients reduces to five.

Note 2: For *nematics* formed by low-molar-mass compounds, the Leslie coefficients are typically in the range  $10^{-2}$  to  $10^{-1}$  Pa s.

### 5.5 Miesowicz coefficient, $\eta_i$ $i = 1, 2$ and $3$ , SI unit: Pa s

Ratio of the shear stress,  $\sigma$ , to the shear velocity gradient,  $\gamma$ , for a *nematic* liquid crystal with a particular *director* orientation, denoted by  $i$ , under the action of an external field:

$$\eta_i = \sigma/\gamma$$

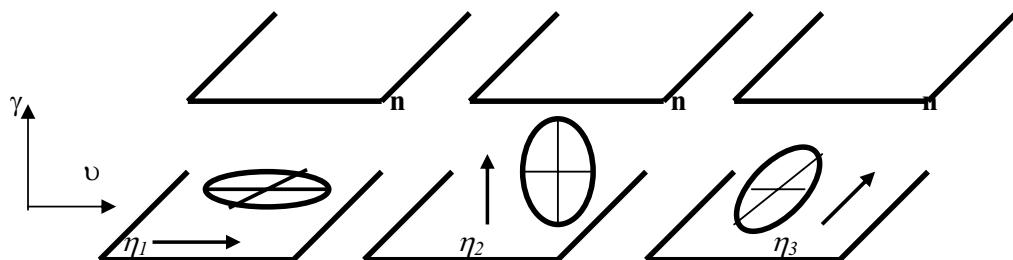
Note 1: The three Miesowicz coefficients ( $\eta_1$ ,  $\eta_2$ , and  $\eta_3$ ) describe the shear flow of a *nematic* phase with three different *director* orientations, (see Fig. 31) namely:  $\eta_1$  for the *director* parallel to the shear-flow axis;  $\eta_2$  for the *director* parallel to the velocity gradient; and  $\eta_3$  for the *director* perpendicular to the shear flow and to the velocity gradient.

Note 2: Usually  $\eta_1 < \eta_2 < \eta_3$ .

Note 3: The Miesowicz coefficients are related to the *Leslie-Ericksen coefficients* by the following equations:

$$\eta_1 = 0.5(\alpha_3 + \alpha_4 + \alpha_6), \eta_2 = 0.5(\alpha_4 + \alpha_5 + \alpha_2), \eta_3 = 0.5(\alpha_4)$$

Note 4: The external field used to align the *director* must be sufficiently large to ensure that it remains aligned during flow.



**Fig. 31.** Scheme of director alignment in the shear flow of velocity  $v$  of a nematic phase and the corresponding Miesowicz coefficients.

### 5.6 friction coefficients, $\gamma_i$ $i = 1$ and $2$ , SI unit: Pa s rotational viscosity coefficients

Coefficients that define the energy dissipation associated with a rotation of the *director* in an incompressible, *nematic* liquid crystal.

Note 1: The rotational viscosity coefficients are of the order of  $10^{-2}$ – $10^{-1}$  Pa s for low-molar-mass liquid crystals; for *polymeric liquid-crystals* their values depend strongly on the molar mass of the polymer.

Note 2: The friction coefficients can be expressed in terms of the *Leslie-Ericksen coefficients* as follows:

$$\gamma_1 = \alpha_3 - \alpha_2$$

$$\gamma_2 = \alpha_6 - \alpha_5$$

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Note 3:  $\gamma_1$  is often called the rotational viscosity or the twist viscosity, i.e., the viscosity associated with the rotation of the *director* without material flow.

### 5.7 backflow

Motion of a liquid crystal associated with the rate of change of the *director* in the direction opposite to that of the action of an external field.

### 5.8 anisotropy of physical properties

Dependence of certain physical properties, like the electric permittivity, refractive index and magnetic susceptibility on direction. It is created by long-range orientational order in a *mesophase*, provided the corresponding molecular property is anisotropic.

Note: The symmetry of the tensor representing the average anisotropic property cannot be lower than the symmetry of the phase.

#### 5.8.1 uniaxial mesophase anisotropy, $\Delta\tilde{\chi}$

Value of a property  $\tilde{\chi}$  parallel to the *director*  $\tilde{\chi}_{\parallel}$  minus that perpendicular to it  $\tilde{\chi}_{\perp}$ :

$$\Delta\tilde{\chi} = \tilde{\chi}_{\parallel} - \tilde{\chi}_{\perp}$$

Note 1: The tilde is used to indicate a property of a liquid-crystal *mesophase*.

Note 2:  $\Delta\tilde{\chi}$  provides a practical measure of the orientational order of a *mesophase* and necessarily vanishes in an isotropic phase.

Note 3: For *mesophases* composed of cylindrically symmetric molecules there is a precise relationship between the magnetic anisotropy,  $\Delta\tilde{\chi}$ , and the second-rank orientational parameter  $\langle P_2 \rangle$ .

$$\Delta\tilde{\chi} = (2/3)(\tilde{\chi}_{zz} - \tilde{\chi}_{xx})\langle P_2 \rangle$$

#### 5.8.2 biaxial mesophase anisotropies, $\Delta\tilde{\chi}$ and $\delta\tilde{\chi}$

With the principal phase axes, corresponding to the three *directors*  $\mathbf{l}$ ,  $\mathbf{m}$ , and  $\mathbf{n}$  (see Definition 3.3, Note 1) labelled X, Y, and Z such that  $\tilde{\chi}_{zz} > \tilde{\chi}_{xx} > \tilde{\chi}_{yy}$ , the major biaxial mesophase anisotropy,  $\Delta\tilde{\chi}$ , is defined by

$$\delta\tilde{\chi} = (\tilde{\chi}_{zz} - \tilde{\chi}_{yy})$$

and the biaxial mesophase anisotropy is

$$\Delta\tilde{\chi} = \tilde{\chi}_{zz} - (1/2)(\tilde{\chi}_{xx} + \tilde{\chi}_{yy})$$

Note 1: The long-range biaxial ordering of the *mesophase* means that the three principal components of a second-rank tensorial property will not normally be the same, hence the two measures of the anisotropy  $\Delta\tilde{\chi}$  and  $\delta\tilde{\chi}$ .

Note 2: At a transition to a *uniaxial mesophase*  $\delta\tilde{\chi}$  vanishes. The **relative biaxiality**,  $\eta$ , is defined as the ratio of  $\delta\tilde{\chi}$  to  $\Delta\tilde{\chi}$ .

## 5.9 ferroelectric effects

Ferroelectric *mesophase* that appears through the breaking of symmetry in a tilted *smectic mesophase* by the introduction of molecular chirality and, hence, *mesophase* chirality.

Note 1: When the numbers of layers with opposite tilt directions are not the same, the *smectic mesophase* has ferroelectric properties.

Note 2: The appearance of a spontaneous polarization,  $| \mathbf{P}_s |$ , in *chiral tilted smectic mesophases* is caused by a long-range ordering of molecular transverse electric dipoles.

Note 3: The polarization  $| \mathbf{P}_s |$  can be switched between two stable states with an external electric field ( $E$ ); these states are stable in zero electric field.

Note 4: The switching time,  $\tau$ , is given by

$$\tau = \gamma_1 \sin \theta / \mathbf{P}_s \cdot \mathbf{E}$$

where  $\gamma_1$  is the twist viscosity (see Definition 5.6, Note 3) and  $\theta$  is the tilt angle.

Note 5: The spontaneous polarization depends on the transverse component,  $\mu_t$ , of the molecular dipole, the number density,  $\rho$ , and the polar or first-rank *order parameter*,  $\langle \cos \varphi \rangle$ , the ensemble average of  $\cos \varphi$ , where  $\varphi$  is the angle between the transverse axis and the minor *director*, see Definition 3.3, by

$$| \mathbf{P}_s | = \rho \mu_t \langle \cos \varphi \rangle$$

Note 6: Typical values of the spontaneous polarization,  $| \mathbf{P}_s |$ , in *chiral smectic C mesophases* are between  $10^{-3}$  and  $10^{-4} \text{ C m}^{-2}$ .

Note 7: When the tilt direction alternates from layer to layer, the *smectic mesophase* is antiferroelectric; such *mesophases* do not possess spontaneous polarization. They can be turned into ferroelectric structures through the application of an electric field.

## 5.10 Fréedericksz transition

Elastic deformation of the *director*, induced by a magnetic induction or electric field, in a uniformly aligned, thin sample of a *nematic* confined between two surfaces.

Note 1: The Fréedericksz transition occurs when the strength of the applied field exceeds a certain threshold value (see Definition 5.12).

Note 2: For the magnitude of the magnetic induction this threshold has the form

$$B_{\text{th}} = (\pi/d)(\mu_0 K_i / \Delta \tilde{\chi})^{1/2}$$

where,  $B_{\text{th}}$  is the threshold magnetic induction (flux density),  $d$  is the thickness of the *nematic* film,  $\mu_0$  is the permeability of a vacuum, and  $\Delta \tilde{\chi}$  is the *magnetic anisotropy*. The particular *elastic constant*  $K_i$  depends on the geometry of the experiment.

Note 3: For an electric field, this threshold has the form

$$E_{\text{th}} = (\pi/d)(\epsilon_0 K_i / \Delta \tilde{\epsilon})^{1/2}$$

where  $\epsilon_0$  is the permittivity of vacuum and  $\Delta \tilde{\epsilon}$  is the dielectric *anisotropy*.

## 5.11 electroclinic effect

Tilt in an A *mesophase* is called the electroclinic effect.

Note: In high polarization materials induced tilt angles as high as  $10^\circ$  have been observed.

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### 5.12 threshold fields

**threshold electric field**,  $E_{\text{th}}$ , SI unit: V m<sup>-1</sup>

**threshold magnetic induction**,  $B_{\text{th}}$ , SI unit: T

Critical electric field strength or magnetic induction necessary to change the equilibrium *director* alignment imposed by constraining surfaces.

Note: See Definition 5.10, Notes 1–3.

### 5.13 electrohydrodynamic instabilities, (EHD instabilities)

Instabilities caused by the anisotropy of conductivity and corresponding to a periodic deformation of the alignment of the *director* in a *nematic monodomain* under the action of a direct current or low-frequency alternating current.

Note 1: See Definition 4.2 for the definition of a *monodomain*.

Note 2: The basic electric parameters determining EHD instabilities are the dielectric anisotropy,  $\Delta\tilde{\epsilon}$ , and the anisotropy of the (ionic) conductivity,  $\Delta\tilde{\sigma}$ .

Distortion of the *director*, space charges and the motion of the fluid are coupled through the applied electric field. Above a given threshold, fluctuations of these quantities are amplified and EHD instabilities develop.

### 5.14 Williams domains

#### Kapustin domains

Regions in a liquid crystal having a specific cellular periodic flow-pattern in the form of long rolls induced by the application of an electric field perpendicular to a *nematic* layer with an initial *planar alignment* of the *director*.

Note 1: The *nematic* liquid crystal must have a negative dielectric anisotropy ( $\Delta\tilde{\epsilon} < 0$ ), and a positive anisotropy ( $\Delta\tilde{\sigma} > 0$ ). The *optical texture* corresponding to the flow pattern consists of a set of regularly spaced, black and white stripes perpendicular to the initial direction of the *director*. These stripes are caused by the periodicity of the change in the refractive index for the extraordinary ray due to variations in the *director* orientation.

Note 2: The *domains* exist over only a small range of electric-field strength.

### 5.15 dynamic-scattering mode, (DSM)

State of a liquid crystal that shows a strong scattering of light due to a turbulent flow resulting from an applied voltage greater than a particular critical value.

Note 1: In DSM the *Williams (Kapustin) domains* become distorted and mobile, and macroscopic *director* alignment is completely disturbed.

Note 2: A liquid crystal in DSM has a complicated *optical texture*.

### 5.16 flexo-electric effect

Electric polarization resulting from a splay or bend deformation of the *director* of a *nematic* liquid crystal.

Note 1: See Fig. 32.

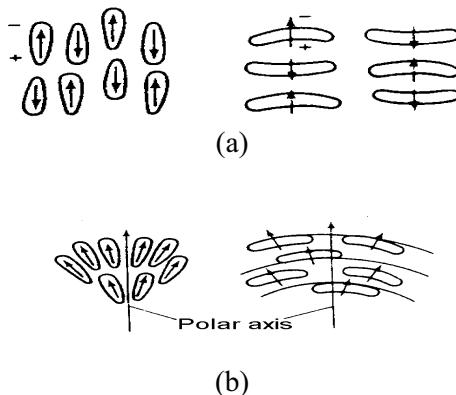
Note 2: The molecular origins of dipolar flexo-electricity are the particular shape anisotropy (e.g., resembling a pear or banana) of the molecules, each of which must also possess a permanent dipole moment.

Note 3: The net polarization,  $\mathbf{P}$ , is proportional to the distortion:

$$\mathbf{P} = e_1 \mathbf{n}(\text{div } \mathbf{n}) + e_3 (\text{rot } \mathbf{n}) \times \mathbf{n}$$

where  $e_1$  and  $e_3$  are the flexo-electric coefficients. They have the units of an electric potential, namely  $\text{J C}^{-1}$ , of arbitrary sign.

Note 4: The flexo-electric effect is the analogue of the piezo-electric effect in solids, where the polarization is induced by a strain that produces a translational deformation of the crystal. The flexo-electric effect in a liquid crystal is caused by a purely orientational deformation.



**Fig. 32.** Schematic representation of the flexo-electric effect. (a) The structure of an undeformed nematic liquid crystal with pear- and banana-shaped molecules; (b) the same liquid crystal subjected to splay and bend deformations, respectively.

### 5.17 flexo-electric domain

*Domain* corresponding to a periodic deformation caused by the inverse flexo-electric effect in a *nematic* liquid crystal.

Note: A flexo-electric domain occurs when  $\Delta\tilde{\epsilon} < 4\pi el/K$  where  $e$  is the flexo-electric coefficient and  $K$  is the *elastic constant*, assuming  $K_1 = K_3 = K$  and  $e_1 = -e_3 = e$  (see Definitions 5.3 and 5.16).

### 5.18 twisted-nematic cell

Twisted *nematic* liquid crystal sandwiched between two glass plates, with the *director* aligned parallel to the plates, with one of the plates turned in its own plane about an axis normal to it.

### 5.19 ‘time-on’ of the electro-optical effect, $\tau_{\text{on}}$ , SI unit: s turn-on time

Time required for the light intensity viewed through crossed polarizers to increase to 90% of the final value from the off-state to the on-state of an electro-optical twisted-nematic cell.

Note: In the off-state the electro-optical cell contains a thin film of a *nematic liquid-crystal* with mutually perpendicular *directors* at the upper and lower glass plates; hence to reach the on-state the *director* performs a 90° twist over the thickness of the liquid crystal film.

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### 5.20 ‘time-off’ of the electro-optical effect, $\tau_{\text{off}}$ , SI unit: s turn-off time

The time required for the light intensity viewed through crossed polarizers to decrease by 90% from the on-state to the off-state of an electro-optical twisted-nematic cell.

Note: See the note to Definition 5.19.

### 5.21 rise time, SI unit: s

Time required by an electro-optical *nematic* cell for a light-intensity change from 10% to 90 % of the maximum intensity on going from the off-state to the on-state.

Note: See the note to Definition 5.19.

### 5.22 fall time, SI unit: s decay time

Time required by an electro-optical twisted-nematic cell for a light-intensity change from 90% to 10 % of the maximum intensity on going from the on-state to the off-state.

Note: See the note to Definition 5.19.

### 5.23 guest-host effect

Field-induced change in the orientation of either dichroic dye molecules (the guest) dissolved in a *mesophase* (the host) or dichroic dye moieties (the guest) of polymers (the host) resulting in changes in the absorption spectrum of a mesomorphic mixture.

## 6 LIQUID CRYSTAL POLYMERS

### 6.1 liquid-crystal polymer, (LCP) polymer liquid-crystal, (PLC) liquid-crystalline polymer

Polymer material that, under suitable conditions of temperature, pressure and concentration, exists as a *LC mesophase*.

### 6.2 main-chain polymer liquid-crystal, (MCPLC) main-chain liquid-crystalline polymer, (MCLCP)

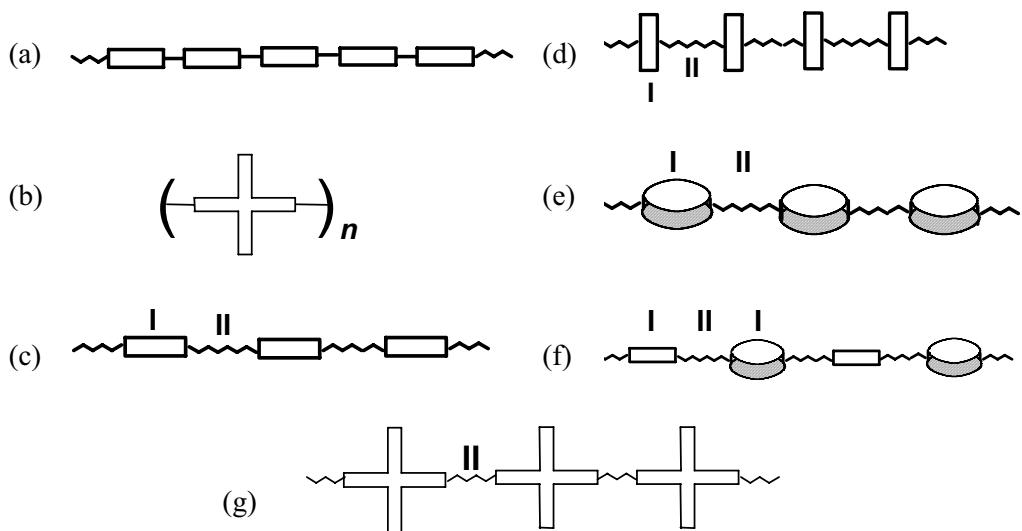
Polymer containing *mesogenic* units in their main chains but not in side-chains.

Note 1: A MCPLC is formed by linking together suitable relatively rigid units directly or through appropriate functional groups (see Fig. 33).

Note 2: The linkage between the rigid units (I) may be (a) direct or (b-g) via flexible spacers (II).

Note 3: A MCPLC with cross-shaped *mesogenic groups* (b or g) is known as a **cruciform (or star) polymer liquid crystal**.

Note 4: The rigid units may, but often do not, possess intrinsic *mesogenic* character.

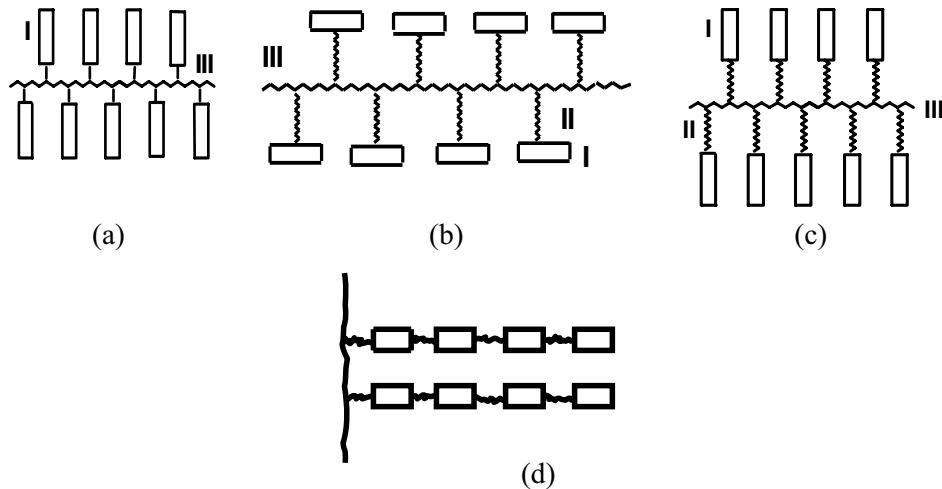


**Fig. 33.** Examples of main-chain polymer liquid crystals: I - *mesogenic group*; II - *spacer*.

### 6.3 side-group or side-chain polymer liquid-crystal, (SGPLC, SCPLC) side-group or side-chain liquid-crystalline polymer, (SGLCP, SCLCP) polymer with mesogenic side-groups or side-chains comb-shaped (comb-like) polymer liquid crystal

Polymer, the molecules of which have *mesogenic units* only in the side-groups or side-chains.

Note 1: The *mesogenic groups* (I) in a SGPLC can be connected to the backbone (III) either (a) directly or (b, c) via flexible *spacers* (II) (see Fig. 34).



**Fig. 34.** Examples of side-group polymer liquid crystals: I - *mesogenic group*; II - *spacer*; III - *backbone*. The terminology ‘side-group’ is used for (a), ‘side-on fixed’ is used for (b), ‘end-on fixed’ for (c) and ‘side-chain’ for (d).

Note 2: The structures as in Fig. 34 can also be used with the proviso that the side-group units are replaced by chains containing *mesogens*.

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Note 3: Examples of polymer backbones are polyacrylates, polymethacrylates, and polysiloxanes; the *spacers* are usually oligomethylene, oligo(oxyethylene), or oligosiloxane.

Note 4: The pendant groups in these polymers have structures compatible with liquid-crystal formation, that is, they are *mesogenic* but not intrinsically mesomorphic. See the examples given in Definitions 2.10; 2.11.2.1.

Note 5: If the *mesogenic* side-groups are rod-like (*calamitic*) in nature, the resulting polymer may, depending upon its detailed structure, exhibit any of the common types of *calamitic mesophases*: *nematic*, *chiral nematic* or *smectic*. Side-on fixed SGPLC, however, are predominantly *nematic* or *chiral nematic* in character. Similarly, disc-shaped side-groups tend to promote *discotic nematic* or *columnar mesophases* while amphiphilic side-chains tend to promote amphiphilic or *lyotropic mesophases*.

Note 6: A plethora of types of copolymers can be produced. For example, non-*mesogenic* side-groups may be used in conjunction with *mesogenic* side-groups and the polymer backbone may be substituted, to various degrees, with side-groups or chains.

### 6.4 spacer

Flexible segment used to link successive *mesogenic* units in the molecules of MCPLCs or to attach *mesogenic* units as side-groups onto the polymer backbone of SGPLCs.

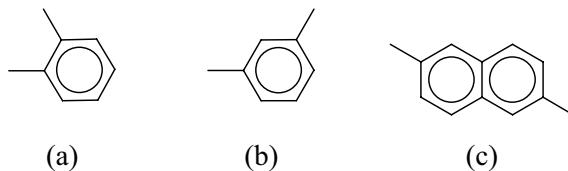
Note 1: Examples of *spacers* are: oligomethylene, oligooxyethylene, or oligosiloxane chains.

Note 2: The term is also used for the group linking two or more *mesogenic* units in *liquid-crystal oligomers*.

### 6.5 disruptor

Chemical group used to disrupt the linearity of the backbone of molecules of MCLCPs.

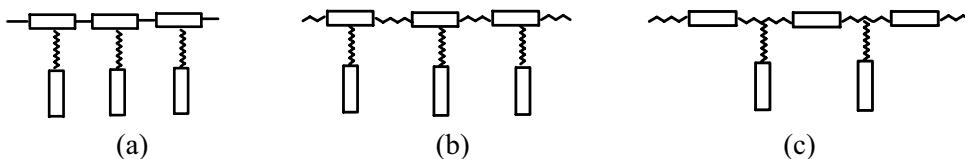
Note: Examples are (a, b) rigid-kink or (c) crankshaft units.



### 6.6 combined liquid-crystalline polymer

*Liquid-crystalline polymer* consisting of macromolecules in which *mesogenic groups* are incorporated both in the main-chain and in the side-groups.

Note: See Fig. 35. The *mesogenic* side-groups can be attached either as lateral substituents to the backbone *mesogenic* moieties that are connected to each other either (a) directly or (b) by *spacers* or (c) they can be attached to the *spacer* incorporated into the main-chain.



**Fig. 35.** Examples of combined liquid-crystalline polymers.

### 6.7 rigid chain

Rod-like chain of a MCPLC with direct links between the *mesogenic groups* for which the persistence length is at least comparable with the contour length and much greater than the diameter.

Note 1: The persistence length is a characteristic of the stiffness of a chain in the limit of infinite chain length.

Note 2: A polymer composed of molecules that have rigid rod-like groups or chains usually does not show thermotropic mesomorphic behaviour because decomposition occurs below its melting point.

Note 3: A polymer composed of molecules that have rigid rod-like groups or chains may form *LC mesophases* in solution under suitable conditions. These are sometimes described as *lyotropic* but, as the solvent does not induce the formation of aggregates or micelles, this term is not appropriate.

### 6.8 semi-rigid chain

Chain for which the contour length is greater than the persistence length but for which their ratio is still below the Gaussian limit.

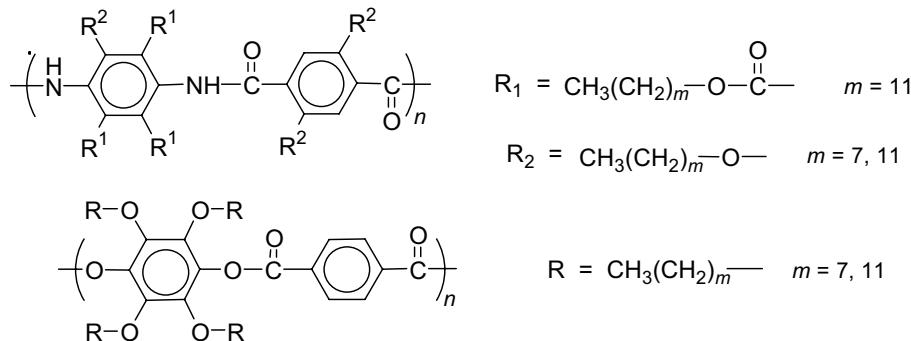
Note: Some polymers composed of semi-rigid chains form *amphiphilic mesogens*.

Examples: polyisocyanates and (2-hydroxyethyl)cellulose.

### 6.9 board-shaped polymer

Polymer chain composed of a rigid backbone to which many lateral side-groups are attached, giving the repeating unit a board-like shape.

Note 1: The rigid backbone often has a polyester, polyamide or poly(ester-amide) type of structure. Examples are:



Note 2: A polymer *LC* consisting of macromolecules of board-like shape can be called a board-shaped polymer *LC*. Such polymers can form *sanidic mesophases*.

### 6.10 liquid-crystal dendrimer dendrimeric liquid crystal dendritic liquid crystal

Highly branched oligomer or polymer of dendritic structure containing *mesogenic groups* that can display *mesophase* behaviour.

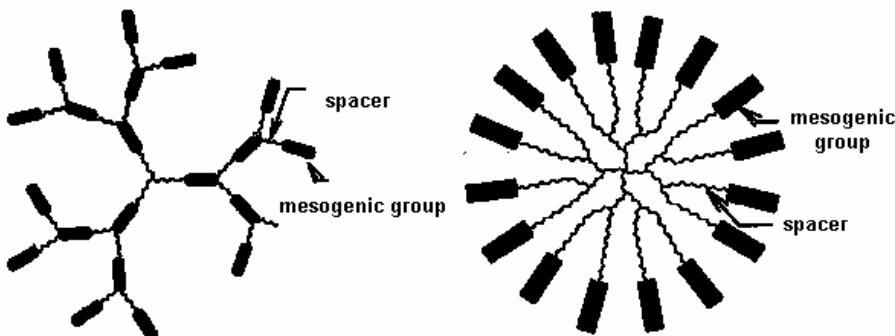
Note 1: See Fig. 36. The *mesogenic groups* can be located along the chains of the molecule (a) or can occur as terminal groups (b).

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Note 2: The *mesogenic groups* can be, e.g., rod-like or disc-like, and can be attached laterally or longitudinally to the flexible *spacers*.

### 6.11 hyperbranched polymer liquid-crystal

Polymer composed of highly branched macromolecules containing *mesogenic groups* of which any linear subchain generally may lead in either direction, to at least two other subchains.



**Fig. 36.** Liquid-crystal dendrimers: (a) with *mesogenic groups* in the whole volume of a macromolecule; (b) with terminal *mesogenic groups*.

### 6.12 banded texture band texture

Alternating dark and bright bands observed, following shear, in a wide range of main-chain *nematic* and *chiral nematic liquid-crystalline polymers*.

Note 1: The bands always lie perpendicular to the prior shear direction.

Note 2: In general, bands form after the cessation of shear, but, under some circumstances, they may appear during the flow process

Note 3: The bands are associated with a periodic variation in the *director* orientation about the flow axis.

## 7 REFERENCES

1. D. Demus, G. W. Gray, H. W. Spiess, V. Vill (Eds.). *Handbook of Liquid Crystals*. Wiley-VCH, New York (1998), Vols. Q, 2a, 2b, and 3, J.
2. W. Brostow (Ed.). *Polymer Liquid Crystals Mechanical and Thermophysical Properties*. Chapman & Hall, London (1996).
3. V. Vill. LIQCRYST 2.1, Database of Liquid Crystalline Compounds for Personal Computers, LCI Publisher GmbH, Hamburg (1996).
4. L. M. Blinov and V. G. Chigrinov. *Electrooptic Effects in Liquid Crystal Materials*, Springer-Verlag, New York (1994).
5. V. P. Shibaev and Lui Lam (Eds.). *Liquid Crystalline and Mesomorphic Polymers*, Springer-Verlag, New York (1994).
6. H. Stegmeyer (Ed.). *Topics in Physical Chemistry*, Vol. 3, *Liquid Crystals*, Springer-Verlag, New York (1994).
7. G. R. Luckhurst and C. A. Veracini (Eds.). *The Molecular Dynamics of Liquid Crystals*, Kluwer, Dordrecht (1994).