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C2C 1600 1601 200 20Y 215 21X 220 226 227 22Y 246 248 250 252 257 259 25Y 270 271 280 29X 29Y 304 305 30Y 313 314 31Y 320 326 337 338 342 34Y 350 351 352 364 366 367 368 36Y 37X 387 400 401 40Y 43X 440 47X 485 488 490 500 50Y 54X 573 574 579 624 625 628 62X 62Y 644 652 658 65X 662 666 66X 672 676 678 67X 68Y 699 69Y 713 73Y 746 761 762 776 779 77Y 799 BK KF KV MB MC NA NR TB TC TJ TR WS ZL
C4X 12

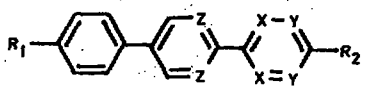
(19)

(54) PYRIMIDINE DERIVATIVES

(71) We, F. HOFFMANN-LA ROCHE & CO., AKTIENGESELLSCHAFT, a Swiss Company of 124—184 Grenzacherstrasse, Basle, Switzerland, do hereby declare the invention for which we pray that a patent may be granted to us, and the method by which it is to be performed, to be particularly described in and by the following statement:—

The present invention relates to pyrimidine derivatives. More particularly, the invention is concerned with pyrimidine derivatives, a process for the manufacture thereof, nematic mixtures for electro-optical purposes containing same and a process for the preparation of said nematic mixtures. The invention is also concerned with an electro-optical apparatus containing said pyrimidine derivatives and with a process for the production of said apparatus.

The pyrimidine derivatives provided by the present invention have the following general formula



I

wherein each of the symbols X represents a nitrogen atom and each of the symbols Y and Z represents —CH— or each of the symbols Y represents a nitrogen atom and each of the symbols X and Z represents —CH— or each of the symbols Z represents a nitrogen atom and each of the symbols X and Y represents —CH— and one of the symbols R_1 and R_2 represents a cyano group and the other represents a straight-chain alkyl group containing 1 to 7 carbon atoms, a straight-chain alkoxy group containing 1 to 7 carbon atoms or a straight-chain alkanoyloxy group containing 2 to 7 carbon atoms.

The pyrimidine derivatives of formula I are particularly valuable as components of nematic mixtures and, for the most part, they possess liquid crystalline properties. The present pyrimidine derivatives possess, inter alia, a very high positive anisotropy of the dielectric constants ($\varepsilon_{11} > \varepsilon_{\perp}$, ε_{11} signifying the dielectric constant along the longitudinal axis of the molecule and $\varepsilon_{\perp}$ denoting the dielectric constant perpendicular thereto).

In an electric field, the pyrimidine derivatives of formula I orientate themselves (because $\varepsilon_{\parallel} > \varepsilon_{\perp}$) with the direction of their largest dielectric constant (i.e. with their longitudinal axes) parallel to the field direction. This effect is used, *inter alia*, in the interaction between embedded molecules and the liquid crystalline molecules (guest-host interaction) described by J. H. Heilmeier and L. A. Zanoni [Applied Physics Letters *13*, 91 (1968)]. A further interesting application of the dielectric field orientation exists in the rotation cell discovered by M. Schadt and W. Helfrich [Applied Physics Letters *18*, (1971)] and in the Kerr cell described in Molecular Crystals and Liquid Crystals *17*, 355 (1972).

The electro-optical rotation cell is essentially a condenser having transparent electrodes, the dielectric of which is formed from a nematic crystal with $\varepsilon_{\parallel} > \varepsilon_{\perp}$. The longitudinal molecular axes of the liquid crystals are arranged in twisted form between the condenser plates in the fieldless state, the twisting structure being determined by the given wall orientation of the molecules. Upon the application of an electric potential to the condenser plates, the molecules adjust themselves with their longitudinal axes in the field direction (i.e. perpendicular to the surface of the plates), by which means linear polarised light is no longer rotated in the dielectric (the liquid crystal is uniaxially perpendicular to the surface of the plates). This effect is reversible and can be used to electrically control the optical transmissivity of the condenser.

In such a "light rotation cell" it is, *inter alia*, desirable to use compounds or mixtures which possess a low threshold potential, this being important, for example, when a rotation cell is used in clocks.

It has now been found in accordance with the present invention that the pyrimidine derivatives of formula I have a particularly large mesophase range with high clearing points and that, accordingly, they are particularly suitable for increasing the clearing points of nematic mixtures. In addition, they not only possess the required large positive anisotropy of the dielectric constants, and accordingly low threshold potentials, in indicating devices based on a field effect, for example, the rotation cell described earlier, but they exhibit a short relay time and a high chemical stability. Furthermore, the pyrimidine derivatives of formula I considerably improve, in indicating devices based on a field effect, the steepness of the optical transmission curves as a function of the potential applied when they are admixed with other nematic substances such as, for example, para-cyano-substituted Schiff's bases, esters or biphenyls. This property renders the pyrimidine derivatives of formula I particularly valuable for multiplex working and for application in indicting devices having a low threshold potential. A further advantage of the present pyrimidine derivatives is that they are colourless. Mixtures which contain the pyrimidine derivatives of formula I are characterised by having a ready orientability and provide a high contrast in indicating devices.

The following pyrimidine derivatives fall within the scope of formula I hereinbefore:

2-(4-Cyanophenyl)-5-(4-methylphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-ethylphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-pentylphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-hexylphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-heptylphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-methoxyphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-ethoxyphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-propoxyphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-butoxyphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-pentyloxyphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-hexyloxyphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-heptyloxyphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-acetoxyphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-propionyloxyphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-butyryloxyphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-valeryloxyphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-hexanoyloxyphenyl)-pyrimidine,
2-(4-cyanophenyl)-5-(4-n-heptanoyloxyphenyl)-pyrimidine,
2-(4-methylphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-ethylphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-n-propylphenyl)-5-(4-cyanophenyl)-pyrimidine,

2-(4-n-butylphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-n-pentylphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-n-hexylphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-n-heptylphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-methoxyphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-ethoxyphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-n-propoxyphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-n-butoxyphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-n-pentyloxyphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-n-hexyloxyphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-n-heptyloxyphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-acetoxyphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-n-propionyloxyphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-n-butyryloxyphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-n-valeryloxyphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-n-hexanoyloxyphenyl)-5-(4-cyanophenyl)-pyrimidine,
2-(4-n-heptanoyloxyphenyl)-5-(4-cyanophenyl)-pyrimidine,
5-methyl-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-ethyl-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-n-propyl-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-n-butyl-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-n-pentyl-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-n-hexyl-2-(4′-cyano-4-biphenylyl)-pyrimidine
5-n-heptyl-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-methoxy-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-ethoxy-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-n-propoxy-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-n-butoxy-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-n-pentyloxy-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-n-hexyloxy-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-n-heptyloxy-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-acetoxy-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-n-propionyloxy-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-n-butyryloxy-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-n-valeryloxy-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-n-hexanoyloxy-2-(4′-cyano-4-biphenylyl)-pyrimidine,
5-n-heptanoyloxy-2-(4′-cyano-4-biphenylyl)-pyrimidine,
2-methyl-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-ethyl-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-propyl-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-butyl-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-pentyl-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-hexyl-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-heptyl-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-methoxy-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-ethoxy-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-propoxy-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-butoxy-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-pentyloxy-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-hexyloxy-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-heptyloxy-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-acetoxy-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-propionyloxy-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-butyryloxy-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-valeryloxy-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-hexanoyloxy-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-n-heptanoyloxy-5-(4′-cyano-4-biphenylyl)-pyrimidine,
2-cyano-5-(4′-methyl-4-biphenylyl)-pyrimidine,
2-cyano-5-(4′-ethyl-4-biphenylyl)-pyrimidine,
2-cyano-5-(4′-n-propyl-4-biphenylyl)-pyrimidine,
2-cyano-5-(4′-n-butyl-4-biphenylyl)-pyrimidine,
2-cyano-5-(4′-n-pentyl-4-biphenylyl)-pyrimidine,
2-cyano-5-(4′-n-hexyl-4-biphenylyl)-pyrimidine,
2-cyano-5-(4′-n-heptyl-4-biphenylyl)-pyrimidine,
2-cyano-5-(4′-methoxy-4-biphenylyl)-pyrimidine,

2-cyano-5-(4'-ethoxy-4-biphenylyl)-pyrimidine,
2-cyano-5-(4'-n-propoxy-4-biphenylyl)-pyrimidine,
2-cyano-5-(4'-n-butoxy-4-biphenylyl)-pyrimidine,
2-cyano-5-(4'-n-pentyloxy-4-biphenylyl)-pyrimidine,
2-cyano-5-(4'-n-hexyloxy-4-biphenylyl)-pyrimidine,
2-cyano-5-(4'-n-heptyloxy-4-biphenylyl)-pyrimidine,
2-cyano-5-(4'-acetoxy-4-biphenylyl)-pyrimidine,
2-cyano-5-(4'-n-propionyloxy-4-biphenylyl)-pyrimidine,
2-cyano-5-(4'-n-butyryloxy-4-biphenylyl)-pyrimidine,
2-cyano-5-(4'-n-valeryloxy-4-biphenylyl)-pyrimidine,
2-cyano-5-(4'-n-hexanoyloxy-4-biphenylyl)-pyrimidine,
2-cyano-5-(4'-n-heptanoyloxy-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-methyl-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-ethyl-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-n-propyl-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-n-butyl-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-n-pentyl-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-n-hexyl-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-n-heptyl-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-methoxy-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-ethoxy-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-n-propoxy-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-n-butoxy-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-n-pentyloxy-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-n-hexyloxy-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-n-heptyloxy-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-acetoxy-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-n-propionyloxy-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-n-butyryloxy-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-n-valeryloxy-4-biphenylyl)-pyrimidine,
5-cyano-2-(4'-n-hexanoyloxy-4-biphenylyl)-pyrimidine, and
5-cyano-2-(4'-n-heptanoyloxy-4-biphenylyl)-pyrimidine.

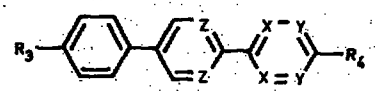
Amongst the pyrimidine derivatives of formula I, those in which one of the symbols R_1 and R_2 represents a cyano group and the other represents a straight-chain alkyl group containing 3 to 7 carbon atoms are preferred. In addition, those pyrimidine derivatives of formula I in which each of the symbols Y represents —CH— are preferred. The pyrimidine derivatives of formula I in which each of the symbols Z represents a nitrogen atom and each of the symbols X and Y represents —CH— are particularly preferred. Further particularly preferred pyrimidine derivatives of formula I are those in which the symbol R_2 represents a cyano group.

As will be evident from the foregoing, those pyrimidine derivatives of formula I in which one of the symbols R_1 and R_2, preferably the symbol R_2, represents a cyano group and the other represents a straight-chain alkyl group containing 3 to 7 carbon atoms and each of the symbols Z represents a nitrogen atom and each of the symbols X and Y represents —CH— are particularly preferred.

Especially preferred pyrimidine derivatives of formula I are:
2-(4-Cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and
2-(4-cyanophenyl)-5-(4-n-hexylphenyl)-pyrimidine.

According to the process provided by the present invention, the pyrimidine derivatives of formula I hereinbefore are manufactured by

(a) reacting a compound of the general formula

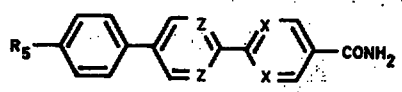


II

wherein one of the symbols R_3 and R_4 represents a straight-chain alkyl group containing 1 to 7 carbon atoms, a straight-chain alkoxy group containing 1 to 7 carbon atoms or a straight-chain alkanoyloxy group containing 2 to 7 carbon atoms and the other represents a halogen atom and the symbols X, Y and Z have the significance given earlier, with copper-(I) cyanide, sodium cyanide or potassium cyanide, or

(b) for the manufacture of pyrimidine derivatives of formula I in which each of the symbols Y represents —CH—, the symbol R_2 represents a cyano group and

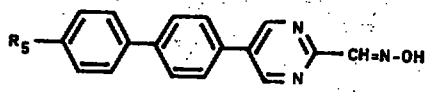
the symbols R_1, X and Z have the significance given earlier, dehydrating a compound of the general formula



III

wherein the symbol R_5 represents a straight-chain alkyl group containing 1 to 7 carbon atoms, a straight-chain alkoxy group containing 1 to 7 carbon atoms or a straight-chain alkanoyloxy group containing 2 to 7 carbon atoms and the symbols X and Z have the significance given earlier, or

(c) for the manufacture of pyrimidine derivatives of formula I in which each of the symbols Y represents a nitrogen atom, the symbol R_2 represents a cyano group and the symbols R_1, X and Z have the significance given earlier, dehydrating a compound of the general formula



IV

wherein R_5 has the significance given earlier.

In embodiment (a) of the foregoing process, a compound of formula II is reacted with copper-(I) cyanide, sodium cyanide or potassium cyanide. This reaction is conveniently carried out in an inert organic solvent such as ethyleneglycol, tetrahydrofuran, dimethylformamide, dimethylsulphoxide, pyridine or acetonitrile. The temperature and pressure are not critical aspects of this reaction. The reaction can be carried out at atmospheric pressure and a temperature between room temperature and the boiling point of the reaction mixture. The halogen atom present in the compound of formula II is preferably a bromine atom.

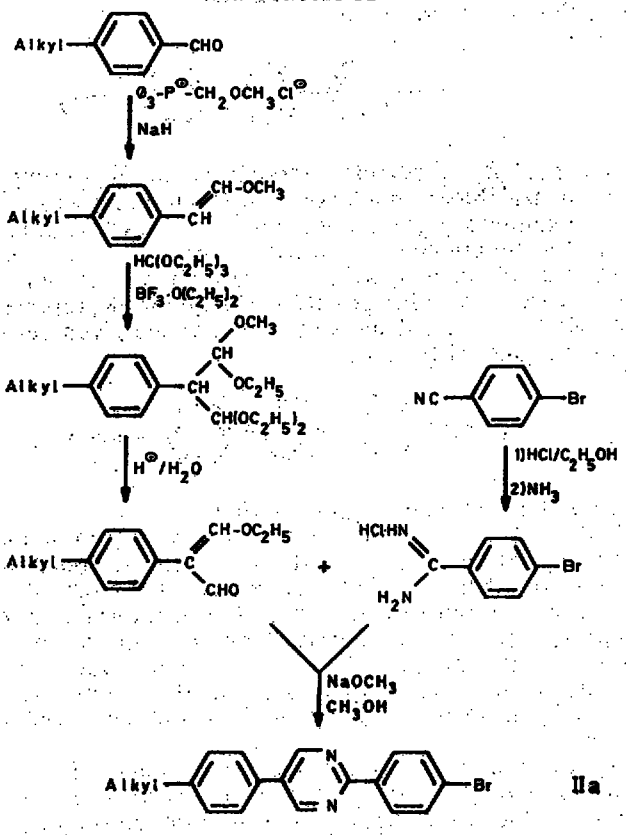
The dehydration of a compound of formula III in accordance with embodiment (b) of the foregoing process can be carried out using any suitable dehydrating agent such as phosphorus oxychloride, phosphorus pentoxide, thionyl chloride or acetic anhydride. The dehydration can be carried out in an inert organic solvent such as a hydrocarbon or a halogenated hydrocarbon, if necessary in the presence of a base such as sodium acetate, pyridine or triethanolamine. The dehydration can, however, also be carried out in the absence of an organic solvent. The dehydration may be carried out at the reflux temperature of the mixture. The pressure is not critical; it is advantageous, however, to carry out the dehydration at atmospheric pressure.

In embodiment (c) of the foregoing process, a compound of formula IV is dehydrated. This dehydration is conveniently carried out using acetic anhydride or using anhydrous sodium acetate in glacial acetic acid. This dehydration may be carried out at the reflux temperature of the mixture. The pressure is not critical; it is advantageous, however, to carry out the dehydration at atmospheric pressure.

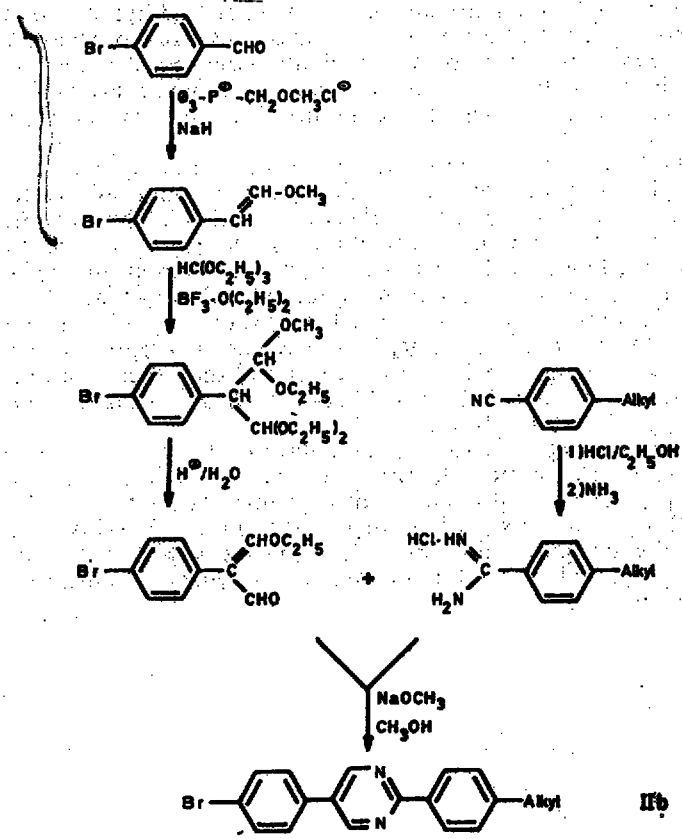
The preparation of the starting materials of formulae II, III and IV is illustrated in Formula Schemes A to I hereinafter for such starting materials in which one of the symbols R_3 and R_4 (or the symbol R_5) represents a straight-chain alkyl group containing 1 to 7 carbon atoms and the other represents a bromine atom. In these Formulae Schemes "Alkyl" means a straight-chain alkyl group containing 1 to 7 carbon atoms.

Throughout the specification and claims, the straight-chain alkyl groups with 1 to 7 carbon atoms are methyl, ethyl, n-propyl, n-butyl, n-pentyl, n-hexyl and n-heptyl groups, the straight-chain alkoxy groups with 1 to 7 carbon atoms are methoxy, ethoxy, n-propoxy, n-butyloxy, n-pentyloxy, n-hexyloxy and n-heptyloxy groups and the straight-chain alkanoyloxy groups with 2 to 7 carbon atoms are acetoxy, n-propionyloxy, n-butyryloxy, n-valeryloxy, n-hexanoyloxy and n-heptanoyloxy groups.

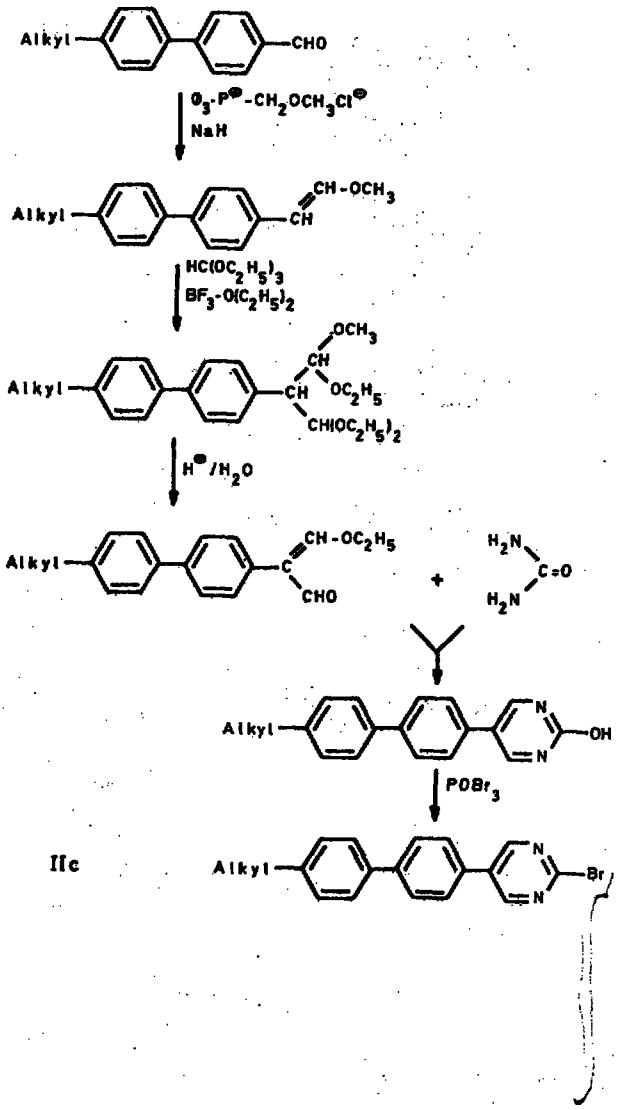
Formula Scheme A



Formula Scheme B

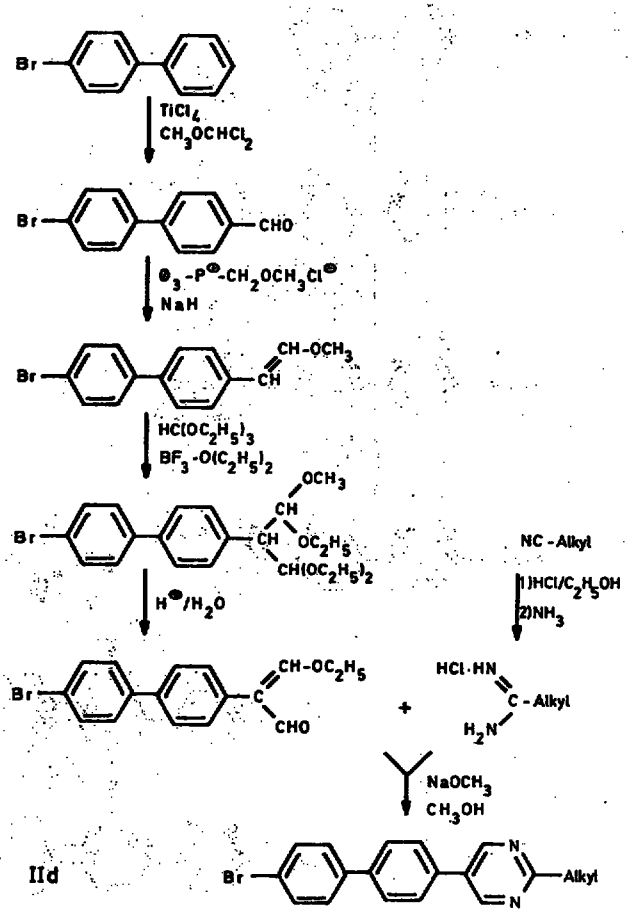


Formula Scheme C



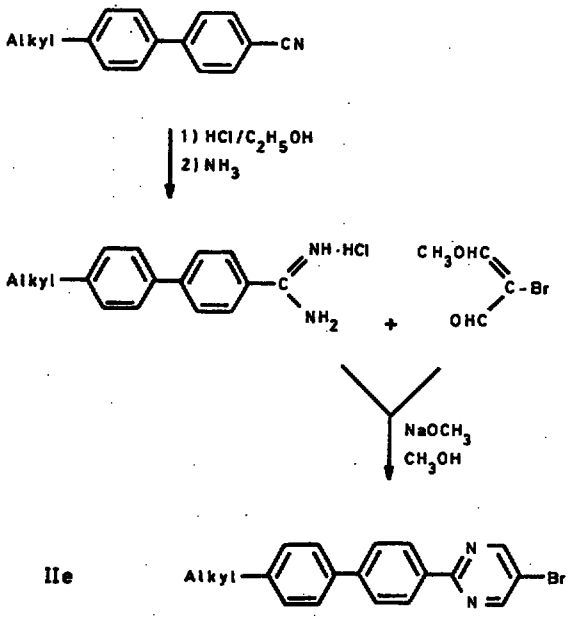
IIc

Formula Scheme D



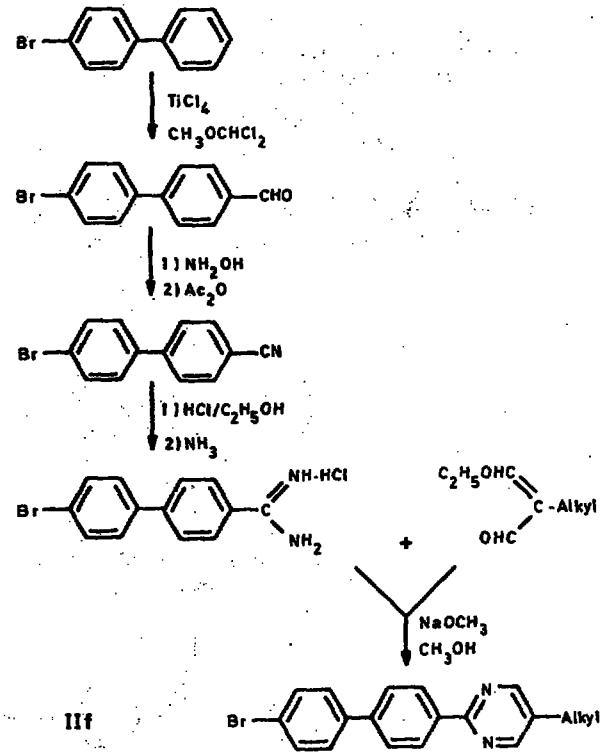
IId

Formula Scheme E

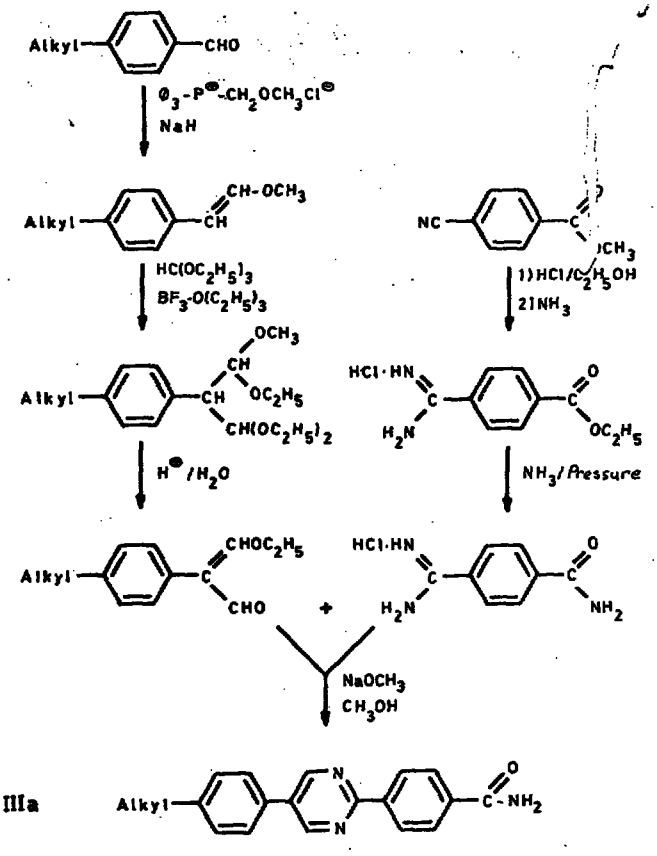


IIe

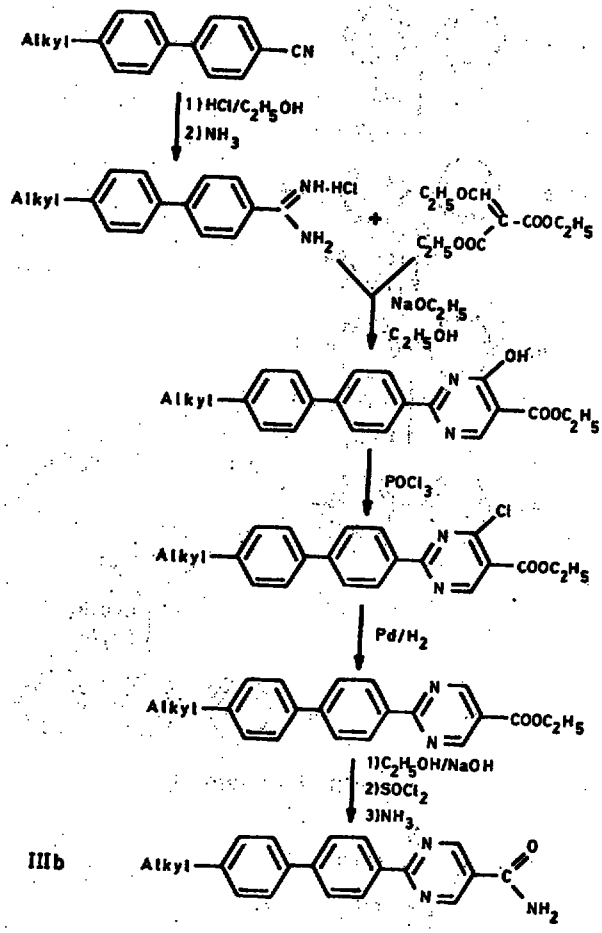
Formula Scheme F



Formula Scheme G

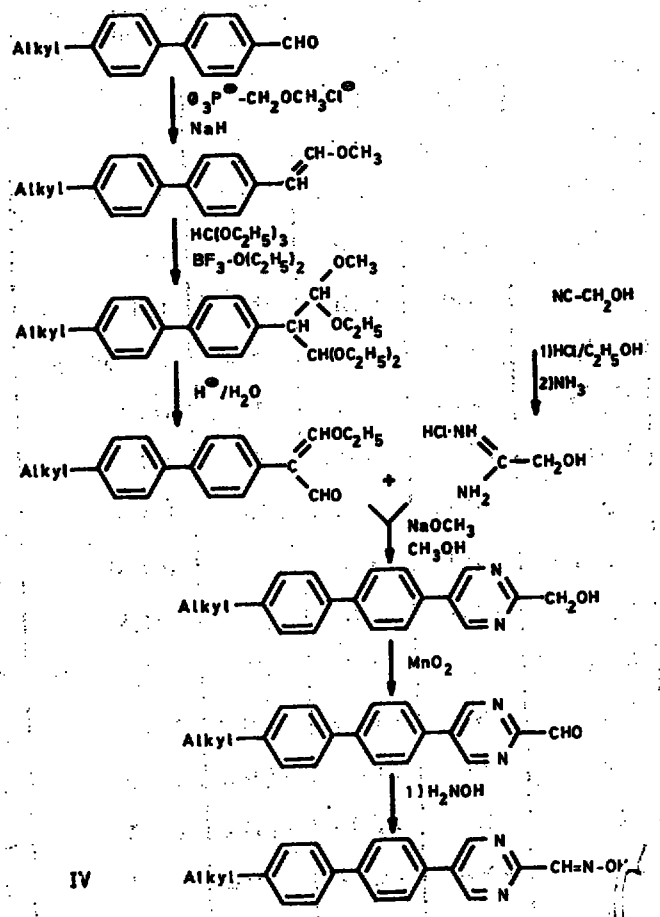


Formula Scheme H



IIIb

Formula Scheme I



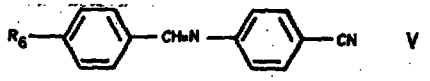
IV

The physical properties of some of the pyrimidine derivatives of formula I are given in the following Table:

TABLE

R_1	R_2	X	Y	Z	Melting point (°C)	Clearing point (°C)
C_3H_7–	–CN	–CH–	–CH–	–N–	154–154.5°	261°
C_4H_9–	–CN	–CH–	–CH–	–N–	94°	246–246.5°
C_5H_{11}–	–CN	–CH–	–CH–	–N–	125.5°	242.5–243°
C_6H_{13}–	–CN	–CH–	–CH–	–N–	93°	232.5°
C_7H_{15}–	–CN	–CH–	–CH–	–N–	104.5°	226°
–CN	C_2H_5–	–CH–	–CH–	–N–	167–167.5°	279–279.5°
–CN	C_3H_7–	–CH–	–CH–	–N–	167°	278.5–279°
–CN	C_4H_9–	–CH–	–CH–	–N–	138.5°	266–266.5°
–CN	C_5H_{11}–	–CH–	–CH–	–N–	131.5°	262.5–263°
–CN	C_6H_{13}–	–CH–	–CH–	–N–	121.5°	250°
–CN	C_7H_{15}–	–CH–	–CH–	–N–	121.5°	245–245.5°
–CN	C_5H_{11}	–N–	–CH–	–CH–	123.5–124°	204.5–205°
C_2H_5–	–CN	–N–	–CH–	–CH–	166°	241°
C_6H_{13}–	–CN	–N–	–CH–	–CH–	132.5°	258.5–259.5°
C_2H_5–	–CN	–N–	–CH–	–CH–	166.3°	240.9°
C_3H_7–	–CN	–N–	–CH–	–CH–	138.7°	232°
C_4H_9–	–CN	–N–	–CH–	–CH–	129.3°	274.6°
C_2H_5–	–CN	–CH–	–CH–	–N–	182°	262.2°
C_3H_7O–	–CN	–CH–	–CH–	–N–	132°	279.7°
C_4H_9O–	–CN	–CH–	–CH–	–N–	119°	271.6°
$C_5H_{11}O$–	–CN	–CH–	–CH–	–N–	85.8°	261°
$C_6H_{13}O$–	–CN	–CH–	–CH–	–N–	94.8°	254.3°
–CN	C_3H_7	–N–	–CH–	–CH–	125.6°	275.7°
–CN	C_4H_9	–N–	–CH–	–CH–	112°	262°
–CN	C_6H_{13}	–N–	–CH–	–CH–	108°	245.5°
–CN	C_7H_{15}	–N–	–CH–	–CH–	110°	241.5°

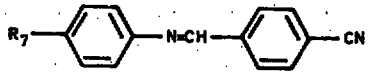
The pyrimidine derivatives of formula I can be used in the form of mixtures with other nematic substances; for example, with compounds of the general formula



V

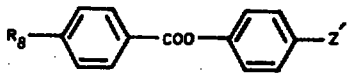
wherein the symbol R_6 represents a straight-chain alkyl group containing 2 to 8 carbon atoms, a straight-chain alkoxy group containing 4 to 7 carbon atoms, a

straight-chain alkanoyloxy group containing 2 to 8 carbon atoms or a straight-chain alkyl-carbonate group containing 2 to 11 carbon atoms,
and/or with compounds of the general formula



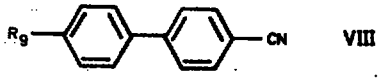
VI

wherein the symbol R_7 represents a straight-chain alkyl group containing 4 to 7 carbon atoms or a straight-chain alkyl-carbonate group containing 2 to 11 carbon atoms,
and/or with compounds of the general formula



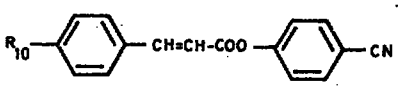
VII

wherein the symbol Z' represents a cyano group, a straight-chain alkyl group containing 1 to 9 carbon atoms, a straight-chain alkoxy group containing 1 to 9 carbon atoms or a straight-chain alkanoyloxy group containing 1 to 10 carbon atoms and the symbol R_8 represents a straight-chain alkyl group containing 4 to 8 carbon atoms, a straight-chain alkoxy group containing 5 to 8 carbon atoms, a straight-chain alkanoyloxy group containing 2 to 8 carbon atoms or a straight-chain alkylcarbonate group containing 3 to 11 carbon atoms,
and/or with compounds of the general formula



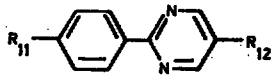
VIII

wherein the symbol R_9 represents a straight-chain alkyl group containing 4 to 8 carbon atoms, a straight-chain alkoxy group containing 4 to 8 carbon atoms, a straight-chain alkanoyloxy group containing 4 to 9 carbon atoms or a straight-chain alkylcarbonate group containing 4 to 11 carbon atoms,
and/or with trans-cinnamic acid esters of the general formula



IX

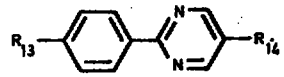
wherein the symbol R_{10} represents a straight-chain alkyl group containing 1 to 8 carbon atoms,
and/or with compounds of the general formula



X

wherein one of the symbols R_{11} and R_{12} represents a cyano group and the other represents a straight-chain alkyl group containing 3 to 9 carbon atoms, a straight-chain alkoxy group containing 2 to 9 carbon atoms or a straight-chain alkanoyloxy group containing 2 to 9 carbon atoms.

The compounds of formula X are novel and can be prepared by dehydrating a compound of the general formula

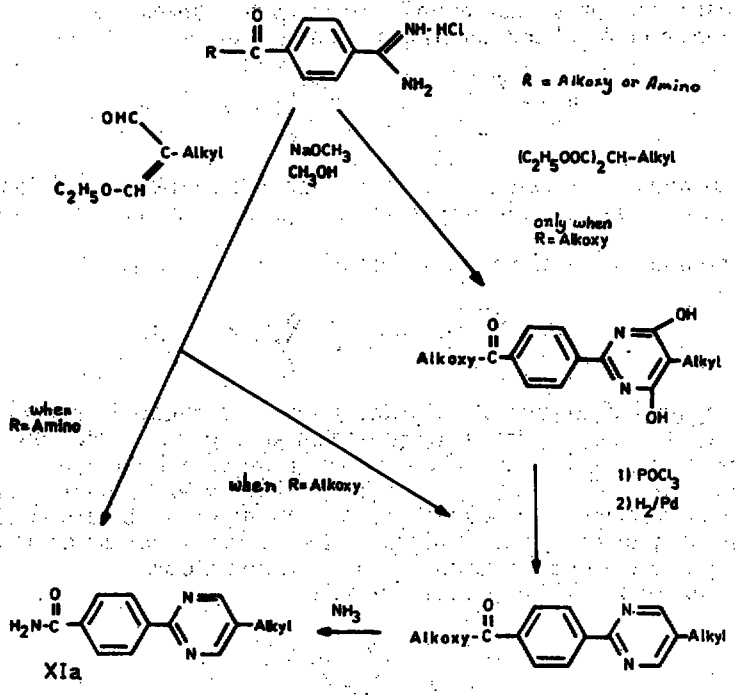


XI

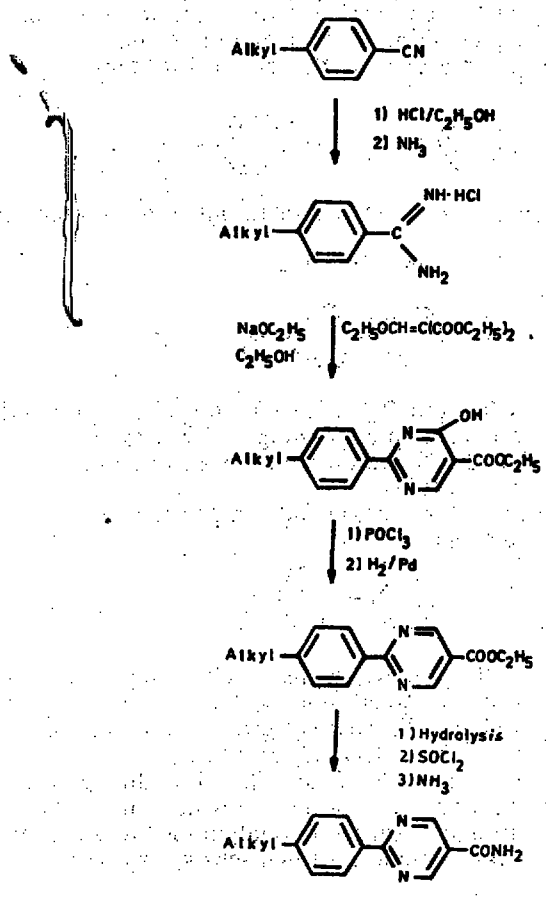
wherein one of the symbols R_{13} and R_{14} represents a straight-chain alkyl group containing 3 to 9 carbon atoms, a straight-chain alkoxy group containing 2 to 9 carbon atoms or a straight-chain alkanoyloxy group containing 2 to 9 carbon atoms and the other represents the $—CONH_2$ group.

The preparation of the compounds of formula XI is illustrated in Formulae Schemes 1 and 2 hereinafter for such compounds in which one of the symbols R_{13} and R_{14} represents a straight-chain alkyl group containing 3 to 9 carbon atoms. In these Formulae Schemes "Alkyl" means a straight-chain alkyl group containing 3 to 9 carbon atoms.

Formula Scheme 1.



Formula Scheme 2.



The pyrimidine derivatives of formula I are present in nematic mixtures for electro-optical purposes in weight ratio which preferably corresponds to the eutectic composition. The amount of a pyrimidine derivative of formula I in a nematic mixture is, however, generally between 0.5 and 20 per cent by weight and preferably between 2 and 15 per cent by weight.

The following mixtures are particularly preferred. All percentages are by weight unless otherwise indicated.

63.4% of 4'-n-pentyl-4-cyanobiphenyl, 31.6% of 4'-n-heptyl-4-cyanobiphenyl and 5.0% of 2-(4-cyanophenyl)-5-(4-n-hexylphenyl)-pyrimidine; melting point <3°C; clearing point 47.4°—48.9°C.

57.0% of 4'-n-pentyl-4-cyanobiphenyl, 28.5% of 4'-n-heptyl-4-cyanobiphenyl, 5% of 5-cyano-2-(4-n-pentylphenyl)-pyrimidine, 5% of 5-cyano-2-(4-n-hexylphenyl)-pyrimidine and 4.5% of 2-(4-cyanophenyl)-5-(4-n-hexylphenyl)pyrimidine; melting point <3°C; clearing point 53.2°—54.7°C.

44.2% of 4'-n-pentyl-4-cyanobiphenyl, 25.0% of 4'-n-pentyloxy-4-cyanobiphenyl, 8.6% of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine, 11.4% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 10.6% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 67.8°—68.9°C.

9.1% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 26.6% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 24.0% of p-[(p-n-pentylbenzyliden)amino]benzonitrile and 2.3% of 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine; melting point <3°C; clearing point 70.3—70.9°C.

8.9% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 23.3% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 36.9% of p-[(p-n-propylphenyl)-pyrimidine; melting point <0°C; clearing point 75.3°—76.8°C.

11.0% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 43.1% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 12.4% of 5-n-heptyl-2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine; melting point <0°C; clearing point 65.8°—66.4°C.

10.4% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 29.5% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 7.4% of p-n-heptylbenzoic acid p'-cyanophenyl ester and 10.7% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 81.2°—82.2°C.

49.3% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 12.1% of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine, 16.1% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 9.0% of 2-(4-cyanophenyl)-5-(4-n-hexylphenyl)-pyrimidine; melting point <0°C; clearing point 96.8°—97.9°C.

6.3% of p-n-butylbenzoic acid p'-cyanophenyl ester 8.0% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 11.5% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 31.9% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 7.0% of 2-(4-cyanophenyl)-5-(4-n-heptylphenyl)-pyrimidine, 9.8% of 2-(4-cyanophenyl)-5-(4-n-hexylphenyl)-pyrimidine and 13.1% of 2-(4-cyanophenyl)-5-(4-n-pentylphenyl)-pyrimidine; melting point <0°C; clearing point 77.9°C.

11.5% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 6.3% of p-n-butylbenzoic acid p'-cyanophenyl ester, 8.0% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 7.0% of 5 - n - pentyl - 2 - (4 - cyanophenyl) - pyrimidine, 9.8% of 5 - n - hexyl-2-(4-cyanophenyl)-pyrimidine, 13.1% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 11.6% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)pyrimidine; melting point <0°C; clearing point 77.5°C.

13.0% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 35.2% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 7.4% of p-n-butyl-benzoic acid p'-cyanophenyl ester, 7.8% of p-n-pentylbenzoic acid p'-cyanophenyl ester, 9.6% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 8.1% of 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 15.2% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 2.6% of 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine; melting point <0°C; clearing point 62.5°C.

12.5% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 34.3% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 7.0% of p-n-butylbenzoic acid p'-cyano-

phenyl ester, 8.7% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 9.7% of p-n-heptylbenzoic acid p'-cyanophenyl ester, 7.5% of 5-n-pentyl-2-(4-cyanophenyl)pyrimidine, 14.0% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine, 2.5% of 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine and 3.6% of p-[(p-ethoxybenzyliden)amino]benzonitrile; melting point <0°C; clearing point 65.0°C.

36.0% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 7.7% of p-n-butylbenzoic acid p'-cyanophenyl ester, 8.1% of p-n-pentylbenzoic acid p'-cyanophenyl ester, 10.0% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 8.4% of 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 15.8% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 13.0% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 81.0°C.

16.8% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 10.2% of p-n-butylbenzoic acid p'-cyanophenyl ester, 11.0% of p-n-pentylbenzoic acid p'-cyanophenyl ester, 14.1% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 10.9% of 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 21.0% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine; and 15.5% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <10°C; clearing point 85.5°C.

16.2% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 9.7% of p-n-butylbenzoic acid p'-cyanophenyl ester, 13.4% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 14.4% of p-n-heptylbenzoic acid p'-cyanophenyl ester, 10.5% of 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 20.2% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 15.1% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <10°C; clearing point 83.5°C.

11.6% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 32.1% of p-n-[(p-n-butylbenzyliden)amino]benzonitrile, 6.4% of p-n-butylbenzoic acid p'-cyanophenyl ester, 8.1% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 8.7% of p-n-heptylbenzoic acid p'-cyanophenyl ester, 7.1% of 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 13.2% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 11.7% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 80.0°C.

10.3% of p-n-butylbenzoic acid p'-cyanophenyl ester, 11.1% of p-n-pentylbenzoic acid p'-cyanophenyl ester, 14.3% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 15.4% of p-n-heptylbenzoic acid p'-cyanophenyl ester, 11.0% of 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 21.2% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 15.6% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <10°C; clearing point 82.5°C.

10.0% of p-n-butylbenzoic acid p'-cyanophenyl ester 10.9% of p-n-pentylbenzoic acid p'-cyanophenyl ester, 13.4% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 11.9% of p-n-heptylbenzoic acid p'-cyanophenyl ester, 10.5% of 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 20.6% of 5-n-heptyl-2-(4-cyanophenyl)pyrimidine, 3.3% of 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine and 15.5% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <10°C; clearing point 88.5°C.

44.5% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 6.6% of p-n-butylbenzoic acid p'-cyanophenyl ester, 6.9% of p-n-pentylbenzoic acid p'-cyanophenyl ester, 8.4% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 7.3% of 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 13.6% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 11.9% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 80.0°C.

15.3% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 9.0% of p-n-butylbenzoic acid p'-cyanophenyl ester, 9.9% of p-n-pentylbenzoic acid p'-cyanophenyl ester, 12.8% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 9.2% of 5-n-pentyl-2-(4-cyanophenyl)pyrimidine, 12.7% of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine, 18.2% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 12.9% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <3°C; clearing point 79.0°C.

18.1% of p-n-butylbenzoic acid p'-cyanophenyl ester, 13.3% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 8.4% of p-n-octylbenzoic acid p'-cyanophenyl ester, 10.4% of 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 14.8% of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine, 19.8% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 15.0% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <10°C; clearing point 78.5°C.

42.4% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 6.0% of p-n-butylbenzoic acid p'-cyanophenyl ester, 7.5% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 4.2% of p-n-octylbenzoic acid p'-cyanophenyl ester, 6.7% of 5-n-pentyl-2-(4-

cyanophenyl)-pyrimidine, 9.3% of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine, 12.3% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 11.2% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 76.0°C.

10.1% of p-n-butylbenzoic acid p'-cyanophenyl ester, 12.0% of p-n-pentylbenzoic acid p'-cyanophenyl ester, 14.2% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 15.2% of p-n-heptylbenzoic acid p'-cyanophenyl ester, 11.1% of 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 21.3% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 16.0% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <3°C; clearing point 82.0°C.

33.1% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 6.7% of p-n-butylbenzoic acid p'-cyanophenyl ester, 7.1% of p-n-pentylbenzoic acid p'-cyanophenyl ester, 8.6% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 7.4% of 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 10.4% of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine, 13.9% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 12.0% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 76.8°C.

7.7% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 23.2% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 34.2% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 11.1% of 5-cyano-2-(4-n-hexylphenyl)-pyrimidine, 7.9% of 5-n-heptyl-2-(4-cyanophenyl) - pyrimidine, 1.6% of 2 - (4 - cyanophenyl) - 5 - (4-n-propylphenyl)-pyrimidine, 8.5% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 5.3% of 2-(4-cyanophenyl)-5-(4-n-hexylphenyl)-pyrimidine; melting point <0°C; clearing point 93.5°C.

10.1% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 29.0% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 40.8% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 2.0% of 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine, 10.6% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 7.3% of 4-cyano-4"-n-pentyl-p-terphenyl; melting point <0°C; clearing point 101°C.

9.8% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 28.2% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 39.9% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 11.4% of 5-cyano-2-(4'-n-hexyl-4-biphenylyl)pyrimidine and 10.4% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 109°C.

10.3% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 29.4% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 40.9% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 5.8% of 5-cyano-2-(4'-n-propyl-4-biphenylyl)pyrimidine, 10.7% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 2.2% of 5-n-pentyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point <0°C; clearing point 102°C.

9.9% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 27.3% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 41.9% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 6.8% of 5-cyano-2-(4'-n-hexyl-4-biphenylyl)-pyrimidine, 10.1% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 4.9% of 2-(4-cyanophenyl)-5-(4-n-hexylphenyl)-pyrimidine; melting point <0°C; clearing point 106°C.

16.0% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 64.2% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 3.7% of 5-cyano-2-(4-n-butyryloxyphenyl)-pyrimidine, 2.6% of 5-cyano-2-(4-n-valeryloxyphenyl)-pyrimidine, 2.2% of 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine and 11.2% of 2-(4-cyanophenyl-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 92.0°C.

11.1% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 31.3% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 43.5% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 2.4% of 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine and 11.4% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 88.0°C.

10.0% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 28.6% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 40.6% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 4.9% of 5-cyano-2-(4-n-butyryloxyphenyl)-pyrimidine, 3.0% of 5-cyano-2-(4-n-valeryloxyphenyl)-pyrimidine, 2.0% of 2-(4-cyanophenyl)-5-(4-n-propylphenyl)pyrimidine and 10.5% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 90.0°C.

9.1% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 26.8% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 38.3% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 6.4% of 5-cyano-2-(4-n-pentylphenyl)-pyrimidine, 4.6% of 5-cyano-2-(4-n-butyloxyphenyl)-pyrimidine, 2.7% of 5-cyano-2-(4-n-

valeryloxyphenyl)-pyrimidine, 1.8% of 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine and 9.8% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 91.5°C.

11.3% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 31.5% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 43.2% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 11.5% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 2.5% of 5-n-pentyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point <0°C; clearing point 87.0°C.

8.8% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 25.9% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 36.9% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 7.4% of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine, 9.4% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine, 9.5% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 1.9% of 5-n-pentyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point <0°C; clearing point 81.0°C.

11.0% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 30.8% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 42.4% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 42.4% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 2.2% of 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine, 11.2% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 2.4% of 5-n-pentyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point <0°C; clearing point 92.5°C.

17.8% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 57.8% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 3.6% of 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine, 16.2% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 4.1% of 5-n-pentyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point <10°C; clearing point 107.5°C.

14.7% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 51.2% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 13.3% of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine, 3.0% of 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine, 14.0% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 3.3% of 5-n-pentyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point <3°C; clearing point 97.5°C.

10.2% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 29.1% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 40.6% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 10.6% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine, 6.9% of 2-(4-cyanophenyl)-5-(4-n-hexylphenyl)-pyrimidine and 21.% of 5-n-pentyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point <0°C; clearing point 99.0°C.

11.3% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 31.5% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 43.2% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 11.5% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 2.5% of 5-n-pentyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point <0°C; clearing point 89.0°C.

35.2% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 7.4% of p-n-butylbenzoic acid p'-cyanophenyl ester, 7.8% of p-n-pentylbenzoic acid p'-cyanophenyl ester, 9.7% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 11.4% of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine, 15.2% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 12.8% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 77.5°C.

37.3% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 8.1% of p-n-butylbenzoic acid p'-cyanophenyl ester, 8.6% of p-n-pentylbenzoic acid p'-cyanophenyl ester, 10.8% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 8.9% of 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 12.5% of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine and 13.5% of 2-(4-cyanophenyl)-5-(4-butylphenyl)-pyrimidine; melting point <3°C; clearing point 81.0°C.

36.3% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 7.8% of p-n-butylbenzoic acid p'-cyanophenyl ester, 10.2% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 12.0% of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine, 16.0% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine, 13.1% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 4.4% of 5-n-hexyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point <0°C; clearing point 87.5°C.

12.4% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 33.9% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 7.0% of p-n-butylbenzoic acid p'-cyanophenyl ester, 9.0% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 10.8% of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine, 14.4% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 12.2% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 79.0°C.

6.7% of p-n-butylbenzoic acid p'-cyanophenyl ester, 7.1% of p-n-pentylbenzoic acid p'-cyanophenyl ester, 8.6% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 33.1% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 7.4% of 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 10.4% of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine, 13.9% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 12.0% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 77.5°C.

7.4% of p-n-butylbenzoic acid p'-cyanophenyl ester, 7.8% of p-n-pentylbenzoic acid p'-cyanophenyl ester, 9.7% of p-n-hexylbenzoic acid p'-cyanophenyl ester, 35.2% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 11.4% of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine, 15.2% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 12.8% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine; melting point <0°C; clearing point 78.0°C.

9.8% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 28.2% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 39.6% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 2.0% of 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine, 10.3% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 9.7% of 5-n-butyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point <0°C; clearing point 105.5°C.

10.3% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 29.3% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 41.4% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 9.8% of 2-(4-cyanophenyl)-5-(4-butylphenyl)-pyrimidine and 9.2% of 5-n-butyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point <0°C; clearing point 100.0°C.

46.8% of 4'-n-pentyl-4-cyanobiphenyl, 23.4% of 4'-n-heptyl-4-cyanobiphenyl, 7.8% of 4'-n-heptyloxy-4-cyanobiphenyl, 2.3% of 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine, 11.3% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 7.7% of 4-cyano-4''-n-pentyl-p-terphenyl; melting point <0°C; clearing point 85.0°C.

43.9% of 4'-n-pentyl-4-cyanobiphenyl, 21.1% of 4'-n-heptyl-4-cyanobiphenyl, 6.7% of 4'-n-hexyloxy-4-cyanobiphenyl, 10.6% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine, 9.9% of 5-n-butyl-2-(4'-cyano-4-biphenylyl)-pyrimidine and 7.2% of 4-cyano-4''-n-pentyl-p-terphenyl; melting point <0°C; clearing point 98.0°C.

43.6% of 4'-n-pentyl-5-cyanobiphenyl, 20.9% of 4'-n-heptyl-4-cyanobiphenyl, 7.6% of 4'-n-octyloxy-4-cyanobiphenyl, 10.5% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine, 9.8% of 5-n-butyl-2-(4'-cyano-4-biphenylyl)-pyrimidine and 7.1% of 4-cyano-4''-n-pentyl-p-terphenyl; melting point <0°C; clearing point 96.0°C.

46.8% of 4'-n-pentyl-4-cyanobiphenyl, 23.4% of 4'-n-heptyl-4-cyanobiphenyl, 7.8% of 4'-n-heptyloxy-4-cyanobiphenyl, 11.3% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 10.6% of 5-n-butyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point <0°C; clearing point 84.5°C.

50.7% of 4'-n-pentyl-4-cyanobiphenyl, 25.4% of 4'-n-pentyloxy-4-cyanobiphenyl, 6.0% of 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 8.9% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 9.0% of 5-n-butyl-2-(4'-cyanobiphenylyl)-pyrimidine; melting point <0°C; clearing point 83.5°C.

44.8% of 4'-n-pentyl-4-cyanobiphenyl, 21.9% of 4'-n-heptyl-4-cyanobiphenyl, 11.7% of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine, 10.8% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 10.1% of 5-n-butyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point <0°C; clearing point 82.0°C.

46.8% of 4'-n-pentyl-4-cyanobiphenyl, 23.4% of 4'-n-heptyl-4-cyanobiphenyl, 7.8% of 4'-n-heptyloxy-4-cyano-biphenyl, 11.3% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 10.6% of 5-n-butyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point <0°C; clearing point 84.0°C.

8.13% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 24.4% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 39.6% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 10.81% of p-[5-(p-n-pentyloxyphenyl)-2-pyrimidinyl]benzonitrile and 16.75% of p-[5-(p-n-pentyloxyphenyl)-2-pyrimidinyl]benzonitrile; melting point <0°C; clearing point 112.5°C.

10.2% of p-[(p-n-propylbenzyliden)amino]benzonitrile, 29.1% of p-[(p-n-butylbenzyliden)amino]benzonitrile, 40.6% of p-[(p-n-hexylbenzyliden)amino]benzonitrile, 9.4% of 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 10.7% of 5-(4-cyanophenyl)-2-(4-n-hexylphenyl)-pyrimidine; melting point <0°C; clearing point 101.6°C.

The following Examples illustrate the process provided by the present invention and also describe the preparation of the novel compounds of formula X:

Example 1.

4.2 g of 4-[5-(4-n-pentylphenyl)-2-pyrimidyl]-benzoic acid amide are left under reflux for 1 hour while stirring in a mixture of 200 ml of ethylene chloride and 2.5 ml of phosphorus oxychloride. The mixture is diluted with ether and washed with 2-*N* sodium hydroxide solution and then with water until neutral. After drying the organic phase over sodium sulphate and evaporation, there is obtained 5-(4-n-pentylphenyl)-2-(4-cyanophenyl)-pyrimidine which is filtered on a short silica gel column and subsequently recrystallised from methylene chloride/methanol; melting point 125.5°C; clearing point 242.5°—243°C.

The starting material can be prepared as follows:

Dry hydrochloric acid gas is passed into a solution of 88.6 g of methyl 4-cyanobenzoate in 190 ml of benzene and 70 ml of methanol for 3 hours at 0°C while stirring. The mixture is left to stand for 5 days at +5°C and the precipitated imido ether is then filtered off. 178 g of this crude product are suspended in 300 ml of methanol and, after cooling to about –40°C, treated with 130 g of liquid ammonia and the mixture is shaken in an autoclave for 24 hours at +70°C. After cooling the mixture to room temperature and evaporation of the ammonia, the crystallised product is filtered off and the crystals are washed with hexane and dried overnight at 50°C under a waterpump vacuum, there being obtained 4-amidino-benzoic acid amide hydrochloride.

46.07 g of 1-(4-n-pentylphenyl)-2-methoxyethylene [prepared as described in Ber. *94*, 1373 (1961)] are added dropwise to a solution of 2 ml of boron trifluoride etherate in 500 ml of ethyl orthoformate, cooled in an ice bath, and the mixture is then further stirred at room temperature. After dilution with ether, extraction with 1-*N* sodium hydroxide solution and water and evaporation of the organic phase, which is previously dried over sodium sulphate, there is obtained 4-n-pentylphenyl-malonic tetraacetal.

7.33 g of 4-n-pentylphenyl-malonic tetraacetal in 20 ml of ethanol are stirred overnight at 50°C under nitrogen with 0.72 ml of water and 2 drops of concentrated sulphuric acid. The acidic pentylphenyl-malonic aldehyde obtained as a byproduct can be separated from the neutral 2-(4-n-pentylphenyl)-3-ethoxy-acrolein by extracting the mixture, diluted with ether, with aqueous sodium carbonate solution.

4.46 g of 2-(4-n-pentylphenyl)-3-ethoxy-acrolein, 3.63 g of the foregoing 4-amidino-benzoic acid amide hydrochloride and 0.0254 mol of sodium methylate (obtained by dissolving 0.584 g of sodium metal in methanol) are suspended in 250 ml of methanol and the mixture is stirred overnight at room temperature under nitrogen. The yellow suspension is then filtered and the residue is washed with a small amount of ethanol and suspended in 1.4 litres of ether for further purification. The suspension is washed with water and then filtered again. Sparingly soluble 4-[5-(4-n-pentylphenyl)-2-pyrimidinyl]-benzoic acid amide is obtained.

The following pyrimidine derivatives are prepared in an analogous manner:

	Melting point	Clearing point
5-(4-n-Propylphenyl)-2-(4-cyanophenyl)-pyrimidine	154°—154.5°C	261°C
5-(4-n-Butylphenyl)-2-(4-cyanophenyl)-pyrimidine	94°C	246.0°—246.5°C
5-(4-n-Hexylphenyl)-2-(4-cyanophenyl)-pyrimidine	93°C	232.5°C
5-(4-n-Heptylphenyl)-2-(4-cyanophenyl)-pyrimidine	104.5°C	226°C
5-(4-Ethylphenyl)-2-(4-cyanophenyl)-pyrimidine	182°C	262.2°C
5-(4-n-Propoxyphenyl)-2-(4-cyanophenyl)-pyrimidine	132°C	279.7°C

	Melting point	Clearing point
5-(4-n-Butoxyphenyl)-2-(4-cyanophenyl)-pyrimidine	119°C	271.6°C
5-(4-n-Pentyloxyphenyl)-2-(4-cyanophenyl)-pyrimidine	85.8°C	261°C
5-(4-n-Hexyloxyphenyl)-2-(4-cyanophenyl)-pyrimidine	94.8°C	254.3°C

Example 2.

1.9 g of 2-(4-n-hexylphenyl)-5-(4-bromophenyl)-pyrimidine in 50 ml of dimethylformamide are heated to reflux for 21 hours with 2.5 g of copper (I) cyanide (content 70 wt%). After cooling, the mixture is stirred with 25 ml of 10% aqueous ethylenediamine solution and then extracted with methylene chloride. The extract is washed again with aqueous ethylenediamine solution and then several times with water until it gives a neutral reaction. The crude product obtained after evaporation is chromatographed on 150 g of silica gel with toluene/1wt% acetone. Initially there are obtained traces of the starting material and then fractions containing pure 2-(4-n-hexylphenyl)-5-(4-cyanophenyl)-pyrimidine. After recrystallisation from ethyl acetate, the product has a melting point of 121.5°C and a clearing point of 250°C.

The starting material can be prepared as follows:

A solution of 15 g of 1-(4-bromophenyl)-2-methoxyethylene [prepared as described in Ber. *94*, 1373 (1961)] in 150 ml of ethyl orthoformate is added dropwise at 0°—5°C to 5 g of boron trifluoride etherate in 200 ml of ethyl orthoformate. The mixture is stirred overnight and reaches room temperature. The mixture is then diluted with ether and washed firstly with soda solution and then with water until it gives a neutral reaction. The crude product obtained after evaporation yields 4-bromophenyl-malonic tetraacetal after recrystallisation from hexane.

In order to partially hydrolyse the foregoing tetraacetal, 4.5 g thereof are dissolved in 10 ml of ethanol, the solution is treated with 0.5 ml of water and 1 drop of concentrated sulphuric acid and the mixture is stirred overnight at 50°C and then worked up in the customary manner. Crude 2-(4-bromophenyl)-3-ethoxy-acrolein is thus obtained and is used in the crude form.

Firstly 2.5 g of crude 2-(4-bromophenyl)-3-ethoxyacrolein in 20 ml of methanol and then 2.4 g of 4-n-hexyl-benzamidine hydrochloric are added to a sodium methylate solution obtained from 0.7 g of sodium in 25 ml of methanol. The mixture is heated to the reflux overnight. The solvent is then partially distilled off, the residue is treated with water and subsequently acidified with dilute hydrochloric acid. The resulting precipitate is filtered off, washed thoroughly with water and ether and dried. The crude 2-(4-n-hexylphenyl)-5-(4-bromophenyl)-pyrimidine of melting point 152.5°—156°C is used in the process without further purification.

The following pyrimidine derivatives were prepared in an analogous manner:

	Melting point	Clearing point
2-(4-Ethylphenyl)-5-(4-cyanophenyl)-pyrimidine	167°—167.5°C	279°—279.5°C
2-(4-n-Propylphenyl)-5-(4-cyanophenyl)-pyrimidine	167°C	278.5°—279°C
2-(4-n-Butylphenyl)-5-(4-cyanophenyl)-pyrimidine	138.5°C	266°—266.5°C
2-(4-n-Pentylphenyl)-5-(4-cyanophenyl)-pyrimidine	131.5°C	262.5°—263°C
2-(4-n-Heptylphenyl)-5-(4-cyanophenyl)-pyrimidine	121.5°C	245°—245.5°C

Example 3.

1.5 g of 5-n-pentyl-2-(4'-bromo-4-biphenylyl)-pyrimidine are heated to reflux for 22 hours with 2.5 g of copper (I) cyanide (content 70%) in 50 ml of dimethylformamide. After cooling, 25 ml of 10% aqueous ethylenediamine solution are added and, after stirring for a short time, the mixture is extracted with methylene chloride. The organic extract is shaken again with 25 ml of ethylenediamine solution and then washed until it gives a neutral reaction. The crude concentrate is chromatographed on silica gel with toluene/1% acetone. Recrystallisation of the pure fractions from ethyl acetate yields 5-n-pentyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point 123.5°—124°C; clearing point 204.5°—205°C.

The starting material can be prepared as follows:

34.5 g of 4-bromobiphenyl in 164 ml of methylene chloride are treated at ca 2°C with 60.6 g of titanium tetrachloride. 20.7 g of dichloromethyl methyl ether are added dropwise at the same temperature over a period of 40 minutes. The cooling means is then removed and the mixture is stirred for 21 hours at room temperature. The mixture is poured on to ice and the product is extracted with ether in the customary manner. Chromatography on silica gel with benzene as the eluting agent initially gives unreacted starting material and then 4'-bromo-4-biphenylaldehyde.

From 17.5 g of 4'-bromo-4-biphenylaldehyde and 4.4 g of hydroxylamine hydrochloride in 35 ml of methanol and 70 ml of pyridine there is obtained, after boiling under reflux, crude oxime which is converted into the nitrile by heating for 15 hours in acetic anhydride. The mixture is concentrated as much as possible on a rotary evaporator. The residue is poured on to ice and dilute sodium hydroxide solution and the product is isolated with ether in the customary manner. After treatment with hexane, the 4'-bromo-4-cyanobiphenyl melts at ca 150°C.

Gaseous hydrochloric acid is passed into a mixture of 5.6 g of 4'-bromo-4-cyanobiphenyl and 1 g of absolute ethanol in 25 ml of toluene until the mixture becomes saturated. After stirring for 3 days at room temperature, the precipitate is filtered off and washed with toluene. The residue is suspended in 5 ml of absolute ethanol whilst still moist and the suspension is treated with 1.3 g of ammonia in the form of a 10% ethanolic solution. After stirring for 3 days at room temperature, the precipitated 4'-bromo-4-biphenylamide hydrochloride is separated, washed with ether and dried.

5.8 g of n-pentyl-malonic tetraacetal in 10 ml of ethanol are stirred overnight at room temperature with 0.75 ml of water and 1 drop of concentrated sulphuric acid. The mixture is then diluted with ether, extracted with sodium carbonate solution, washed neutral and evaporated.

1.42 g of the thus-obtained crude 2-n-pentyl-3-ethoxy-acrolein are dissolved in a sodium ethylate solution (obtained from 580 mg of sodium in 40 ml of ethanol) and 2.6 g of the 4'-bromo-4-biphenylamidine hydrochloride obtained as described earlier. The mixture is then stirred for 3 days at room temperature. After some of the solvent has been distilled off, water is added and the mixture is extracted with chloroform in the customary manner. Upon crystallisation from ethanol, there is obtained 5-n-pentyl-2-(4'-bromo-4-biphenyl)-pyrimidine in the form of needles of melting point 137°C and clearing point 197°C.

The following pyrimidine derivatives can be prepared in an analogous manner:

5-n-Propyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point 125.6°C; clearing point 275.7°C.

5-n-Butyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point 112°C; clearing point 262°C.

5-n-Hexyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point 108°C; clearing point 245°C.

5-n-Heptyl-2-(4'-cyano-4-biphenylyl)-pyrimidine; melting point 110°C; clearing point 241.5°C.

Example 4.

4.31 g of 2-(4'-n-hexyl-4-biphenylyl)-pyrimidine-5-carboxylic acid amide are boiled for 2 hours under reflux with 75 ml of phosphorus oxychloride and the excess reagent is removed *in vacuo*. Toluene is then added and the mixture is concentrated twice *in vacuo*. The residue is taken up in methylene chloride and chromatographed on silica gel 60. Elution with methylene chloride/2% acetone yields 5-cyano-2-(4'-n-hexyl-4-biphenylyl)-pyrimidine which is purified by recrystallisation from acetone/hexane and distillation at 180°C in high vacuum; melting point 132.5°C; clearing point 258.5°—259.5°C.

The starting material can be prepared as follows:

Hydrochloric acid gas is passed into a solution of 5.0 g of 4'-n-hexyl-4-cyano-biphenyl in 3.8 ml of absolute ethanol and 4.8 ml of absolute benzene for 8 hours while stirring and cooling to 0°C and the mixture is left to stand overnight at room temperature. After evaporation *in vacuo*, the mixture is treated with 100 ml of absolute ether and 4'-n-hexyl-4-biphenyl-imidoethyl ether hydrochloride is isolated by filtration. This crude salt is suspended in 7.6 ml of absolute ethanol and stirred for 40 hours with 10.7 g of a 16% (g/g) solution of ammonia in ethanol. The clear solution is evaporated *in vacuo* and the residue is treated with 100 ml of absolute ether. 4-n-Hexyl-4-biphenyl-amidine hydrochloride is isolated by filtration.

A mixture of 6.0 g of 4'-n-hexyl-4-biphenyl-amidine hydrochloride and 4.9 g of diethyl ethoxymethylene-malonate is stirred in a sodium ethylate solution (obtained from 0.867 g of sodium and 80 ml of ethanol) for 40 minutes at room temperature and for 40 minutes under reflux. The yellow mixture is then evaporated *in vacuo* and the residue suspended in 95 ml of water and acidified with 15 ml of glacial acetic acid. Filtration, washing with water and drying yields crude ethyl 2-(4'-n-hexyl-4-biphenylyl)-4-hydroxy-pyrimidine-5-carboxylate which can be purified by sublimation at 185°C in a high vacuum; melting point 218.0°C.

6.95 g of the above hydroxypyrimidine are boiled for 1 hour under reflux with 50 ml of phosphorus oxychloride. The excess reagent is evaporated off *in vacuo* and the residue is chromatographed in methylene chloride on silica gel 60. Elution with methylene chloride and methylene chloride/2% acetone yields ethyl 2-(4'-n-hexyl-4-biphenylyl)-4-chloro-pyrimidine-5-carboxylate which can be purified by distillation at 180°C in a high vacuum; melting point 91.6°—91.9°C; clearing point 112.6°—112.7°C.

6.2 g of the above chloropyrimidine are suspended in 300 ml of ethanol and hydrogenated in the presence of 0.4 g of 5% palladium-on-charcoal and 2.17 g of anhydrous potassium acetate at room temperature until 1 mol of hydrogen has been absorbed. The catalyst is separated and rinsed with methylene chloride and the evaporation residue is dissolved in benzene, diluted with an equivalent amount of hexane and chromatographed on silica gel 60. Elution with hexane/benzene (1:1) and benzene initially yields a small amount of starting material and then ethyl 2-(4'-n-hexyl-4-biphenylyl)-pyrimidine-5-carboxylate. This carboxylate can be purified by distillation at 180°C in a high vacuum; melting point 129.2°C; clearing point 181°C.

5.12 g of ethyl 2-(4'-n-hexyl-4-biphenylyl)-pyrimidine-5-carboxylate are boiled under reflux for 3 hours with 150 ml of ethanol and 6.1 g of sodium hydroxide in 45 ml of water and the mixture is evaporated *in vacuo*. 50 ml of water and 100 ml of 20% hydrochloric acid are added to the residue. Filtration, washing with water and drying yields 2-(4'-n-hexyl-4-biphenylyl)-pyrimidine-5-carboxylic acid which can be converted into the acid chloride by boiling for 2 hours with 30 ml of thionyl chloride. The excess reagent is removed *in vacuo* and the residual acid chloride is suspended in 60 ml of absolute dioxane and added while stirring to a solution of 80 ml of dioxane saturated with ammonia at room temperature. Ammonia is passed into the mixture for a further 4 hours and the mixture is left to stand overnight at room temperature. The mixture is then evaporated to dryness and the residue is stirred for 30 minutes with 100 ml of water, filtered, rinsed with water and dried. There is thus obtained colourless 2-(4'-n-hexyl-4-biphenylyl)-pyrimidine-5-carboxylic acid amide which can be purified by sublimation at 205°C in a high vacuum; melting point 260°C.

The following pyrimidine derivatives can be prepared in an analogous manner:

5-Cyano-2-(4'-ethyl-4-biphenylyl)-pyrimidine; melting point 166°C; clearing point 241°C.

5-Cyano-2-(4'-n-propyl-4-biphenylyl)-pyrimidine; melting point 138.7°C; clearing point 232°C.

5-Cyano-2-(4'-n-butyl-4-biphenylyl)-pyrimidine; melting point 129.3°C; clearing point 274.6°C.

Example 5.

1.9 g of 4-(5-n-heptylpyrimid-2-yl)-benzoic acid amide are left for 80 minutes while stirring under reflux in a mixture of 40 ml of ethylene chloride and 0.63 ml of phosphorus oxychloride. The mixture is diluted with ether and washed with 2-*N* sodium hydroxide solution and then with water until neutral. After drying the

organic phase over sodium sulphate and evaporation, there are obtained 1.9 g of 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine which is distilled in a high vacuum; melting point 44.2°—44.7°C; clearing point 50.1°—50.4°C.

The starting material can be prepared as follows:

0.07 mol of 2-n-heptyl-malonic tetraethyl acetal in 35 ml of ethanol is stirred for 15 hours at 50°C under nitrogen with 0.14 mol of water and 2 drops of concentrated sulphuric acid. The acidic 2-heptyl-malonic aldehyde obtained as a byproduct can be separated from the neutral 2-n-heptyl-3-ethoxy-acrolein by extracting the mixture, diluted with ether, with aqueous sodium carbonate solution.

A suspension consisting of 0.1 mol of ethyl 4-amidinobenzoate hydrochloride, 0.1 mol of 2-n-heptyl-3-ethoxyacrolein and 0.14 mol of sodium ethylate in 100 ml of methanol is stirred overnight at room temperature under nitrogen. After the customary working-up and separation into basic and acidic portions, ethyl 4-(5-n-heptylpyrimid-2-yl)-benzoate and 4-(5-n-heptylpyrimid-2-yl)-benzoic acid are obtained.

A. 4.4 g of ethyl 4-(5-n-heptylpyrimid-2-yl)-benzoate dissolved in 50 ml of methanol/dichloromethane (1:1) are treated with 30 ml of liquid ammonia in a laboratory autoclave and the mixture is then warmed to 90°C for 5 hours (pressure: 16 atmospheres absolute). The mixture is evaporated to dryness and the more sparingly soluble amide is separated from unreacted educt. 4-(5-n-Heptylpyrimid-2-yl)-benzoic acid amide is obtained.

B. 2.3 g of 4-(5-n-heptylpyrimid-2-yl)-benzoic acid and 1.9 ml of thionyl chloride are left in 100 ml of benzene for 8 hours under reflux and the mixture is then evaporated to dryness on a vacuum film evaporator. The resulting residue is dissolved in 50 ml of dichloromethane and ammonia is passed into the solution at room temperature for 2 hours. 4-(5-n-Heptylpyrimid-2-yl)-benzoic acid amide is obtained in virtually quantitative yield.

Example 6.

15.58 g of 4-(5-n-hexylpyrimid-2-yl)-benzoic acid amide are left in a mixture of 350 ml of ethylene chloride and 5.58 ml of phosphorus oxychloride for 90 minutes under reflux while stirring. The mixture is diluted with ether and washed with 2-*N* sodium hydroxide solution and then with water until neutral. After drying the organic phase over sodium sulphate and evaporation, there are obtained 14.6 g of 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine which is distilled in a high vacuum; melting point 53.5°—54.5°C; clearing point 35.5°—36.5°C.

The starting material can be prepared as follows:

0.1 mol of 2-n-hexyl-malonic tetraethyl acetal in 40 ml of ethanol is stirred at 50°C under nitrogen for 18 hours with 0.2 mol of water and 3 drops of concentrated sulphuric acid. The acidic 2-hexyl-malonic aldehyde obtained as a byproduct can be separated from the neutral 2-n-hexyl-3-ethoxy-acrolein by extracting the mixture, diluted with ether, with aqueous sodium carbonate solution.

89 g of methyl 4-methylimido-benzoate hydrochloride suspended in 150 ml of methanol are treated at –40°C with 60 ml of liquid ammonia, the suspension is transferred to a laboratory autoclave, pressurised to 30 atmospheres of nitrogen and left for 24 hours at 70°C. The crystallised product is filtered off, washed with hexane and dried at 40°C under a vacuum (14 mm). 72 g of 4-amidino-benzoic acid amide hydrochloride are obtained.

0.082 mol of 4-amidino-benzoic acid amide hydrochloride suspended in a solution of 0.082 mol of 2-n-hexyl-3-ethoxyacrolein and 0.14 mol of sodium methylate in 150 ml of methanol is stirred overnight at room temperature under nitrogen. The precipitate obtained by diluting the mixture with 3 litres of ether is filtered off, washed with water until neutral and dried at 40°C in a vacuum drying cabinet. 17.9 g of 4-(5-n-hexylpyrimid-2-yl)-benzoic acid amide of melting point 231.6°—233.0°C are obtained.

Example 7.

A mixture of 12.6 g (37.8 mmol) of ethyl 2-(p-n-pentylphenyl)-4-chloro-pyrimidine-5-carboxylate, 1.1 g of 5% palladium-on-charcoal, 5.6 g (57.0 mmol) of anhydrous potassium acetate and 156 ml of ethanol is hydrogenated at room temperature until 1 mol of hydrogen has been absorbed, this taking 1 hour. The catalyst is filtered off, the filtrate is evaporated *in vacuo* and any starting material present is separated by chromatography on silica gel using benzene and benzene/

2% acetone as the solvent. The pure colourless ethyl 2-(p-n-pentylphenyl)-pyrimidine-5-carboxylate melts at 85.1°—86.7°C after distillation at 130°C in a high vacuum (bulb-tube).

After the addition of 21 ml of ethanol, 10.2 g (34.2 mmol) of ethyl 2-(p-n-pentylphenyl)-pyrimidine-5-carboxylate are boiled under reflux for 1 hour with a solution of 15.8 g of sodium hydroxide in 105 ml of water. After cooling, the mixture is made congo-acid with 82 ml of 20% hydrochloric acid and the precipitated 2-(p-n-pentylphenyl)-pyrimidine-5-carboxylic acid is separated, washed with water, dried and further reacted in the crude form.

9.3 g (34.4 mmol) of 2-(p-n-pentylphenyl)-pyrimidine-5-carboxylic acid are boiled under reflux for 2 hours with the exclusion of moisture with 50 ml of thionyl chloride, the excess reagent is removed *in vacuo* and the residual 2-(p-n-pentylphenyl)-pyrimidine-5-carboxylic acid chloride is dissolved in 100 ml of absolute dioxan and added while stirring to a solution of 200 ml of absolute dioxan saturated with ammonia at room temperature, a colourless precipitate forming. Ammonia is then passed into the mixture for a further 4 hours, the mixture is left to stand overnight at room temperature, evaporated *in vacuo* and the residue stirred with 100 ml of water for 30 minutes. The precipitate is separated, washed with water and dried. The resulting crude 2-(p-n-pentylphenyl)-pyrimidine-5-carboxamide is used without further purification.

9.1 g (33.8 mmol) of 2-(p-n-pentylphenyl)-pyrimidine-5-carboxamide are boiled under reflux for 2 hours with the exclusion of moisture with 100 ml of phosphorus oxychloride. The excess reagent is then removed *in vacuo* and the mixture is evaporated twice with toluene *in vacuo*. The residue is taken up in methylene chloride and chromatographed on 100 g of silica gel in methylene chloride. Elution with methylene chloride and methylene chloride/2% acetone yields 5-cyano-2-(4-n-pentylphenyl)-pyrimidine which is recrystallised from acetone/hexane and sublimed at 120°C in a high vacuum to constant melting point. The pure colourless product melts at 96.0°—96.2°C and has a clearing point of 109.0°C.

The starting material (melting point 58.5°—59.2°C) can be prepared as described by A. R. Todd and F. Bergel. J. Chem. Soc. *1937*, 366 from p-n-pentylbenzamidine hydrochloride and diethyl ethoxymethylenemalonate with sodium ethylate in ethanol and subsequent treatment of the resulting ethyl 2-(p-n-pentylphenyl)-4-hydroxy-pyrimidine-5-carboxylate (melting point 193.9°—194.4°C) with phosphorus oxychloride.

Example 8.

A mixture of 15.6 g (45.0 mmol) of ethyl 2-(p-n-hexylphenyl)-4-chloro-pyrimidine-5-carboxylate, 1.3 g of 5% palladium-on-charcoal, 6.7 g (68.5 mmol) of anhydrous potassium acetate and 150 ml of dioxane is hydrogenated at room temperature until 1 mol of hydrogen has been absorbed, this taking 70 hours. The working-up is carried out as described in Example 7. The pure colourless ethyl 2-(p-n-hexylphenyl)-pyrimidine-5-carboxylate melts at 83.2°—83.9°C after distillation at 125°C in a high vacuum.

After the addition of 28 ml of ethanol, 14.1 g (45.0 mmol) of ethyl 2-(p-n-hexylphenyl)-pyrimidine-5-carboxylate are reacted as described in Example 7 with a solution of 20.8 g of sodium hydroxide in 140 ml of water and the mixture is worked-up as described in Example 7. The dry 2-(p-n-hexylphenyl)-pyrimidine-5-carboxylic acid is used in crude form.

In a manner analogous to that described in Example 7, 12.0 g (42.4 mmol) of 2-(p-n-hexylphenyl)-pyrimidine-5-carboxylic acid are reacted with the exclusion of moisture with 80 ml of thionyl chloride and worked-up. The residual 2-(p-n-hexylphenyl)-pyrimidine-5-carboxylic acid chloride is dissolved in 120 ml of absolute dioxan while warming and added to a solution of 200 ml of absolute dioxan saturated with ammonia at room temperature whilst stirring. The mixture is further treated as described in Example 7 and worked-up. A sample of the resulting crude 2-(p-n-hexylphenyl)-pyrimidine-5-carboxamide is purified by sublimation at 180°C in a high vacuum; melting point 250.2°—258.3°C.

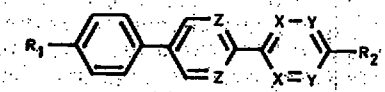
In a manner analogous to that described in Example 7, 11.5 g (40.6 mmol) of 2-(p-n-hexylphenyl)-pyrimidine-5-carboxamide are reacted with the exclusion of moisture with 100 ml of phosphorus oxychloride worked-up and purified. The pure colourless 5-cyano-2-(4-n-hexylphenyl)-pyrimidine melts at 86.3°—87.8°C (smectic), becomes nematic at 101.3°C and has a clearing point of 102.6—103.2°C.

The starting material (melting point 59.4°—60.5°C) can be prepared as

described by A. R. Todd and F. Bergel, J. Chem. Soc. *1937*, 366 from p-n-hexylbenzamidine hydrochloride and diethyl ethoxymethylene-malonate with sodium ethylate in ethanol and subsequent treatment of the resulting ethyl 2-(p-n-hexylphenyl)-4-hydroxy-pyrimidine-5-carboxylate (melting point 189.6°—191.0°C) with phosphorus oxychloride.

WHAT WE CLAIM IS:—

1. Pyrimidine derivatives of the general formula



I

wherein each of the symbols X represents a nitrogen atom and each of the symbols Y and Z represents —CH— or each of the symbols Y represents a nitrogen atom and each of the symbols X and Z represents —CH— or each of the symbols Z represents a nitrogen atom and each of the symbols X and Y represents —CH— and one of the symbols R_1 and R_2 represents a cyano group and the other represents a straight-chain alkyl group containing 1 to 7 carbon atoms, a straight-chain alkoxy group containing 1 to 7 carbon atoms or a straight-chain alkanoyloxy group containing 2 to 7 carbon atoms.

2. Pyrimidine derivatives according to claim 1, wherein one of the symbols R_1 and R_2 represents a cyano group and the other represents a straight-chain alkyl group containing 3 to 7 carbon atoms.

3. Pyrimidine derivatives according to claim 2, wherein the symbol R_2 represents a cyano group.

4. Pyrimidine derivatives according to any one of claims 1 to 3 inclusive, wherein each of the symbols Y represents —CH—.

5. Pyrimidine derivatives according to any one of claims 1 to 4 inclusive, wherein each of the symbols Z represents a nitrogen atom.

6. Pyrimidine derivatives according to any one of claims 1 to 5 inclusive, wherein one of the symbols R_1 and R_2 represents a cyano group and the other represents a straight-chain alkyl group containing 3 to 7 carbon atoms, each of the symbols Z represents a nitrogen atom and each of the symbols X and Y represents —CH—.

7. Pyrimidine derivatives according to claim 6, wherein the symbol R_2 represents a cyano group.

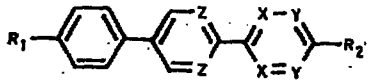
8. 5-(4-n-Pentylphenyl)-2-(4-cyanophenyl)-pyrimidine.
9. 5-(4-n-Propylphenyl)-2-(4-cyanophenyl)-pyrimidine.
10. 5-(4-n-Butylphenyl)-2-(4-cyanophenyl)-pyrimidine.
11. 5-(4-n-Hexylphenyl)-2-(4-cyanophenyl)-pyrimidine.
12. 5-(4-n-Heptylphenyl)-2-(4-cyanophenyl)-pyrimidine.
13. 2-(4-n-Hexylphenyl)-5-(4-cyanophenyl)-pyrimidine.
14. 2-(4-Ethylphenyl)-5-(4-cyanophenyl)-pyrimidine.
15. 2-(4-n-Propylphenyl)-5-(4-cyanophenyl)-pyrimidine.
16. 2-(4-n-Butylphenyl)-5-(4-cyanophenyl)-pyrimidine.
17. 2-(4-n-Pentylphenyl)-5-(4-cyanophenyl)-pyrimidine.
18. 2-(4-n-Heptylphenyl)-5-(4-cyanophenyl)-pyrimidine.
19. 5-n-Pentyl-2-(4'-cyano-4-biphenylyl)-pyrimidine.
20. 5-Cyano-2-(4'-n-hexyl-4-biphenylyl)-pyrimidine.
21. 5-Cyano-2-(4'-ethyl-4-biphenylyl)-pyrimidine.
22. 5-(4-Ethylphenyl)-2-(4-cyanophenyl)-pyrimidine.
23. 5-(4-n-Propoxyphenyl)-2-(4-cyanophenyl)-pyrimidine.
24. 5-(4-n-Butoxyphenyl)-2-(4-cyanophenyl)-pyrimidine.
25. 5-(4-n-Pentyloxyphenyl)-2-(4-cyanophenyl)-pyrimidine.
26. 5-(4-n-Hexyloxyphenyl)-2-(4-cyanophenyl)-pyrimidine.
27. 5-n-Propyl-2-(4'-cyano-4-biphenylyl)-pyrimidine.
28. 5-n-Butyl-2-(4'-cyano-4-biphenylyl)-pyrimidine.
29. 5-n-Hexyl-2-(4'-cyano-4-biphenylyl)-pyrimidine.
30. 5-n-Heptyl-2-(4'-cyano-4-biphenylyl)-pyrimidine.
31. 5-Cyano-2-(4'-n-propyl-4-biphenylyl)-pyrimidine.
32. 5-Cyano-2-(4'-n-butyl-4-biphenylyl)-pyrimidine.

33. A process for the manufacture of the pyrimidine derivatives of formula I given in claim 1, which process comprises

described by A. R. Todd and F. Bergel, J. Chem. Soc. *1937*, 366 from p-n-hexyl-benzamidine hydrochloride and diethyl ethoxymethylene-malonate with sodium ethylate in ethanol and subsequent treatment of the resulting ethyl 2-(p-n-hexyl-phenyl)-4-hydroxy-pyrimidine-5-carboxylate (melting point 189.6°—191.0°C) with phosphorus oxychloride.

WHAT WE CLAIM IS:—

1. Pyrimidine derivatives of the general formula



I

wherein each of the symbols X represents a nitrogen atom and each of the symbols Y and Z represents —CH— or each of the symbols Y represents a nitrogen atom and each of the symbols X and Z represents —CH— or each of the symbols Z represents a nitrogen atom and each of the symbols X and Y represents —CH— and one of the symbols R_1 and R_2 represents a cyano group and the other represents a straight-chain alkyl group containing 1 to 7 carbon atoms, a straight-chain alkoxy group containing 1 to 7 carbon atoms or a straight-chain alkanoyloxy group containing 2 to 7 carbon atoms.

2. Pyrimidine derivatives according to claim 1, wherein one of the symbols R_1 and R_2 represents a cyano group and the other represents a straight-chain alkyl group containing 3 to 7 carbon atoms.

3. Pyrimidine derivatives according to claim 2, wherein the symbol R_2 represents a cyano group.

4. Pyrimidine derivatives according to any one of claims 1 to 3 inclusive, wherein each of the symbols Y represents —CH—.

5. Pyrimidine derivatives according to any one of claims 1 to 4 inclusive, wherein each of the symbols Z represents a nitrogen atom.

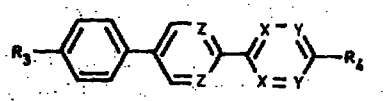
6. Pyrimidine derivatives according to any one of claims 1 to 5 inclusive, wherein one of the symbols R_1 and R_2 represents a cyano group and the other represents a straight-chain alkyl group containing 3 to 7 carbon atoms, each of the symbols Z represents a nitrogen atom and each of the symbols X and Y represents —CH—.

7. Pyrimidine derivatives according to claim 6, wherein the symbol R_2 represents a cyano group.

8. 5-(4-n-Pentylphenyl)-2-(4-cyanophenyl)-pyrimidine.
9. 5-(4-n-Propylphenyl)-2-(4-cyanophenyl)-pyrimidine.
10. 5-(4-n-Butylphenyl)-2-(4-cyanophenyl)-pyrimidine.
11. 5-(4-n-Hexylphenyl)-2-(4-cyanophenyl)-pyrimidine.
12. 5-(4-n-Heptylphenyl)-2-(4-cyanophenyl)-pyrimidine.
13. 2-(4-n-Hexylphenyl)-5-(4-cyanophenyl)-pyrimidine.
14. 2-(4-Ethylphenyl)-5-(4-cyanophenyl)-pyrimidine.
15. 2-(4-n-Propylphenyl)-5-(4-cyanophenyl)-pyrimidine.
16. 2-(4-n-Butylphenyl)-5-(4-cyanophenyl)-pyrimidine.
17. 2-(4-n-Pentylphenyl)-5-(4-cyanophenyl)-pyrimidine.
18. 2-(4-n-Heptylphenyl)-5-(4-cyanophenyl)-pyrimidine.
19. 5-n-Pentyl-2-(4'-cyano-4-biphenylyl)-pyrimidine.
20. 5-Cyano-2-(4'-n-hexyl-4-biphenylyl)-pyrimidine.
21. 5-Cyano-2-(4'-ethyl-4-biphenylyl)-pyrimidine.
22. 5-(4-Ethylphenyl)-2-(4-cyanophenyl)-pyrimidine.
23. 5-(4-n-Propoxyphenyl)-2-(4-cyanophenyl)-pyrimidine.
24. 5-(4-n-Butoxyphenyl)-2-(4-cyanophenyl)-pyrimidine.
25. 5-(4-n-Pentyloxyphenyl)-2-(4-cyanophenyl)-pyrimidine.
26. 5-(4-n-Hexyloxyphenyl)-2-(4-cyanophenyl)-pyrimidine.
27. 5-n-Propyl-2-(4'-cyano-4-biphenylyl)-pyrimidine.
28. 5-n-Butyl-2-(4'-cyano-4-biphenylyl)-pyrimidine.
29. 5-n-Hexyl-2-(4'-cyano-4-biphenylyl)-pyrimidine.
30. 5-n-Heptyl-2-(4'-cyano-4-biphenylyl)-pyrimidine.
31. 5-Cyano-2-(4'-n-propyl-4-biphenylyl)-pyrimidine.
32. 5-Cyano-2-(4'-n-butyl-4-biphenylyl)-pyrimidine.

33. A process for the manufacture of the pyrimidine derivatives of formula I given in claim 1, which process comprises

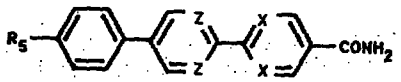
(a) reacting a compound of the general formula



II

, wherein one of the symbols R_3 and R_4 represents a straight-chain alkyl group containing 1 to 7 carbon atoms, a straight-chain alkoxy group containing 1 to 7 carbon atoms or a straight-chain alkanoyloxy group containing 2 to 7 carbon atoms and the other represents a halogen atom and the symbols X, Y and Z have the significance given in claim 1,
with copper (I) cyanide, sodium cyanide or potassium cyanide, or

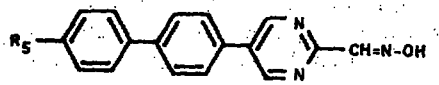
(b) for the manufacture of pyrimidine derivatives of formula I in which each of the symbols Y represents —CH—, the symbol R_2 represents a cyano group and the symbols R_1, X and Z have the significance given in claim 1, dehydrating a compound of the general formula



III

wherein the symbol R_5 represents a straight-chain alkyl group containing 1 to 7 carbon atoms, a straight-chain alkoxy group containing 1 to 7 carbon atoms or a straight-chain alkanoyloxy group containing 2 to 7 carbon atoms and the symbols X and Z have the significance given in claim 1,
or

(c) for the manufacture of pyrimidine derivatives of formula I in which each of the symbols Y represents a nitrogen atom, the symbol R_2 represents a cyano group and the symbols R_1, X and Z have the significance given in claim 1, dehydrating a compound of the general formula



IV

wherein the symbol R_5 has the significance given above.

34. A process according to claim 33, wherein one of the symbols R_1 and R_2 represents a cyano group and the other represents a straight-chain alkyl group containing 3 to 7 carbon atoms.

35. A process according to claim 34, wherein the symbol R_2 represents a cyano group.

36. A process according to any one of claims 33 to 35 inclusive, wherein each of the symbols Y represents —CH—.

37. A process according to any one of claims 33 to 36 inclusive, wherein each of the symbols Z represents a nitrogen atom.

38. A process according to any one of claims 33 to 37 inclusive, wherein one of the symbols R_1 and R_2 represents a cyano group and the other represents a straight-chain alkyl group containing 3 to 7 carbon atoms, each of the symbols Z represents a nitrogen atom and each of the symbols X and Y represents —CH—.

39. A process according to claim 38, wherein the symbol R_2 represents a cyano group.

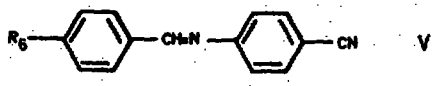
40. A process according to claim 33, wherein the pyrimidine derivative which is manufactured is as claimed in any of claims 8 to 32.

41. A process for the manufacture of the pyrimidine derivates of formula I given in claim 1, substantially as hereinbefore described with reference to Examples 1 to 4.

42. Pyrimidine derivatives of formula I given in claim 1, when manufactured by the process claimed in any one of claims 33 to 41 inclusive.

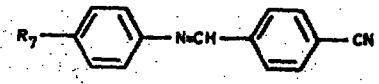
43. A nematic mixture for electro-optical purposes which contains one or more of the pyrimidine derivatives of formula I given in claim 1 and other nematic substances.

44. A nematic mixture according to claim 43 which contains at least one pyrimidine derivative of formula I given in claim 1 and at least one compound of the general formula



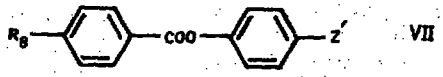
wherein the symbol R_6 represents a straight-chain alkyl group containing 2 to 8 carbon atoms, a straight-chain alkoxy group containing 4 to 7 carbon atoms, a straight-chain alkanoyloxy group containing 2 to 8 carbon atoms or a straight-chain alkylcarbonate group containing 2 to 11 carbon atoms.

45. A nematic mixture according to claim 43 which contains at least one pyrimidine derivative of formula I given in claim 1 and at least one compound of the general formula



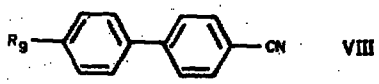
wherein the symbol R_7 represents a straight-chain alkyl group containing 4 to 7 carbon atoms or a straight-chain alkylcarbonate group containing 2 to 11 carbon atoms.

46. A nematic mixture according to claim 43 which contains at least one pyrimidine derivative of formula I given in claim 1 and at least one compound of the general formula



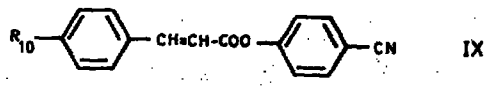
wherein the symbol Z' represents a cyano group, a straight-chain alkyl group containing 1 to 9 carbon atoms, a straight-chain alkoxy group containing 1 to 9 carbon atoms or a straight-chain alkanoyloxy group containing 1 to 10 carbon atoms and the symbol R_8 represents a straight-chain alkyl group containing 4 to 8 carbon atoms, a straight-chain alkoxy group containing 5 to 8 carbon atoms, a straight-chain alkanoyloxy group containing 2 to 8 carbon atoms or a straight-chain alkylcarbonate group containing 3 to 11 carbon atoms.

47. A nematic mixture according to claim 43 which contains at least one pyrimidine derivative of formula I given in claim 1 and at least one compound of the general formula



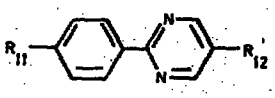
wherein the symbol R_9 represents a straight-chain alkyl group containing 4 to 8 carbon atoms, a straight-chain alkoxy group containing 4 to 8 carbon atoms, a straight-chain alkanoyloxy group containing 4 to 9 carbon atoms or a straight-alkylcarbonate group containing 4 to 11 carbon atoms.

48. A nematic mixture according to claim 43 which contains at least one pyrimidine derivative of formula I given in claim 1 and at least one trans-cinnamic acid ester of the general formula



wherein the symbol R_{10} represents a straight-chain alkyl group containing 1 to 8 carbon atoms.

49. A nematic mixture according to claim 43 which contains at least one pyrimidine derivative of formula I given in claim 1 and at least one compound of the general formula



wherein one of the symbols R_{11} and R_{12} represents a cyano group and the other represents a straight-chain alkyl group containing 3 to 9 carbon atoms, a straight-chain alkoxy group containing 2 to 9 carbon atoms or a straight-chain alkanoyloxy group containing 2 to 9 carbon atoms.

50. A nematic mixture according to any one of claims 43 to 49 inclusive, wherein said pyrimidine derivative is a pyrimidine derivative as set forth in any one of claims 8 to 32 inclusive.

51. A nematic mixture according to claim 50 which contains p-[(p-n-propylbenzyliden)amino]benzonitrile, p-[(p-n-butylbenzyliden)amino]benzonitrile, p-n-butylbenzoic acid p'-cyanophenyl ester, p-n-hexylbenzoic acid p'-cyanophenyl ester, 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine, 5-n-hexyl-2-(4-cyanophenyl)-pyrimidine and 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine.

52. A nematic mixture according to claim 50 which contains p-[(p-n-butylbenzyliden)amino]benzonitrile, p-n-butylbenzoic acid p'-cyanophenyl ester, p-n-pentylbenzoic acid p'-cyanophenyl ester, p-n-hexylbenzoic acid p'-cyanophenyl ester, 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine.

53. A nematic mixture according to claim 50 which contains p-n-butylbenzoic acid p'-cyanophenyl ester, p-n-pentylbenzoic acid p'-cyanophenyl ester, p-n-hexylbenzoic acid p'-cyanophenyl ester, p-n-heptylbenzoic acid p'-cyanophenyl ester, 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 5-n-heptyl-2-(4-cyanophenyl)-pyrimidine and 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine.

54. A nematic mixture according to claim 50 which contains p-[(p-n-propylbenzyliden)amino]benzonitrile, p-[(p-n-butylbenzyliden)amino]benzonitrile, p-[(p-n-hexylbenzyliden)amino]-benzonitrile, 5-cyano-2-(4-n-hexylphenyl)-pyrimidine, p-[(p-5-n-heptyl-2-(4-cyanophenyl)-pyrimidine, 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine, 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 2-(4-cyanophenyl)-5-(4-n-hexylphenyl)-pyrimidine.

55. A nematic mixture according to claim 50 which contains p-[(p-n-propylbenzyliden)amino]benzonitrile, p-[(p-n-butylbenzyliden)amino]benzonitrile, p-[(p-n-hexylbenzyliden)amino]-benzonitrile, 5-cyano-2-(4'-n-propyl-4-biphenylyl)-pyrimidine, 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 5-n-pentyl-2-(4'-cyano-4-biphenylyl)-pyrimidine.

56. A nematic mixture according to claim 50 which contains p-[(p-n-propylbenzyliden)amino]benzonitrile, p-[(p-n-butylbenzyliden)amino]benzonitrile, p-[(p-n-hexylbenzyliden)amino]-benzonitrile, 5-cyano-2-(4-n-pentylphenyl)-pyrimidine, 5-cyano-2-(4-n-butoxyphenyl)-pyrimidine, 5-cyano-2-(4-n-valeryloxyphenyl)-pyrimidine, 2-(4-cyanophenyl)-5-(4-n-propylphenyl)-pyrimidine and 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine.

57. A nematic mixture according to claim 50 which contains p-[(p-n-propylbenzyliden)amino]benzonitrile, p-[(p-n-butylbenzyliden)amino]benzonitrile, p-[(p-n-hexylbenzyliden)amino]-benzonitrile, 2-(4-cyanophenyl)-5-(4-n-butylphenyl)pyrimidine and 5-n-butyl-2-(4'-cyano-4-biphenylyl)-pyrimidine.

58. A nematic mixture according to claim 50 which contains 4'-n-pentyl-4-cyanobiphenyl, 4'-n-pentyloxy-4-cyanobiphenyl, 5-n-pentyl-2-(4-cyanophenyl)-pyrimidine, 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 5-n-butyl-2-(4'-cyano-4-biphenylyl)-pyrimidine.

59. A nematic mixture according to claim 50 which contains p-[(p-n-propylbenzyliden)amino]benzonitrile, p-[(p-n-butylbenzyliden)amino]benzonitrile, p-[(p-n-hexylbenzyliden)amino]-benzonitrile, p-[5-(p-n-butylphenyl)-2-pyrimidinyl]benzonitrile and p-[5-(p-n-pentyloxyphenyl)-2-pyrimidinyl]benzonitrile.

60. A nematic mixture according to claim 50 which contains p-[(p-n-propylbenzyliden)amino]benzonitrile, p-[(p-n-butylbenzyliden)amino]benzonitrile, p-[(p-n-hexylbenzyliden)amino]-benzonitrile, 2-(4-cyanophenyl)-5-(4-n-butylphenyl)-pyrimidine and 5-(4-cyanophenyl)-2-(4-n-hexylphenyl)-pyrimidine.

61. A process for the preparation of nematic mixtures, which process comprises mixing one or more of the pyrimidine derivatives of formula I given in claim 1 with other nematic substances.

62. A process according to claim 85, wherein one or more of the pyrimidine derivatives of formula I given in claim 1 is/are mixed with one or more compounds of formula V given in claim 44.

63. A process according to claim 61, wherein one or more of the pyrimidine derivatives of formula I given in claim 1 is/are mixed with one or more compounds of formula VI given in claim 45.

64. A process according to claim 61, wherein one or more of the pyrimidine derivatives of formula I given in claim 1 is/are mixed with one or more compounds of formula VII given in claim 46.

65. A process according to claim 61, wherein one or more of the pyrimidine derivatives of formula I given in claim 1 is/are mixed with one or more compounds of formula VIII given in claim 47.

66. A process according to claim 61, wherein one or more of the pyrimidine derivatives of formula I given in claim 1 is/are mixed with one or more trans-cinnamic acid esters of formula IX given in claim 48.

67. A process according to claim 61, wherein one or more of the pyrimidine derivatives of formula I given in claim 1 is/are mixed with one or more compounds of formula X given in claim 49.

68. A process according to any one of claims 61 to 67 inclusive, wherein one or more of the pyrimidine derivatives set forth in claims 8 to 32 inclusive is/are used.

69. A process according to claim 68, wherein compounds as specifically recited in any one of claims 51 to 60 respectively are mixed.

70. A process for the production of an electro-optical apparatus, which process comprises introducing one or more of the pyrimidine derivatives of formula I given in claim 1 into a suitable cell in admixture with other nematic substances.

71. A process according to claim 70, wherein a mixture containing at least one of the pyrimidine derivatives of formula I given in claim 1 and at least one compound of formula V given in claim 44 is introduced.

72. A process according to claim 70, wherein a mixture containing at least one of the pyrimidine derivatives of formula I given in claim 1 and at least one compound of formula VI given in claim 45 is introduced.

73. A process according to claim 70, wherein a mixture containing at least one of the pyrimidine derivatives of formula I given in claim 1 and at least one compound of formula VII given in claim 46 is introduced.

74. A process according to claim 70, wherein a mixture containing at least one of the pyrimidine derivatives of formula I given in claim 1 and at least one compound of formula VIII given in claim 47 is introduced.

75. A process according to claim 70, wherein a mixture containing at least one of the pyrimidine derivatives of formula I given in claim 1 and at least one trans-cinnamic acid ester of formula IX given in claim 48 is introduced.

76. A process according to claim 70, wherein a mixture containing at least one of the pyrimidine derivatives of formula I given in claim 1 and at least one compound of formula X given in claim 49 is introduced.

77. A process according to any one of claims 70 to 76 inclusive, wherein a mixture containing at least one of the pyrimidine derivatives set forth in claims 8 to 32 inclusive is introduced.

78. A process according to claim 77, wherein a mixture of compounds as specifically recited in any one of claims 51 to 60 respectively is introduced.

79. An electro-optical apparatus containing a pyrimidine derivative of formula I given in claim 1 in liquid crystalline condition.

80. An electro-optical apparatus according to claim 79 containing a pyrimidine derivative as set forth in any one of claims 8 to 32 inclusive in liquid crystalline condition.

81. An electro-optical apparatus containing a liquid crystalline mixture as set forth in any one of claims 43 to 60 inclusive.

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