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Ona Adomėnienė^a, Povilas Adomėnas^a, Antanas Gleiznys^a, Aldona Beganskienė^a, Lidija Poloudina^a & Yasuyuki Gotoh^b

^a Laboratory of Liquid Crystals, Vilnius University, Naugarduko 24, Vilnius, 2006, LITHUANIA

^b Chisso Corporation, 7-3, Marunouchi 2-Chome, Chiyoda-ku, Tokyo, 100-8333, JAPAN

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Mesomorphic Properties of New 5-Alkyl-2-Pyrimidinols Esters

ONA ADOMĖNIENĖ^a, POVILAS ADOMĖNAS^a,
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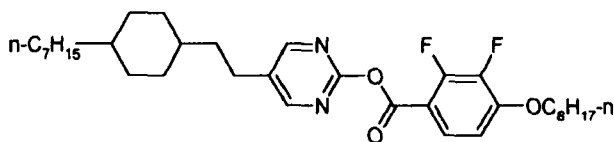
^a*Laboratory of Liquid Crystals, Vilnius University Naugarduko 24, Vilnius 2006, LITHUANIA* and ^b*Chisso Corporation 7-3, Marunouchi 2-Chome, Chiyoda-ku, Tokyo 100-8333, JAPAN*

A synthesis of a number of 5-alkyl-2-pyrimidinol esters was conducted, their mesomorphic properties were examined. Two ring esters of said pyrimidinols are nonmesomorphic, while three ring esters are typical mesogens, forming nematic either nematic-smectic mesophases.

Keywords: 5-alkyl-2-pyrimidinol; mesomorphic; nematic

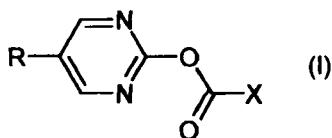
Pyrimidine unit is the most popular heterocycle among those used for synthesis of mesomorphic compounds for practical applications.

Nevertheless, not all combinations containing pyrimidine unit have been exploited in equally detail. So, if Dr. Volkmar Vill's database LiqCryst 3.1 contains 3761 compound possessing pyrimidine unit, it contains only 18 compounds which are 2-pyrimidinol derivatives and just one which is 5-alkyl-2-pyrimidinol ester [1], namely:



Cr 73.0° Sc 115.0° N 134.0° Is

We got an idea that some practically important compounds might occur among much more simple esters of 5-alkyl-2-pyrimidinols. In this work we made an attempt of a systematic evaluation of mesomorphic properties of structurally simple 5-alkyl-2-(substituted)carbonyloxy-pyrimidines:

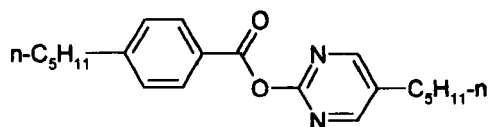


In this abbreviation, R is a straight alkyl group, X – 4-substituted phenyl, 4-(4-alkylcyclohexyl)phenyl, 4-(4-alkylcyclohexyl)cyclohexyl unit.

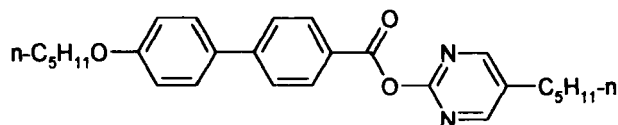
The target compounds (I) were obtained by a classical reaction of

5-alkyl-2-pyrimidinols with appropriate acid chlorides in pyridine solution. After an usual work-up, reaction products were purified by multiple crystallization, sometimes by chromatography on silicagel. 2-Hydroxypyrimidines may exist in hydroxyl- either amide form, so one may expect formation of some amount of N-acylated product. In our experiments, we didn't notice a presence of such type amides. The key start compounds, 5-alkyl-2-pyrimidinols, were obtained by a condensation of 2-alkylmalonic aldehydes tetraacetals hydrolysis products with carbamide at controlled pH values.

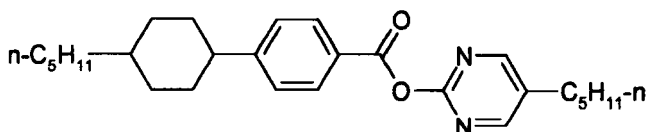
In the case of simple 4-alkylbenzoates, the compounds (I) are rather low – melting nonmesomorphic compounds, whereas an introduction of an additional phenyl or cyclohexane ring led to compounds I forming nematic either nematic-smectic mesophase in a wide temperature range.



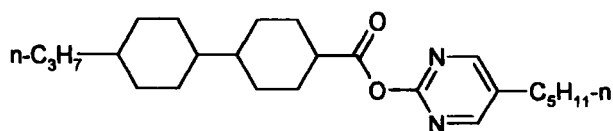
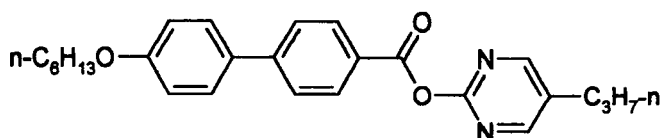
Cr 39.0° Is



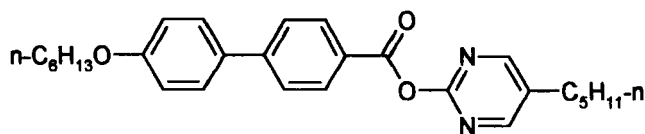
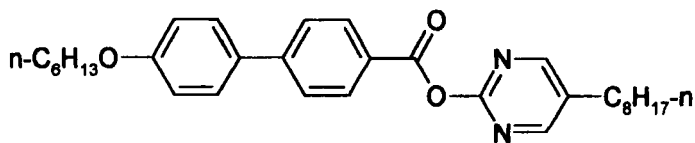
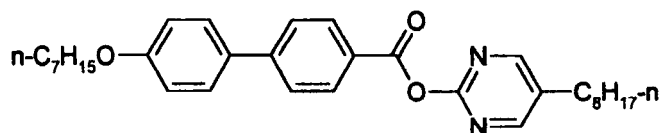
Cr 101° N 171° Is

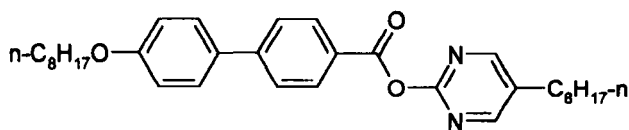


Cr 92° N 168° Is

Cr 146° (S_F 130°) N 180° Is

Cr 78° N 140° Is

Cr 68° S_C 142° N 154° IsCr 53.5° S_C 86.5-87.3° N 150° IsCr 71-71.5° S_C 120° N 134.5° Is



Cr 80.5-82.5⁰ S₂ 86.5-87.3⁰ S₁ 150-151⁰ Is

That's evident from the given phase transition temperatures that three-ring benzoates of 5-alkyl-2-pyrimidinols possess mesomorphic properties typical to that of other similar structure mesogens. They may be regarded as possible components of liquid crystalline materials for practical use, at least in smectic type materials.

References

- [1] Reiffenrath V., Krause J., Weber G., Finkenzeller U., Waechter A., Geelhar T., Coates D., Sage I.C., Greenfield S. (Merck): Pat. DE 3.906.019 (27.2.89).