Tuning the Mesogenic Properties of 5-Alkoxy-2-(4-alkoxyphenyl)pyrimidine Liquid Crystals: The Effect of Fluoro-Substituted Phenoxy End-Groups

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Notwithstanding variations of alkyl chain length, tuning mesogenic properties of smectic liquid crystals for FLC formulation often focuses on structural modifications of the rigid core.¹ However, Goodby and others have shown that the introduction of end-groups on one alkyl chain can have profound effects on mesogenic properties.² In our ongoing study of smectic liquid crystals with ‘de Vries-like’ properties,³ we seek new end-groups that promote the formation of smectic layers and enhance lamellar ordering.

In this presentation, we will report on the effect of mono- and difluorination of the phenoxy end-group on the mesogenic properties of 2-phenylpyrimidine derivatives QL11-m/n, and on correlations of the mesogenic properties to dimerization energy calculations (MP2/6-311++G(d,p)) for models of the corresponding phenoxy end-groups in parallel and antiparallel geometries. For example, we found that an ortho-fluoro substituent on the phenoxy end-group of QL11-8/8 causes a broadening of the SmC phase (QL20-8/8-2F) whereas a para-fluoro substituent (QL20-8/8-4F) causes a complete suppression of the SmC phase, even on cooling. The SmC-promoting effect of the ortho-fluoro substituent appears to be compounded in the 2,6-difluoro derivative QL22-8/8-2,6F₂. Although similar substituent effects are well documented for mesogens with fluoro-substituted cores,¹ this effect is unprecedented for mesogens with aromatic end-groups and suggests that tuning of the molecular tilt in FLC formulations might be achievable via relatively subtle structural modifications in fluoro-terminated components.

References:

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