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Computer simulation of the molecules of thermotropic substituted biphenyls

Abulyaissova L K
Buketov State University of Karagandy, Kazakhstan

The conformational properties of thermotropic 4-alkyl- or 4-alkoxy-4'-cyanobiphenyl have been studied. The substances are in a variety of leading companies producing liquid crystal materials due to the absence of color, low viscosity, stability, low melting temperatures. The geometry of the molecules of 4-*n*-pentyl-4'-cyanobiphenyl (BP-5), 4-*n*-pentoxy-4'-cyanobiphenyl (OBP-5), 4-*n*-octyl-4'-cyanobiphenyl (BP-8) and 4-*n*-decyl-4'-cyanobiphenyl (BP-10) was optimized by the molecular- mechanical method with force field MM2 and quantum-chemical method B3LYP/6-31G(d). The dependence of the mesomorphic properties of substances and the structural parameters of molecules on the length and nature of the non-rigid fragments has been examined.

Biography

Abulyaissova L K is an Associate Professor of Chemistry in Faculty of Physical and Analytical Chemistry at the Karagandy State University, Republic of Kazakhstan. She has published more than 70 papers and presentations in both international and national journals and scientific conferences. She is the author/co-author of 2 textbooks and the member of the International Liquid Crystal Society.

lyazzat.kz07@mail.ru

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