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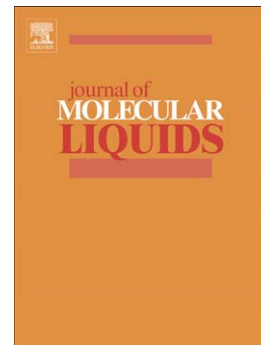
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Odd-even alternation in molecular structure and self-assembling of some macrocyclic polyethers

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ABSTRACT

It was found that the alternation of the melting points of $3n$ -crown- n retains its amplitude within a large range of the number of oxygen atoms ($n = 4 - 8$) in the crown's ring. This behavior is different from that observed for the compounds having n -alkyl chain, where the odd-even effect gradually disappears with increasing number of carbon atoms in the chain. So, the molecular structures of crown ethers containing in their rings even or odd number of oxygen atoms essentially differ from each other and the differences do not disappear when the ring increases. On the basis of temperature behavior of the increment of orientational entropy it was found that in liquid 12-crown-4 and 15-crown-5, the molecules self-organize into entities where the molecules are arranged in a head-to-tail way, while the molecules of 18-crown-6 are behaving quite differently: self-assemblies with antiparallel orientation of the molecular dipoles are predominant.

Keywords:

12-crown-4, 15-crown-5, 18-crown-6, Static Permittivity, Orientational entropy, Self-assembling

1. Introduction

Odd-even alternations of physical properties such as the melting point of n -alkanes and some n -alkyl derivatives, have been reported in numerous papers [1-3]. In particular, the derivatives which form the thermotropic liquid crystalline phases exhibit a spectacular alternation of the clearing temperature, where the compounds with even number of the carbon atoms in n -alkyl chain show the temperatures higher than the odd analogues [4]. Usually, however, the odd-even effect is very pronounced at a relatively low number ξ of $-\text{CH}_2-$

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