LIQUID CRYSTALS. PROPERTY ESTIMATION

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At present more than 100,000 compounds forming mesophases are synthesized [1]. However, for the majority of them (~98 %) only temperatures and enthalpies of phase transitions are known. To enlarge of industrial application areas, it is necessary to have a complete set of data on physical and thermodynamic properties of individual mesogens and mixtures [2]. For property evaluation, a scheme based on the minimum experimental information (molecular structure) is used. The normal boiling temperature is selected as the key property. Applicability of the group-contribution methods has been first tested on p-substituted "model substances", (i.e. compounds having a structure typical for calamitic mesogens, for which a set of physical properties had been well studied). Methods, that gave the minimum difference between the estimated and experimental data, have been tested on liquid crystalline substances. Scheme for the estimation of density, surface tension, thermodynamic properties in mesophase and in isotropic state, is proposed. Precision is enough for engineering calculations. Existing prediction methods for temperatures and enthalpies of phase transitions are analyzed. Different correlation dependencies have been tested on a large volume of experimental data from [3].

It is also demonstrated applicability of the group-contribution methods for mixture properties estimations. It is possible to calculate physical properties for mixtures and phase diagrams of binary and ternary systems containing liquid crystals basing on the activities of components (the UNIFAC-Dortmund method).

1. S. Pestov, V. Vill. *Liquid Crystals*. / In: *Springer Handbook of materials data*. /eds.: W. Martienssen, H. Warlimont. Springer, Berlin, 2018. P. 955-988.

2. M.G. Tomilin, S.M. Pestov. *Properties of liquid crystalline materials*. Polytechnika, St.-Peterbourg, 2005. 296 p. (in Russ.)

3. S.M. Pestov. *Physical properties of liquid crystals.* / ed.: V. Vill / *Landolt-Boernstein. New Series.* VIII/5A. Springer, Berlin, 2003. 492 p.