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# Analysis of the Influence of the Molecular Volume to Predict Experimental Pressure-Temperature Behavior in the Isotropic-Nematic Phase Transition of PAP, 5CB, MBBA and EBBA

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**Abstract** In this work, we have analyzed the experimental pressure-temperature behavior at the isotropic-nematic phase transition of the liquid crystals PAP, 5CB, MBBA, and EBBA at 1 atm by using the HERSW Convex Peg model in conjunction with the IPCM model. We have calculated the molecular volume values for the hard and attractive cores from theoretical quantum calculations at the PM3, PM6, B3LYP/6-311++G(d,p)//PM6, and M06/6-311++G(d,p)//PM6 levels of theory. The results suggest that the best theoretical prediction of the experimental pressure-temperature behavior is obtained when the molecular volume is evaluated at the DFT level.

**Keywords** Phase transitions · Isotropic-nematic · Convex peg

## 1 Introduction

A liquid crystal (LC) is an aggregation state whose properties are intermediate between a crystalline solid and an amorphous liquid [1]. It is important to mention that under appropriate conditions, the axis of the molecules in an LC can be aligned in a particular direction. Thus, if one modifies such direction, a variety of arrangements and phase transitions may be obtained. Moreover, these LC phase transitions may be induced by electric or magnetic fields [2–4]. These phase transitions have technological importance because they can be used to modify the optical properties of LCs without changing its composition [5]. Therefore, the development of predictive theories that allow the correct prediction of LC phase transitions is of great fundamental and applied interest.

Specifically, PAP (4-4′-bis (ethyloxy) azoxybenzene), 5CB (4–pentyl–4′-cyanobiphenyl), MBBA (4–methoxybenzilidene–4′-butylaniline), and EBBA (4–ethoxybenzilidene–4′-butylaniline) liquid crystals have attracted a great interest in view of their potential applications in scientific and technological fields. These liquid crystals exhibit isotropic-nematic (I-N) phase transitions which can be used in the fabrication of liquid crystal displays (LCD) [6–10]. However, the presence of heating lamps in such LCD may cause an increment on the temperature, around of 50 °C. These operating conditions may modify the optical properties of these LCs [11]. Also, in the electronic industry, these LCs can be used as temperature indicators to locate the precise site where an electronic component fails due to overheating, short circuit, or even a bad design. If one considers that in such place there will be an increment of the current density, then a hot spot will be located in this site. Thus, the sensibility of LCs to temperature gradients allows to identify, through a change in their coloration, the site of the fail by mean of the technique so called liquid crystal thermography (LCT) [12, 13]. In addition, the PAP, MBBA, and EBBA nematic liquid crystals can be used as lubricants because they are able to diminish the friction between surfaces [14]. For example, the viscosity of MBBA exhibits a lower value in the nematic phase in comparison to the isotropic phase [15]. Also, in this LC, the nematic ordering and low friction coefficient values are maintained when the temperature is above the

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