Orientational order and conformations in biaxial nematic phase of the bent-core A131 liquid crystal by means of ab initio calculations and ^{13}C Solid State NMR

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Liquid crystalline phases formed by bent-core or V-shaped molecules have recently attracted considerable interest, since these molecules belong to one of the predicted molecular topologies that should form a biaxial nematic phase (N_b) [1, 2].
The aim of this study is to seek the most probable conformational states within the bent-shaped core of A131. The conformers found in the Potential Energy Surface (PES) of the 5-ring model of A131 mesogen belong to two distinct structural groups, namely the *banana-shaped* and the *hockey stick-shaped* forms. The chemical shielding tensors (CSTs) of the aromatic carbons, for the prevalent conformers found, have been calculated using GIAO-DFT methods and compared to those experimentally determined by means of 2D Super technique [3]. The agreement is found to be satisfactory, especially if taking into account the complexity of the system under investigation. The verified CSTs have been used to obtain more reliable structural and local orientational order parameters in the uniaxial and biaxial nematic phases of A131.
Implications of the new ordering information are discussed in light of the conformational states found by DFT calculations. The local order parameters S and D of the aromatic rings are found to be useful, particularly with the aid of DFT results, in postulating the preferred conformers adopted by A131 in its two nematic phases [4].

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