Molecular packing of mesogenic bicyclohexylnitrile compounds

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The method of symmetry breaking potential and first order cluster expansion technique for the partition functions adopted for the theory of ordering in liquid crystals has been extended to symmetric and asymmetric molecules. The order parameter is calculated as a function of temperature and packing coefficient as a function of position of double bond in alkenyl chain length for homologous series of 4–alkenyl bicyclohexylnitrile Compounds [1-4]. The theoretical calculations adopted the method of Shivaprakash et al [5], account fairly well for the gradient differences in the order parameters of symmetric and asymmetric molecules and packing coefficients. Variation of order parameter with temperature for $1d_1$CC is shown in Figure 1.

It is of interest to compare the molecular packing formula given by Kitaigorodsky [6] of the homologous series of 4–alkenyl bicyclohexylnitrile compounds. Compound $1d_1$CC & $3d_1$CC possess double bond after the first carbon chain from cyclohexyl ring and exhibit nearly same packing coefficient. On the other hand, compounds $1d_3$CC & $0d_3$CC possess double bond after the third carbon chain from cyclohexyl ring and exhibit nearly same packing coefficient.

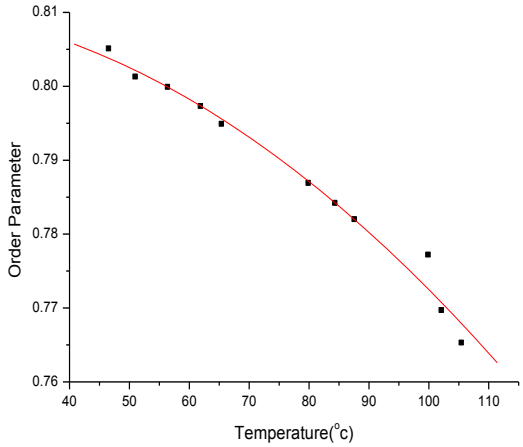

Figure 1. Variation of order parameter with temperature for $1d_1$CC

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