SUPERSONIC JET SPECTROSCOPY AND DENSITY FUNCTONAL CALCULATIONS OF PROTOTYPICAL LIQUID CRYSTALLINE MOLECULES

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We use laser-desorption supersonic jet spectroscopy in conjunction with novel density functional computer simulation to investigate the conformational behaviour of 4-cyanobiphenyl and its 4'-alkyl substituted derivatives. 4-pentyl-4'-cyanobiphenyl(5CB) is considered to be the prototypical nematic liquid crystalline molecule, 4-cyanobiphenyl(0CB) and the shorter chain 4-alkyl-4'-cyanobiphenyls(1-4CB) constitute mesogenic fragments of 5CB. The aim of studying these molecules is to explore the relationship between molecular structure and flexibility and liquid crystalline properties.

Density functional *ab initio* computer simulations are being carried out [1] to predict the conformational energy landscapes of 5CB and related molecules. These calculations predict the behaviour of *isolated* molecules, but the available experimental data is generally concerned with the *condensed phase.* The supersonic jet technique provides a unique route to the observation and spectroscopic characterisation of *isolated* molecular conformers, and thus to experimental data with which to definatively test the validity of the density functional calculations.

1. S.J. Clark, C.J. Adam, D.J. Cleaver and J. Crain, Liquid Crystals, 1997, **22**, 477.