

## Supramolecular self-organisation of C60 containing supemesogens

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A molecular model of cubic building blocks(1,2) is used to describe the mesomorphism of fullerene containing conical fullerenomesogens(3-8). The model takes explicitly into account both molecular flexibility and submolecular partitioning into chemically distinct regions. Calculations based on density functional molecular theory and on Monte Carlo computer simulations are used to rationalize the self-organisation exhibited by these systems in terms their molecular structure. The theoretical calculations are applied for a variety of C60 functionalisations, ranging from dendromesogenic branch monoadducts to conical multiadducts of C60. The theoretical calculations reproduce the rich phase polymorphism exhibited by these systems which includes nematic and various types of positionally ordered smectic and columnar mesophases. Detailed analysis of the theoretical calculations and comparison to experimental results are presented. In spite of its many simplifications, the coarse grained molecular models accounts remarkably well for the phase polymorphism of these systems and offers valuable insights into the supramolecular nature of the LC phases. Going a step further from the available experimental results, we study the phase behaviour of mixtures of functionalised fullerenes with nonbonded ones. Our calculations predict that a small fraction of non-bonded fullerenes may cause severe changes to the column morphology of the columnar phases or even to totally destabilise the columnar in favour of the lamellar molecular organisation

### References

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