Computational studies of shape-persistent polyphenylene dendrimers

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Polyphenylenes – compounds containing benzene rings linked by σ-bonds – form an increasingly important class of organic materials, as the benzene ring is an extremely flexible modulus for the construction of a wide range of structures and can bear a large range of active functionality. Also, the delocalized π-systems on adjacent rings can overlap to form extended conjugate systems.

In particular, 3D polyphenylene dendrimers show a variety of interesting properties:

- they are colorless, chemically inert and thermally stable (> 450°C);
- have a good solubility in organic solvents, but are easily precipitated in polar solvents;
- can be thoroughly characterized by spectroscopy and
- are shape persistent.

Further, these peculiar structures may be used as scaffolds with a wide variety of functionality, enabling them to be used as functional nanoparticles with a vast range of possible applications. For example, the controllable coating of the surface of the dendrimers with moieties such as amino and carboxy groups should not only provide a means for obtaining water solubility but also, through attachment of, for example, polyethylene oxide or peptide chains, biocompatibility and/or biodegradability.

In this way, we can prepare functionalized nanoparticles, which potential biological applications: the attachment of an antigen or a biological substrate, for instance, might enable them to be used in biological sensors or drug delivery systems.

In this work we have performed a thorough characterization, by computer simulations, of the first three generation of three polyphenylene dendrimeric families,

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both underivatized and substituted with amino and carboxy groups in a solvated environment, with the purpose of studying the relevant structure-property relationships to be exploited in biomedical applications.