POLYPHENYLENE DENDRIMERS

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The most attractive property of polyphenylene dendrimers is their rigidity. They retain the molecular symmetry and monodispersity of the usual, commercially available alyphatic dendrimers, while the composition of the dendritic branches makes them self-supporting. In solution flexible dendrimers usually form a globular 3D-structure in which the dendritic branches are evenly distributed over the whole molecular volume, however, it has been shown that, depending on the generation of the particular dendrimer, their peripheral groups tend to fold back into the interior of the molecule. Moreover, when being adsorbed on a surface (or by the removal of the solvent), they often tend to flatten out.

In contrast to this behaviour, it has been shown that rigid dendrimers based on polyphenylenes have stiff branches and the backfolding in solutions is impossible. Furthermore, when polyphenylene dendrimers are absorbed on a mica substrate their original shape is retained. These features and their size, lying in the low nanometer scale, make these molecules attractive candidates for several applications such as supports for functional groups and as hosts for smaller guest molecules.

We have studied the free volume in a series of rigid polyphenylene dendrimers by positron lifetime spectroscopy (PLTS) and molecular dynamics calculations, in order to assess the expected relationship between the size (number of generations, molecular weight) of these molecules and the intramolecular free volume. We have found that the size of these inner free volumes is stable, and increases with the increasing number of generations.