MODELING OF MOLECULAR INTERACTIONS AND INCLUSION PHENOMENA OF AMINOACIDS AND NUCLEOTIDES IN A SYNTHETIC DENDRINMER

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As a new class of materials, dendrimers (or starburst polymers) have recently awakened great interest in the scientific community. Despite the substantial difficulties encountered in their synthesis, a wide range of these substances have been produced and, although only in part, characterized.

Starburst dendrimers possess three major architectural components: an initiator core, an interior and an exterior. By definition or construction, these three components are interdependent and reflect a unique molecular genealogy. As we progress from the initiator core to an advanced dendrimer stage (or *generation*), this molecular genealogy manifests itself in a variety of ways. Thus, beginning with the core, molecular details are sequentially transcribed and stored to produce interior and, ultimately, exterior features which are characteristic of that dendrimer family. In this fashion, interior features such as size, chemical composition, flexibility and topology are developed and manifested as stored molecular information.

The interior of a dendrimer consists of a scaffolding upon which surface properties such as shape, reactivity, stoichiometry, congestion, special kinetic features, flexibility and fractal character can be generated and controlled. These surface features may reflect in several interesting attributes, such as divergent recognition and exo-reception properties, which find an analogy in biological processes like, for instance, antibody-antigen recognition and protein-protein interactions.

These are by no means the only fascinating aspects of these molecules. In fact, many other potential applications spring from their unusual architecture, which include nanoscale catalysis and reaction vessels, micelle mimics, magnetic imaging agents, immuno-diagnostics, agents for controlled drug delivery, chemical sensors, information-processing materials, high-performance polymers, adhesive and coatings, separation media and molecular antennae for adsorbing light energy and funneling it to a central core (as occur in photosynthetic systems).

Due to their unique structural properties, dendrimeric molecules can also form inclusion complexes with different guest molecules, comprising conventional drugs, L-alpha-aminoacids and peptide-proteic drugs. This ability could be exploited, in principle, in the abatement of the toxicity and side effects of various drugs, in the increase of their availability and also in the mediation of biological receptor-substrate interactions.

In this work we have performed a detailed computational study of host-guest inclusion complexes between the synthetic poly(aryl ether) dendrimer VAL-OH and a selected series of L-alpha-aminoacids and nucleotides, aimed at understanding the nature of the driving force and mechanism, leading to their formation. Relative complexation energies for the complexes and the solvation free energies for the single guest molecules were also calculated.