Abstract Thesis

The main objective of this thesis is the study of boron cluster compounds in solution, their interaction with polymers and the formation of nanostructures. Most of the work was focused around cobalt bis(dicarbollide) (COSAN) but the incorporation of carborane into polymers was also studied. The idea was to close the knowledge gap around the way COSAN aggregates and continue the line of the laboratory in leading this topic. Therefore, we performed in-depth analysis of isothermal titration calorimetry curves to determine the aggregation number at concentrations around the critical micellar concentration (CMC). Thus, the aggregation number obtained was an improvement over previous data obtained a much higher concentration. The use of acetonitrile as a cosolvent in the micellization process helped formulate a model describing how C-H bonds in the COSAN micelles are directed towards the inside of the micelle. Furthermore, COSAN was used as a model drug for loading nanocarriers composed of hydrophobic core and charged corona. The importance of this work relies on the creation of guidelines for drug loading into similar polymeric vectors in order to determine how the nanocarrier will be affected. With the help of coarse-grained simulations, we determined that changes in the hydrophobicity of the loaded drug will have a deep impact on the solubility of the nanocarrier. Notably, a slight increase in hydrophobicity of loaded drug triggers the collapse of polymer chains in the corona therefore limiting the loading capacity of such systems. Lastly, a triblock terpolymer containing carboranes was used to determine the effect of such clusters in the self-assembly. To determine the direct effect of carborane a diblock copolymer was synthesized with the exact composition as the terpolymer minus the short carborane block. The carborane block allowed for terpolymer to self-assemble either as worms or spherical micelles depending on the solvent mixture, whereas the diblock was only capable of forming spherical micelles. Furthermore, the terpolymer micelles worked as a dual stimuli responsive system to F^- ions and pH change. The changes were tracked via fluorescence with pH working as an ON/OFF switch for the fluorescence of the micelles.

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