579c Determining the Octanol-Water Partition Coefficient for Poss Systems

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Recent reports have highlighted the potentially hazardous nature of nanomaterials.[1,2,3]. It has for example been shown that carbon nanotubes can accumulate in the lungs of rats[4,5] and that buckminsterfullerenes (C60) can bind to and deform DNA sequences.[6] We are interested in understanding whether a novel class of nanomaterials, polyhedral oligomeric silsesquioxanes (POSS), could constitute an environmental hazard. POSS are of the molecular formula $(SiO_{1.5}R)_8$ where R is typically an organic functional group used to tether the POSS molecule to a polymer chain. POSS molecules have been proposed as building-blocks for novel organic-inorganic hybrid nanocomposite materials. As a result a rapidly increasing number of POSS monomers are being synthesized and novel applications are continuously being proposed. However, at present, neither the thermodynamic properties of systems that contain POSS monomers, nor the environmental impact of POSS-based materials are satisfactorily understood.

We report molecular dynamics simulations to evaluate both the thermodynamic properties of POSS molecules, and their potential environmental impact. We concentrate on the properties of POSS systems at infinite dilution in order to compute the octanol/water partition coefficient, which is obtained from the change in free energy for a POSS molecule being transferred from water to octanol. The change in free energy is prototypical to that of transferring the particle from water to a lipid bilayer. We consider H terminated and octa-functionalized POSS monomers to assess the effect of POSS chemical composition on the partitioning. We also explore the solvent structure around the POSS monomers and correlate this information with results for the water/octanol partition coefficient.

Keywords: POSS, water/octanol partition coefficient, solvent structure References

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