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Influence of End Groups in Polymer Aggregates: A Neutron Scattering Study

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Polymer solutions have been studied in great detail in the past, however the influence of the end groups has been mostly overlooked. Recent works found the existence of polymeric micelles, when these possessed hydrophobic end groups. We investigated the solution behavior and the occurrence of micelle-like structures for (semi)-dilute systems. Using RAFT polymerization, we synthesized PNIPAM chains that are hydrophobically terminated. We also investigated these polymers after cleavage of the hydrophobic end groups. The influence of end groups regarding the solution behavior was analyzed using rheology, while the cloud points of the polymer solutions were measured via temperature dependent extinction spectroscopy. To characterize the dimensions of the polymer coils and potential aggregates dynamic light scattering was used. Small angle neutron scattering (SANS) was used, which provided insight into the internal structure of the samples. Through these, we were able to determine the ratio between individual polymer chains and the micelles. The rheological and cloud point measurements show a dependence on the end group for all polymers with molecular weights below 100 kDa. This suggest that the end groups influence not only molecular-scale interactions but also macroscopic properties of polymer solutions. SANS measurements indicate that, at low concentrations, micelles exist as individual structures. Upon increasing the concentration, micelles aggregate, leading to a distinct structure factor contribution in the scattering profile. SANS also facilitates the calculation of the size and aggregation number of these micelles. Our studies demonstrated that the terminal groups of a polymer have a substantial influence on its overall behavior in solution. This effect is especially pronounced for shorter polymers. Using SANS, we were able to gain insight into structural organization and aggregation behavior of these systems as a function of concentration and molecular weight.