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Molecular brushes investigated by scattering methods

Molecular brushes consist of a polymeric backbone with densely grafted side chains. In case a molecular brush contains both hydrophobic and hydrophilic segments, it takes on an elongated shape, which makes it a potential drug carrier in the human body . Poly(2-oxazoline)-based molecular brushes are especially well-suited to this purpose due to their high biocompatibility .
In the present work, a bottle brush copolymer with a hydrophobic poly(2-isopropenyl-2-oxazoline) backbone and hydrophilic side chains of poly(2-ethyl-2-oxazoline); P(iPOx)-g-P(EtOx), is investigated with respect to its size and inner structure in aqueous solution in dependence on temperature. Experimental results from dynamic light scattering show two different kinds of particles, namely 5 nm and 120-220 nm. We attribute the smaller value to the single molecular brush, and the larger one to aggregates or byproduct from the synthesis. The solution becomes turbid at 48℃, which is assumed to be due to the aggregate formation because the thermoresponsive P(EtOx) sidechains collapse and become hydrophobic. As a further step, temperature-resolved small-angle neutron scattering experiment were performed, revealing that the molecular brush does not have the shape of an elongated particle, as expected, but rather forms prolate ellipsoids with equatorial and polar radii of 7 nm and 2.5 nm, respectively. Thus, more advanced modeling is needed to fully describe the inner structure.

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