

用介观动力学模拟Pluronic L64/水/p-Xylene体系的相分离

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摘要 用介观动力学在介观层次上对不同组分的PluronicL64/水/p-xylene三元体系的相分离进行了研究,得到了和实验相吻合的结果。计算表明对于纯p-xylene溶剂和有少量水的p-xylene溶剂,体系没有发生相分离,随着水的含量增加,体系发生了明显的相分离,产生了不同形态的胶团。本研究还通过对比不同溶剂组分下的体系介观形貌,讨论了水在体系相分离中的作用。同时通过分析模拟了1000步后体系中水的分布,证实了胶团核中存在自由水(freewater)的猜想。

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Simulation of the phase separation of the pluronic L64/water/p-xylene system using mesodyn

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Abstract The phase separation of the Pluronic L64/water/p-xylene system in mesoscopic region was simulated using MesoDyn and the results which are in agreement with the experiment results. Phase separation of the system did not take place in pure p-xylene or in the presence of a small amount of water, but with increasing of the concentration of water, phase separation of the system took place markedly and formed micelles with different shapes. This paper also compares th emesoscopic morphology formations of systems at different concentrations of solvents and discusses the effect of water during the phase separation. By analysing the water distributions of the systems after 1000 simulation steps, we can proved that free water do exist in the micellar core.

Key words [PHASE SEPARATION](#) [NON IONIC SURFACTANTS](#) [INTERACTIONS](#)

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