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研究论文

亚苄基山梨醇衍生物在有机溶剂中的自组装及凝胶化研究

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摘要 从分子结构的差异、亲溶剂作用、分子几何构型、
相转变热焓以及溶剂极性等方面研究了三种亚苄基山梨醇衍生物凝胶剂在有机溶剂中的自组装和凝胶化机理. 三种衍生物凝胶剂在结构上的差别仅在于亚苄基上甲基取代基数量不同. 结果表明:
由于亲溶剂作用的增加和分子几何构型的优化, 含甲基多的凝胶剂在有机溶剂中的自组装能力强,
表现在具有低的最低凝胶化浓度和高的相转变温度. 而溶剂极性的增强,
使三种衍生物凝胶剂形成的凝胶相转变温度降低.
偏光显微镜照片表明该凝胶剂在正辛醇凝胶中的聚集体晶型不同.
场发射扫描电镜照片表明三种衍生物凝胶剂自组装形成相互缠绕的纤维束网络结构. 紫外吸收光谱表明,
对比其溶液态, 三种衍生物聚集体苯环的K带发生红移, 表明π-π堆积作用是亚苄基山梨醇衍生物凝胶剂自组装的驱动力之一; 红移的幅度随苯环上甲基数量的增加而增加,
这与三种衍生物形成的分子凝胶的热稳定性相吻合.

关键词 亚苄基山梨醇衍生物 自组装 分子凝胶

分类号

Self-assembly and Gelation of Benzylidene Sorbitol Derivatives in Organic Solvents

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Abstract The self-assembly and gelation of benzylidene sorbitol derivatives, 1,3:2,4-di-*O*-benzylidene-*D*- sorbitol (DBS), 1,3:2,4-di-*O*-*p*-methylbenzylidene-*D*-sorbitol (MDBS) and 1,3:2,4-di-*O*-*m*,*p*-dimethylbenzyl- idene-*D*-sorbitol (DMDBS) as gelators were investigated based on their molecular structure, solvophilic effect, enthalpies of phase transition and the polarity of solvents. Structural differences among the three gelators are only in the varied amount of methyl groups on the benzene ring. It was found that the ability of self-assembly for the three gelators was related to the amount of methyl groups. The lower minimum gelation concentration (MGC) and higher phase transition temperature for MDBS and DMDBS usually imply higher ability of self-assembly due to the more methyl groups in comparison with DBS. The large polarity of solvents causes decrease of phase transition temperature of the gels formed by these three gelators. Polarized optical images of the gels show that the ag-gregates of the three gelators are spherulite crystallite and other types of crystallite in *n*-octanol. FE-SEM images show entangled fiber-like aggregates of the gelators, which in turn form a three-dimensional network in *n*-octanol gels. UV spectra of the *n*-octanol gels formed by the three gelators indicate that the K bands of benzene rings are red shifted. It reveals that the π-π stack is one of the driving forces for the self-assembly of the gelators. The extent of red shifts of K bands depends on the amount of methyl groups in benzene rings which is in accord with the stabilities of the gels formed by such three gelators.

Key words benzylidene-*D*-sorbitol derivative self-assembly molecular gel

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