

研究论文

**Li<sup>+</sup>在PC+DMF混合溶剂中优先溶剂化的<sup>13</sup>C NMR研究**

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**摘要** 利用<sup>13</sup>C NMR光谱技术研究了Li<sup>+</sup>在碳酸丙烯酯(PC)+*N,N*-二甲基甲酰胺(DMF)混合溶剂中的优先溶剂化现象. 根据溶剂分子中碳原子的化学位移随锂盐浓度的变化关系, 确定了与Li<sup>+</sup>发生配位的原子. 碳原子的配位位移值随混合溶剂组成的变化关系表明, 在LiClO<sub>4</sub>+PC+DMF混合物中, DMF分子对Li<sup>+</sup>的溶剂化作用较PC分子强. 定量计算得到, 在*n*(PC): *n*(DMF)=1: 1 (摩尔比)的混合溶剂中, PC与DMF分子数在Li<sup>+</sup>第一溶剂化层中的比率为0.12, 说明Li<sup>+</sup>优先被DMF分子溶剂化.

**关键词** [锂离子](#) [碳酸丙烯酯](#) [N,N-二甲基甲酰胺](#) [优先溶剂化](#) [<sup>13</sup>C NMR](#)

分类号

**<sup>13</sup>C NMR Studies on the Preferential Solvation of Li<sup>+</sup> in PC + DMF Mixed Solvents**

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**Abstract** The preferential solvation of Li<sup>+</sup> in propylene carbonate (PC) and *N,N*-dimethylformamide (DMF) mixed solvents has been studied by <sup>13</sup>C NMR technique at various solvent and lithium salt concentration. The difference in the chemical shifts of the solvent with and without the electrolyte was attributed to the coordination of the solvent to Li<sup>+</sup>. Based on the observed dependence of the <sup>13</sup>C NMR chemical shift for the solvents on the composition of the electrolyte, the coordinated atoms of the solvents to Li<sup>+</sup> have been determined. The solvation ability of DMF to Li<sup>+</sup> was found to be stronger than PC from the variation of coordination shift with the molar fraction of PC. It was shown that the molar ratio of PC to DMF molecules in the first solvation shell of Li<sup>+</sup> was 0.12 in the ternary solution with equal mole of PC and DMF. These results indicated that Li<sup>+</sup> was solvated preferentially by DMF molecules in the LiClO<sub>4</sub>+PC+DMF mixtures.

**Key words** [lithium cation](#) [propylene carbonate](#) [N,N-dimethylformamide](#) [preferential solvation](#) [<sup>13</sup>C NMR](#)

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