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Studies on Room Temperature Ionic Liquid Prepared from $InCl_3$-MBIC

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Abstract: The phase diagram of $InCl_3$-MBIC was constructed by DSC method. A clear, colorless and mobile ionic liquid was obtained and liquid down to 258 K. Both Raman scattering and *ab initio* calculations indicate that $InCl_4^-$ is the predominant anion.

Keywords: Ionic liquid, Raman scattering, phase diagram, $InCl_3$, MBIC, *ab initio* calculation.

Room temperature ionic liquids (RTIL) have been studied for many years, but have recently begun to receive greater attention because of their possible uses, especially with respect to green chemistry. RTILs based on mixture of $AlCl_3$ and dialkylimidazolium chloride were most widely studied. To expand our knowledge of RTIL chemistry and because of our interest in the chemistry of Indium[1], we decided to determine whether similar salts could be prepared by replacing $AlCl_3$ with $InCl_3$. There are a limited number of reports of ionic liquid based on metals other than Al[2]. In this paper, such an ionic liquid has been prepared by directly mixing $InCl_3$ and 1-methy1-3-buty-limidazolium chloride (MBIC) under dry nitrogen atmosphere.

Results and Discussion

Each peak of DSC traces means a transition temperature of $InCl_3$-MBIC system corresponding to given composition. The phase diagram (see **Figure 1**) was drawn according to DSC traces and x means mole fraction of $InCl_3$ in $InCl_3$-MBIC mixture. From **Figure 1**, there is a narrow area of liquid at about x= 0.50 and liquid down to 258 K, that is, a colorless clear, transparent and mobile liquid was observed in experiments. Since there was only one peak on DSC trace at x=0.50, it could be recognized that a pure compound with anion $InCl_4^-$ formed.

Figure 1 Phase diagram for binary system $InCl_3$-MBIC

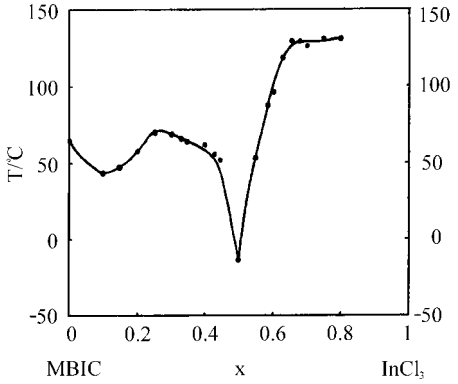
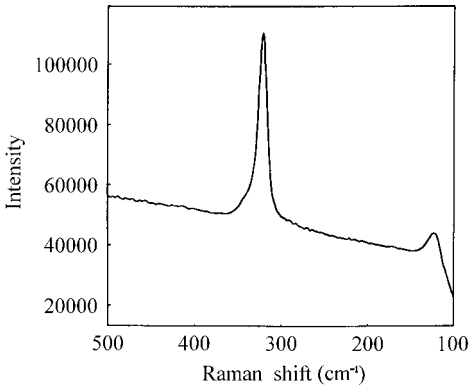


Figure 2 Raman spectrum of ionic liquid at x=0.50



Ab initio Hartree-Fock calculations with 3-21G* basis set were performed to predict the structures, energies, bond lengths and vibrational (Raman) frequencies of In (III) chloride complexes. All calculations were carried out using GaussNet 2000. For example, a Hartree-Fock geometry optimization of $InCl_4^-$ found the most stable structure to be a tetrahedron with In-Cl bond length of 2.423 Å which is in good agreement with the structure determined by Trotter *et al*[3]. The experimentally determined Raman spectrum of the low-wave number range of the ionic liquid with x=0.50 is shown in **Figure 2**. The primary feature is a band with maximum at 321.4 cm^{-1} responding to calculated frequency 321.5 cm^{-1}. The fact shows that only an anion $InCl_4^-$ exists in the liquid at x=0.50 and it could also be confirmed by DSC trace for liquid of the same component.

Acknowledgments

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