Asian Journal of Chemistry; Vol. 23, No. 10 (2011), 4358-4360

ASIAN JOURNAL OF CHEMISTRY

www.asianjournalofchemistry.co.in

Physical and Chemical Properties of 1-Butyl-3-methylimidazolium *bis*(trifluoromethanesulfonyl)imide [Bmim]NTf_2 Ionic Liquid

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(*Received*: 12 October 2010; *Accepted*: 15 June 2011) AJC-10047

Some physical and chemical properties of ionic liquid 1-butyl-3-methylimidazolium *bis*(trifluoromethanesulfonyl)imide ([Bmim]NTf_2) were measured and analyzed separately. At 20 ºC, the density of [Bmim]NTf_2 was 1.4682 g cm^{-3} and the viscosity was 56.0 m Pas. The relationship of viscosity (η) and temperature (t) was η (mPas) = 87.66-1.58 t (ºC). [Bmim]NTf_2 is insoluble in water and most petroleum aromatics solvents but soluble in some molecular solvents. The conductivity was related with temperature, solvent and concentration. The conductivity increased as temperature increase or the concentration increased. [Bmim]NTf_2 had excellent the chemical-stability and thermostability.

Key Words: Ionic liquids, [Bmim]NTf_2, Density, Viscosity, Dissolvability, Conductivity, Thermostability.

INTRODUCTION

Ionic liquids are becoming a new generation of green solvent because of their special characters such as small vapour tension and non-involatility, chemical-stability and thermostability, high conductivity, wide electrochemical window, excellent solubility to many organic compounds and "can being designed", *etc*[1-5]. Recently they were beginning to be applied in many fields such as extraction separation, organic reaction, electrochemistry, catalytic process, namoparticles preparation[6-10]. Each of ionic liquids has superior to ordinary organic solvents in one or several aspects. Different ionic liquid has different speciality according to its composition and structure. Here, some physical and chemical properties of [Bmim]NTf_2 prepared by reported method[11], such as density, viscosity, heat stability, conductivity, dissolvability and solubility in general organic solvents and in petroleum hydrocarbon, were measured separately.

RESULTS AND DISCUSSION

Density: The density of [Bmim]NTf_2 was measured by a densimeter in 20 ºC. The average density was 1.468 g cm^{-3}.

Viscosity: The viscosity of [Bmim]NTf_2 was measured at different temperature by the digital viscometer (NDJ-5S, Shanghai Nirun Intelligent Technology Co., Ltd.) (Fig. 1). It indicated that the viscosity decreases as the temperature increases. The temperature had great effect on the viscosity of ionic liquids. The relationship of viscosity (η) of [Bmim]NTf_2 with the temperature (t) by regression analysis according to the experimental data was:

$$\eta\ (\text{mPaos}) = 87.66-1.58\ t\ (^{\circ}\text{C})$$

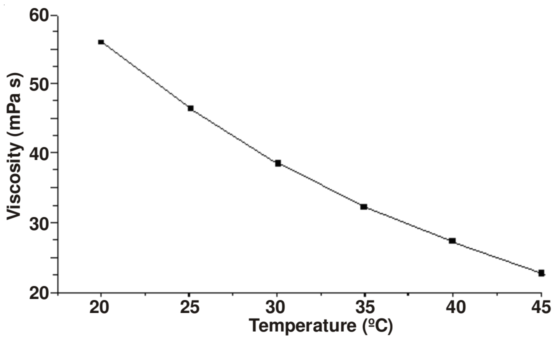

Fig.1. The curve of viscosity of [Bmim]NTf_2 *versus* temperature

Dissolvability and solubility: Ionic liquids have very low vapour tension and good dissolvability and can be used to dissolve many organic or inorganic compounds and polymers. They are excellent solvents for many chemical reactions. The dissolvabilities of ionic liquids need to be systemically investigated before they are utilized well. [Bmim]NTf_2 prepared in this paper was hydrophobic. The dissolvabilities of [Bmim]NTf_2 in conventional volatile molecular solvents, petroleum hydrocarbon solvents were shown in Tables 1 and 2.

Conductivity and influencing factors: The conductivity of [Bmim]NTf_2 was measured in different concentration, different temperature and different solvents separately. The influencing factors to the conductivity were discussed.

TABLE-1
DISSOLVABILITY OF $[Bmim]NTf_2$ IN SOME MOLECULAR SOLVENTS

Solvent	Water	Methanol	Acetone	Chloroform	Ether	Ethyl accetate
Dissolvability	Insoluble	Soluble	Soluble	Slightly Soluble	Insoluble	Soluble

TABLE-2
DISSOLVABILITY OF IONIC LIQUIDS IN SOME PETROLEUM AROMATICS SOLVENTS

Solvent	*n*-Hexane	Cyclohexane	Petroleum ether	Tetrachloride carbon
Dissolvability	Insoluble	Insoluble	Insoluble	Slightly soluble

Effect of solvents: The conductivities of different concentration (0.006, 0.020, 0.035, 0.050 g mL^{-1}) of $[Bmim]NTf_2$ in different solvents (acetone, methanol, 1,2-dichloromethane, ethyl acetate) were measured at room temperature (Fig. 2).

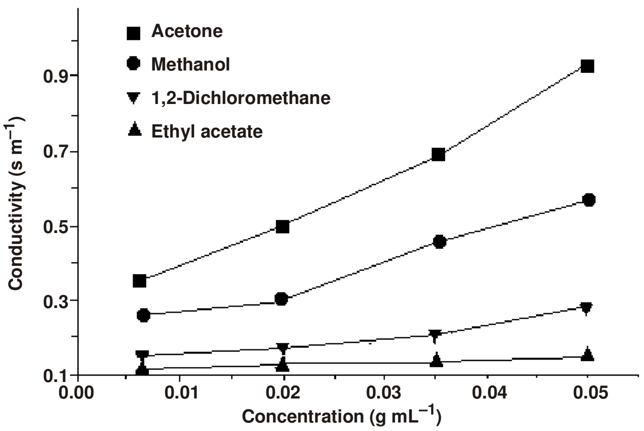

Fig. 2. Conductivities of $[Bmim]NTf_2$ in different solvents

It showed that the conductivities of $[Bmim]NTf_2$ in different solvents were not same. At same concentration, the conductivity of $[Bmim]NTf_2$ in acetone was highest, that in ethyl acetate was lowest. Actually, main factors influencing the conductivity of ions were viscosity, density, ionic size and molecular weight, *etc*, thereinto, the viscosity was dominant. The conductivity was inverse ratio to the viscosity in a wide range. The viscosity of ionic liquid was determined by hydrogen bond and the van der Waals force. The van der Waals force of the ionic liquid in ethyl acetate was higher than that in acetone or methanol. Therefore, the conductivity of $[Bmim]NTf_2$ in ethyl acetate was lowest.

Effect of concentration: The conductivities of $[Bmim]NTf_2$ in acetone at different concentration (0.006, 0.010, 0.015, 0.020, 0.030 g mL^{-1}) were measured at room temperature (Fig. 3). It showed that the conductivity increased as the concentration increased.

Effect of temperature: The conductivity of 0.015 g mL^{-1} $[BMImt]NTf_2$ in acetone was measured at different temperature (20, 30, 40, 50 ºC) (Fig. 4). It showed that the conductivity of $[BMImt]NTf_2$ in acetone solvent increased as temperature increased.

Thermostability of $[Bmim]NTf_2$: Ionic liquids have less vapour tension. The upper limit of service temperature is decided by thermo-decomposable temperature. The curves of DTA and TG of $[Bmim]NTf_2$ was measured by the integrated thermo-analytical apparatus (ZRY-1P, Shanghai optics instrument factory) and showed in Fig. 5. The sample had a little loss of weight at 80-150 ºC. This was caused by volatilization of water and volatile organic solvents such as ethanol present in the sample. When the temperature was above 370 ºC, the sample lost weight quickly and the decomposition occurred. The sample arrived at constant weight and the rate of weight loss was 98.3 % as temperature was above 600 ºC. It indicated that thermal stability of $[Bmim]NTf_2$ was much higher than that of common organic solvents. The decomposition of $[Bmim]NTf_2$ was an exothermal reaction and began at about 370 ºC.

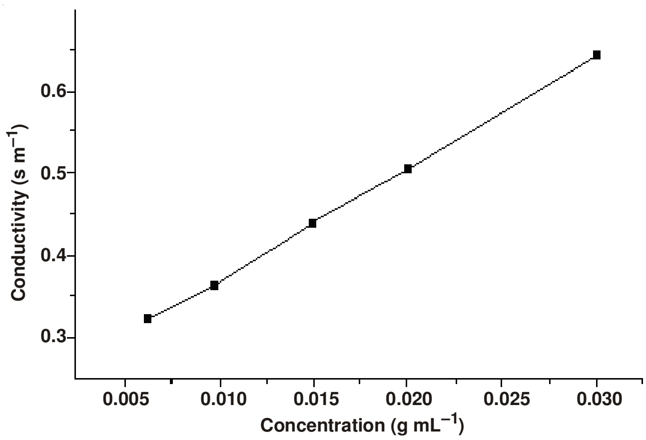

Fig. 3. Conductivities of $[Bmim]NTf_2$ at different concentration in acetone

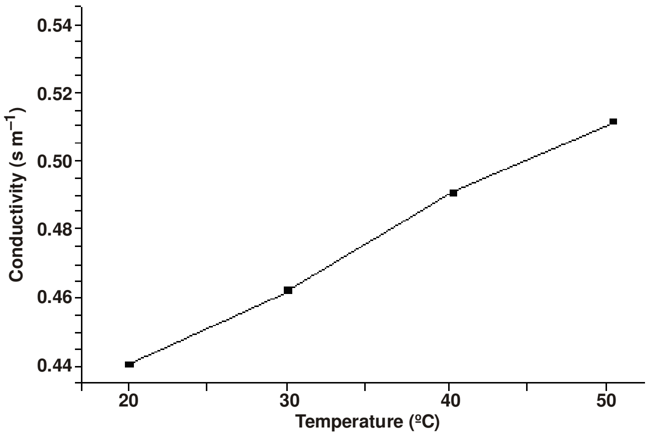

Fig.4 Conductivity of $[Bmim]NTf_2$ at different temperature

Conclusion

Some physical and chemical data of $[Bmim]NTf_2$ ionic liquid were measured and analyzed. The density of $[Bmim]NTf_2$ was 1.4682 g cm^{-3} at 20 ºC. The viscosity was

56.0 m Pas at 20 ºC. It was strongly affected by temperature and decreased quickly as the temperature increased. The relationship of viscosity (η) and temperature (t) was η (m Pas) = 87.66-1.58 t (ºC). [Bmim]NTf_2 was insoluble in water and in most of the aromatics petroleum solvents. It could dissolve in some molecular solvents such as methanol, acetone, *etc*. The conductivity was related with temperature, solvent and concentration. The conductivity increased as temperature increases or the concentration of [Bmim]NTf_2 increased. The kind of solvent had great effect on the conductivity of [Bmim]NTf_2. The conductivity was highest when acetone was chosen as solvent and was lowest in case of acetic acid as solvent. [Bmim]NTf_2 presented excellent chemical-stability and thermostability by TG and DTA analysis and it did not decompose until the temperature arrive at 370 ºC.

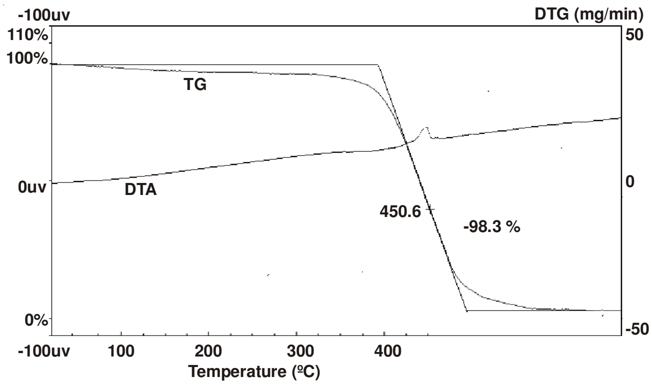

Fig. 5. DTA and TG of [Bmim]NTf_2 (Experimental conditions: Sample weight: 7.66 mg, Temperature-rising speed: 10 ºC/min, TG range:10 mg, Gas source: nitrogen gas, DTA range:100uv, Gas flux: 60 mL/min, DTG range: 50 mg/min)

ACKNOWLEDGEMENTS

The authors would like to acknowledge the support provided by the Yunnan Province Science and Technology Department for the Program of Yunnan Province's Training Young-middle-aged Reserve of Scientific and Technological Principal (Grant No. 2006PY01-50) and the fund of Yunnan Province's Applied Basic Research Plan (Grant No. 2006E00 32M). The authors also acknowledged the support from Department of Yunnan Province Education for the fund of Science Research (Grant no. ZD2010003).

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