

## CHAPTER VI

### CONCLUSIONS AND RECOMMENDATIONS

Heteroaromatic compounds, such as imidazole, benzimidazole and pyrazole, have been studied as an alternative proton conduction system to overcome the problem of losing water, which plays a role as the proton carrier in the commercially available electrolyte membrane (Nafion), due to evaporation at temperature higher than 100°C. Unfortunately, most of the researches concern only about the application of those functional groups in polymeric membrane whereas the points about the orientation of the heterocyclic resonance and its consequent hydrogen bond networks, which are the key factors to initiate proton conductivity, are still left behind. Considering about this point, the author believes that building up a well-defined structure to understand the proton transfer route based on the specific molecular arrangement is a good approach to develop the material and achieve the goal from fundamental knowledge. Thus, the dissertation focuses on the development of the model compounds that possibly induce the formation of hydrogen bond network based on their molecular packing structures.

To achieve the goal, a series of benzimidazole model compounds, i.e., mono-, di- and tri-functional benzimidazole was developed and studied. In Chapter III, the Di- and trifunctional benzimidazole compounds, **1** and **2**, were designed and successfully synthesized by the reaction between acid chloride and diamine. The Compounds showed highly thermally stable property over 400 °C. Characterizations revealed the possibly well-packed structure with intermolecular hydrogen bond network similar to the one observed in benzimidazole. For compound **2**, X-ray structure analysis illustrated the molecular complex between one molecule of **1** and six molecule of 2-propanol resulting in the solvent-assisted intramolecular hydrogen bonds network. The neat packing structure of **1** and **2** showed higher thermal stability than that of benzimidazole implying the stronger molecular interaction than single benzimidazole unit. The works clarified a possibility of di- and trifunctional benzimidazole to form hydrogen bond network as desired.

The study on the benzimidazole model compounds was further extended to the conductivity measurement in Chapter IV. The incorporation of all benzimidazole

compounds in SPEEK was found to improve thermal stability of the polymer matrix. Among the model compounds, BTBI was found to be the most effective molecule to improve thermal degradation property of SPEEK with as high as 130 °C higher than that of the pure polymer at the blending content of 15 phr. For proton conduction study, addition of the model compounds offered the water-independent proton transfer property to the SPEEK membrane. Consequently, proton conductivity of the membrane could be enhanced under increasing temperature even in dry condition. In addition, the work revealed that the stronger intermolecular interaction of the heteroaromatic compound leads to the better proton transfer property.

The last part of the work (Chapter V) demonstrated clearly the formation of hydrogen bond network channels derived by the molecular packing and hydrogen bond interaction of the difunctional benzimidazole model compounds via X-ray structural analyses. The work revealed that by increasing the number of benzimidazole unit from mono- to di-functional benzimidazole, the structure of hydrogen bond network was changed from the “isolated channel type” to the “layered interlinked channel type”. Solvent molecules were also found to significantly affect the hydrogen bond network as they initiated a unique “solvent-assisted intramolecular hydrogen bond network” in BTBI but obstruct the formation of intermolecular hydrogen bond network in BDBI.

The further research that should to be done on these model compounds are (i) analyzing the crystal structure of the pristine trifunctional benzimidazole compound, (ii) determining the conductivity of the pure benzimidazole model compounds, and (iii) extending the study on benzimidazole model compound to the polyfunctional molecule.