Proton Conducting Motion Study in Magnetic Coordination Polymers

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Electric energy is generated by the movement of electrons, a negatively charged particle in an energy system. For the compensation of the charge, positively charged particles such as a cation must move to the opposite direction of the electrons. Among the various positively charged ions, a proton, the smallest cation, is commonly involved in biological and chemical energy systems. The proton pump or proton channels are common proton transport systems in biology. However, the detailed study of proton motion and mechanism has been scarcely done in chemical proton transport systems. For the study of proton conduction mechanisms in chemical systems, structural elucidation of the system is one of the most critical issues and coordination polymers (CPs) provide a unique platform due to their designability, crystallinity, and porosity. In addition, the modulation of proton conductivity in CPs using external stimuli should be also studied such as magnetic property of CPs, which is unprecedented due to the weak magnetic interaction to the moving protons. In this study, we employed various magnetic and non-magnetic CPs, which is denoted as metal formates, $M(HCO_2)_2$, where M = Mg(II), Co(II), Ni(II), Zn(II) for the study of the proton conduction behavior and mechanism. The structure of MOFs was analyzed by single-crystal structure analysis, which was further confirmed by powder X-ray diffraction (PXRD) analysis. Interestingly, the structure of MOFs was changed upon exposure to humidity and proton conductivity and water vapor adsorption follow similar trends to the structure change. The details of the framework structure and the related proton conductivity depending on the external stimuli such as the magnetism or relative humidity were studied. For the detailed understanding of proton motion in the crystal structure, ^2H NMR was used to propose a proton conduction mechanism in the MOFs. In addition, for the detailed analysis of proton position and dynamics, neutron diffraction and quasi-elastic neutron scattering (QENS) techniques were also employed. The details of this work will be presented.