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Proton dynamics in ice VII

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Proton dynamics in the hydrogen bonds, in particular, dissociation and recombination of water molecules is a basic process of physical and chemical phenomena in many chemical systems and life systems [1]. In this talk, we study the proton conductivity of ice VII [2], which may exist in astronomical icy bodies, from the view point of the transport theory of ionic defects and rotation defects in ice, and from view point of molecular dynamics simulation of the hydrogen and oxygen atoms. The figure shows the temperature-pressure dependence of conductivity obtained by the two methods. The peak of conductivity is interpreted from the view point of (A) collaboration of conduction of ion defects and rotation defects and (B) transition from ”plastic phase”[3] to ”crystalline phase”. On the basis of these viewpoints, we discuss the measurement of electric conductivity [4] and possible effects on the proton chemistry in ice VII.

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Figure: Temperature and pressure dependence of the electrical conductivity Ice VII: the filled circles are the result of molecular dynamics, and the surface represents the fit by transport theory.

Keywords: ice, high pressure phase, proton dynamics, electric conductivity, point defect, plastic phase