

PROTON SOLVATION AND TRANSPORT
IN COMPLEX ENVIRONMENTS

by

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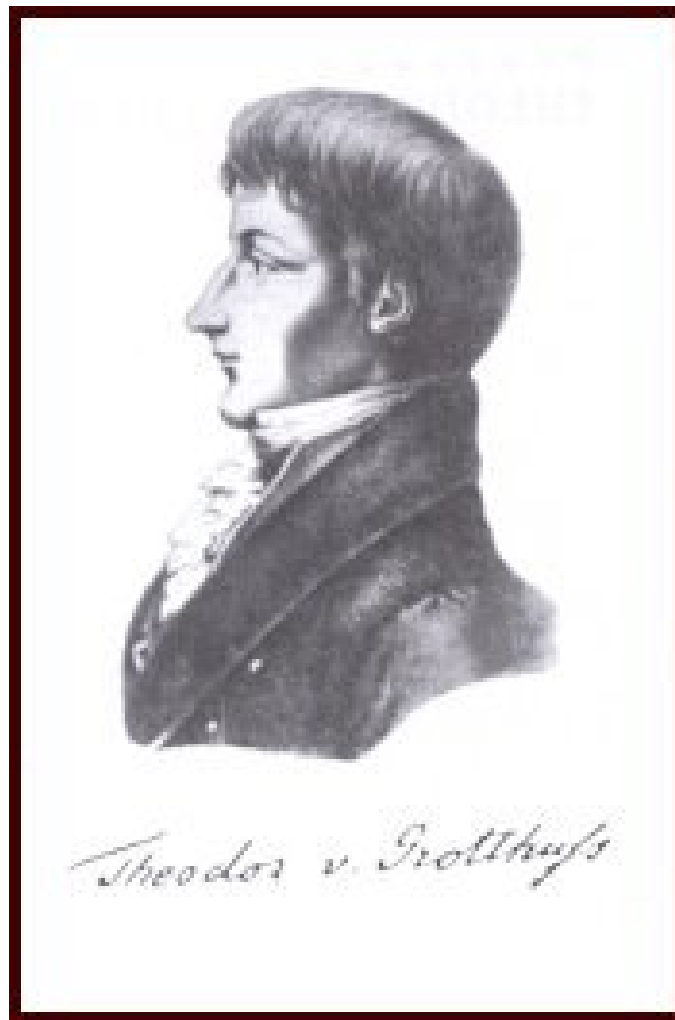
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ABSTRACT

Proton solvation and transport is a central element in innumerable fundamental chemical processes, from seemingly simple acid-base reactions to the exceedingly complicated proton transport channels integral to cellular respiration. The uniqueness of the hydrated proton, relative to other simple monovalent cations, complicates our understanding of transport and solvation in even simple neat fluids. Fortunately, computer modeling has proven valuable in describing the microscopic mechanism and structures inherent in proton transport and solvation. This dissertation will describe the use of computer modeling to characterize proton solvation in pure and mixed liquids with an emphasis on the behavior near mixed dielectrics, as well as the transport mechanism and defining solvation structures in the more complicated surroundings of a hydrated electrolytic polymer.

I dedicate this thesis to my parents
Stand and Karen Petersen,
for raising me to be curious,
and to my wife Dr. Emily Petersen,
for inspiring me beyond my congenital laziness.



Theodore Christian Johann Dietrich von Grotthuss (1785-1822)

“Atoms are round bits of wood invented by Mr. Dalton” –unknown (1887)

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