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Title:	Hydrogen bonding in protonated water clusters: An atoms-in-molecules perspective
Authors:	Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	Carrier concentration Hydrogen bonds Molecular structure Protonated water clusters Protonation Water Solvation shells Solvation
Issue Date:	2007
Publisher:	American Chemical Society
Citation:	Journal of Physical Chemistry A, 111 (51), pp. 13287-13290.
Abstract:	This article highlights the results of a detailed study of hydrogen bonding in the first and the second solvation shells of Eigen ( $\text{H}_3\text{O}^+$ ) and Zundel ( $\text{H}_5\text{O}_2^+$ ) cations solvated by water in a stepwise manner. It is evident from the results that an electron density analysis clearly distinguishes the first and the second solvation shell and helps in quantifying the strength of hydrogen bonding in these clusters.
Description:	Only IISERM authors are available in the record.
URI:	<a href="http://pubs.acs.org/doi/abs/10.1021/jp0775909">http://pubs.acs.org/doi/abs/10.1021/jp0775909</a> ( <a href="http://pubs.acs.org/doi/abs/10.1021/jp0775909">http://pubs.acs.org/doi/abs/10.1021/jp0775909</a> )
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