



**Hydrated Electron
Formation**

VUV pulse



**Scavenging
by NO_3^-**

Recombination

The Hydrated Electron

Katrin Siefermann



The Hydrated Electron:

The Hydrated Electron Edwin James Hart, Michael Anbar, 1970 **The Structure of the Hydrated Electron in Bulk and at Interfaces** Jennifer Ryan Casey, 2014

Since its discovery over fifty years ago the hydrated electron has been the subject of much interest. Hydrated electrons, which are free electrons in water, are found in fields ranging from biochemistry to radiation chemistry, so it is important that we understand the structure and dynamics of this species. Because of its high reactivity, the hydrated electron's structure has proven difficult to pin down, especially its molecular details. One electron mixed quantum/classical molecular dynamics simulations have proven useful in helping elucidate the structure of the hydrated electron. The picture most commonly presented from these studies is one of the electron residing in a cavity, disrupting the local water structure much like an anion, the size of bromide. Our group has recently proposed a completely different structure for the hydrated electron, which arose from rigorous calculations of a new electron-water potential. The picture that emerged was of an electron that does not occupy a cavity but instead draws water within itself; this non-cavity electron resides in a region of enhanced water density. The one-electron cavity and non-cavity models all predict similar experimental observables that probe the electronic structure of the hydrated electron, such as the optical absorption spectrum, which makes it difficult to determine which model most accurately describes the true structure of the hydrated electron. In this thesis, we work to calculate experimental observables for various simulated cavity and non-cavity models that are particularly sensitive to the local water structure near the electron, in an effort to distinguish the various models from each other. Two particular observables we are interested in are the resonance Raman spectrum and the temperature-dependent optical absorption spectrum of the hydrated electron. We find that for both of these experiments, only the non-cavity model has qualitative agreement with experiment; the cavity models miss the experimental temperature dependence in the optical absorption spectrum and show the wrong trends in the resonance Raman spectrum. We also explore the differences between non-cavity and cavity models by quantifying the electron-water overlap, referring to the non-cavity model as an inverse plum pudding, where the water molecules are embedded within the electron density. Finally, we examine hydrated electrons in the presence of an air-water interface. Experiments indicate that most likely electrons do not reside at the surface, and if they do, they have structural and dynamical properties reminiscent of the bulk. Our calculated Potentials of Mean Force indicate that both cavity and non-cavity electrons prefer to be solvated by the bulk, but that the cavity electron has a local free energy minimum near the surface. These calculated interfacial cavity electrons behave very differently than cavity electrons in the bulk, in direct contrast to experimental evidence. From the work presented in this thesis, it is clear that the non-cavity electron is the most appropriate one-electron model we have for the structure of the hydrated electron.

Studies on the Hydrated Electron Geraldine Anne Kenney, 1970 *The Hydrated Electron [by] Edwin J. Hart [and] Michael Anbar* Edwin James Hart, 1970 **Radiolysis of Liquid Hydrocarbons** Edwin J. Hart, Thomas J.

Hardwick, Christiane Ferradini, 1966 *The Hydrated Electron* Claudio Romero, 1987 *Studies on the Hydrated Electron [microform]* Geraldine Anne (Geraldine Anne Kenney-Wallace) Kenney, 1970 Structural Model of the Hydrated Electron Makoto Natori, 1966 **Diffusive Transport of the Hydrated Electron: A Pseudoclassical Model**, 1992 In order to elucidate the factors responsible for the enhanced diffusion rate of the hydrated electron compared to halide ions a pseudoclassical simulation technique that mimics the adiabatic dynamical response of the electron is applied to halide like ions in water for different solute solvent potential models Both the adiabatic and classical diffusive behavior are evaluated and compared to the quantum dynamics of the hydrated electron It is shown that the adiabatic response per se is essential but only partially responsible for the diffusion rate enhancement of the excess electron Specific features of the solute solvent interaction potential must also be taken into account for a realistic description of the electron mobility These include the nature of the short range repulsion associated with the spatial confinement of the excess electron and the partial penetration of the excess electronic distribution into the first hydration shell When these effects are also incorporated into the pseudoclassical model both the solvated electron dynamics and solvation structure are closely reproduced by the model system The Hydrated Electron and Its Reactions at High Temperatures Hilbert Christensen, 1986 New Perspectives on Hydrated Electrons Katrin Siefermann, 2010-12 Since the discovery of the hydrated electron in 1962 scientists have speculated over its vertical binding energy VBE In this book the author describes the sophisticated experiments which finally made this quantity accessible and additionally revealed fascinating information about electrons bound at the liquid water surface These results are crucial for understanding many electron transfer and attachment processes ranging from radiation induced DNA damage to atmospheric chemistry This book examines solvated electrons in liquid water and at liquid water interfaces explaining their binding energies lifetimes and the implications of these physical properties *Developing the Hydrated Electron Dosimeter and Investigation of the G-value of Hydrated Electrons* Giang Bui, 2021 Hydrated electron e_{aq} dosimetry uses absorption spectrophotometry to monitor the concentration of e_{aq} leading to the determination of absorbed dose This technique has been employed in radiotherapy applications in the high dose per pulse regime 10 100 Gy per pulse for the past 60 years however our recent prototype has confirmed its suitability in the low dose per pulse regime

Inorganic Chemistry in Aqueous Solution Jack Barrett, 2003 Inorganic Chemistry in Aqueous Solution is aimed at undergraduate chemistry students but will also be welcomed by geologists interested in this field *Radiochemistry and Nuclear Chemistry - Volume I* Sandor Nagy, 2009-08-25 Radiochemistry and Nuclear Chemistry theme is a component of Encyclopedia of Chemical Sciences Engineering and Technology Resources in the global Encyclopedia of Life Support Systems EOLSS which is an integrated compendium of twenty one Encyclopedias The content of the Theme on Radiochemistry and Nuclear Chemistry provides the essential aspects and a myriad of issues of great relevance to our world such as Isotope Effects Isotope Separation and Isotope Fractionation Radiometric Dating and Tracing Radiochemical

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Excess Electrons in Dielectric Media Christiane Ferradini, Jean-Paul Jay-Gerin, 1991-08-05 This book provides a comprehensive review of the present knowledge and current problems concerning physical chemical aspects of the behavior of excess electrons in various media The book's 13 chapters strike a balance between theoretical and experimental accounts and provide in depth presentations of specific subjects Among the several topics discussed in this stimulating volume are primary interactions transport and relaxation of excess electrons of a few tens of electron Volts in various solid and liquid materials energetics and transport properties of electrons after thermalization in non polar dielectric liquids quantum simulation methods and electron solvation in polar liquids and of excess electrons trapped in polar matrices at low temperature Applications of these concepts are discussed as well including hot electron transport in silicon dioxide the fate of excess electrons created in polar dielectric liquids by photoelectrochemical methods or by cathodic generation and excess electron production and decay in organic microheterogeneous systems Researchers instructors and engineers working in the radiation sciences condensed matter physics chemical physics biophysics photochemistry and the biochemistry of electron transfer and electrochemistry should consider this book to be an invaluable reference resource

Reactions of the Hydrated Electron Michael Anbar, Israel. Waada leenergya atomit, 1965

The Radiation Chemistry of Water Ivan Draganic, 2012-12-02 The Radiation Chemistry of Water tackles radiation induced changes in water and explains the behavior of irradiated water with some changes in aqueous solutions This book deals primarily with short lived species like the hydroxyl radical hydrated electron and hydrogen atom which cause the chemical changes in irradiated water and aqueous solutions These species and their origin properties and dependence of their yields on various factors are discussed in several chapters Other topics also covered are the diffusion kinetic model of water radiolysis and some general cases radiation sources and dosimetry This book is most useful to students in the fields of radiation chemistry physical chemistry radiobiology and nuclear technology

Surfactants in Solution K.L. Mittal, P. Botherel, 2013-03-09 This and its companion Volumes 4 and 6 document the proceedings of the 5th International Symposium on Surfactants in Solution held in Bordeaux France July 9 13 1984 This symposium was the continuation of the series of symposia initiated in 1976 in Albany New York under the title Micellization Solubilization and Microemulsions The next two symposia were labelled Solution Chemistry of Surfactants and Solution Behavior of Surfactants Theoretical and Applied Aspects held in Knoxville TN in 1978 and Potsdam

N Y in 1980 respectively In 1982 at the time of the 4th Symposium in this series it became amply evident that there was a definite need to have more a generic title to describe these biennial events and after much deliberation it was decided that an appropriate title would be Surfactants in Solution as both the aggregation and adsorption aspects of surfactants were addressed So the 4th Symposium was held in 1982 in Lund Sweden under this new rubric and it was decided to continue these symposia in the future under this appellation Naturally the Bordeaux Symposium was dubbed as the 5th International Symposium on Surfactants in Solution and our logo became SIS which is very apropos and appealing It was in Bordeaux that the decision was made to hold the 6th SIS Symposium in New Delhi and it is scheduled for August 18 22 1986 in the capital of India

Quantum Electrochemistry John O'M. Bockris, Shahed U. M. Khan, 2012-12-06 The origin of this book lies in a time before one of the authors J O M B left the University of Pennsylvania bound for the Flinders University His collaboration with Dennis Matthews at the University of Pennsylvania had contributed a singular experimental datum to the quantum theory of electrode processes the variation of the separation factor with potential which could only be interpreted in terms of a quantum theory of electrode kinetics The authors came together as a result of graduate work of one of them S U M K on the quantum mechanics and photo aspects of electrode processes and this book was written during a postdoctoral fellowship held by him at the Flinders University Having stated the book's origin it is worthwhile stating the rationalizations the authors had for writing it Historically quantization in electrochemistry began very early 1931 in the applications of the quantum theory to chemistry See the historical table on pages xviii xix There was thereafter a cessation of work on the quantum theory in electrochemistry until a continuum dielectric viewpoint based on Born's equation for solvation energy began to be developed in the 1950s and snowballed during the 1960s

The Solvated Electron in Radiation Chemistry
Aleksēi Konstantinovich Pikaev, 1971

Unveiling the Magic of Words: A Review of "**The Hydrated Electron**"

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