



The Hydrated Electron

Albert A Gayle



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 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 **Studies on the Hydrated Electron** Geraldine Anne Kenney, 1970 The Hydrated

Electron and Its Reactions at High Temperatures Hilbert Christensen, 1986 Studies on the Hydrated Electron [microform]
 Geraldine Anne (Geraldine Anne Kenney-Wallace) Kenney, 1970 *Reactions of the Hydrated Electron* Michael Anbar, Israel.
 Waada leenergya atomit, 1965 The Hydrated Electron Claudio Romero, 1987 *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 **Reactions of the**
Hydrated Electron with Polynucleotides Peter Chilver Shragge, 1970 **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 **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 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

Fundamentals of Radiation Chemistry A. Mozumder, 1999-08-16 This book describes the physical and chemical effects of radiation interaction with matter Beginning with the physical basis for the absorption of charged particle radiations Fundamentals of Radiation Chemistry provides a systematic account of the formation of products including the nature and properties of intermediate species Developed from first principles the coverage of fundamentals and applications will appeal to an interdisciplinary audience of radiation physicists and radiation biologists Only an undergraduate background in chemistry and physics is assumed as a prerequisite for the understanding of applications in research and industry Provides a working knowledge of radiation effects for students and non experts Stresses the role of the electron both as a radiation and as a reactant species Contains clear diagrams of track models Includes a chapter on applications Written by an expert with more than thirty years of experience in a premiere research laboratory Culled from the author's painstaking research of journals and other publications over several decades

Free-Radical-Induced DNA Damage and Its Repair Clemens Sonntag, 2006-03-20 The free radical chemistry of DNA had been discussed in some detail in 1987 in my book The Chemical Basis of Radiation Biology Obviously the more recent developments and the concomitant higher level of understanding of mechanistic details are missing Moreover in the living cell free radical DNA damage is not only induced by ionizing radiation but free radical induced DNA damage is a much more general phenomenon It was therefore felt that it is now timely to review our present knowledge of free radical induced DNA damage induced by all conceivable free radical generating sources Originally it had been thought to include also a very important aspect the repair of DNA damage by the cell's various repair enzymes Kevin Prise Cancer Campaign Gray Laboratory London was so kind to agree to write this part However an adequate description of this strongly expanding area would have exceeded the allocated space by much and this section had to be omitted The directors of the Max Planck Institut für Strahlenchemie now MPI für Bioanorganische Chemie Karl Wieghardt and Wolfgang Lubitz kindly allowed me to continue to use its facilities after my retirement in 2001 Notably our librarian Mrs Jutta Theurich and her right hand help Mrs Rosemarie Schreier were most helpful in getting hold of the literature I thank them very much Without their constant help this would have been very difficult indeed

Survey of Progress in Chemistry Arthur Scott, 2012-12-02 Survey of Progress in Chemistry Volume 5 is a collection of papers that provides the transmission of instructive material and information from the real chemical world to the classroom teacher or instructor One paper reviews the HSAB principle hard and soft acid bases and notes that it can be regarded as an experimental principle to describe various chemical phenomena in both qualitative and quantitative terms The principle can be applied in correlating and storing large amounts of data and in predicting results Another paper shows that an experiment concerning eliminations induced either by halide ions in dipolar aprotic solvents or by mercaptide ions in alcohols can be essentially normal E2 reactions The microwave spectrum can also be used in identifying compounds and in quantitative analysis Another paper discusses the physical and chemical consequences of electron hydration and its many possible uses such as in the treatment

of cancer and food preservation One paper examines the fluorescence processes which occur in a liquid scintillator including the uses of liquid scintillation in determining the solubility of gases or the production of isotopes This collection is suitable for professors in chemistry students who are taking advanced courses in chemistry and other groups of chemists who are interested to know what is happening beyond their specialized work and research **Nuclear Science Abstracts** ,1975

NSA is a comprehensive collection of international nuclear science and technology literature for the period 1948 through 1976 pre dating the prestigious INIS database which began in 1970 NSA existed as a printed product Volumes 1 33 initially created by DOE s predecessor the U S Atomic Energy Commission AEC NSA includes citations to scientific and technical reports from the AEC the U S Energy Research and Development Administration and its contractors plus other agencies and international organizations universities and industrial and research organizations References to books conference proceedings papers patents dissertations engineering drawings and journal articles from worldwide sources are also included Abstracts and full text are provided if available *Novel Imaging and Spectroscopy* Jinfeng Yang,2020-06-03 Imaging and spectroscopy are the most important and challenging techniques for not only research on materials science chemistry and biology but also medical diagnoses In this book we have collected information on several novel imaging and spectroscopic techniques including time resolved electron diffraction microscopy for materials science various spectroscopes for physics and chemistry and high resolution computed tomography for medical science We think that the content in each chapter is impressive and we hope this book will contribute to future instrument developments and new applications *Encyclopedia of Interfacial Chemistry* ,2018-03-29 Encyclopedia of Interfacial Chemistry Surface Science and Electrochemistry Seven Volume Set summarizes current fundamental knowledge of interfacial chemistry bringing readers the latest developments in the field As the chemical and physical properties and processes at solid and liquid interfaces are the scientific basis of so many technologies which enhance our lives and create new opportunities its important to highlight how these technologies enable the design and optimization of functional materials for heterogeneous and electro catalysts in food production pollution control energy conversion and storage medical applications requiring biocompatibility drug delivery and more This book provides an interdisciplinary view that lies at the intersection of these fields Presents fundamental knowledge of interfacial chemistry surface science and electrochemistry and provides cutting edge research from academics and practitioners across various fields and global regions

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