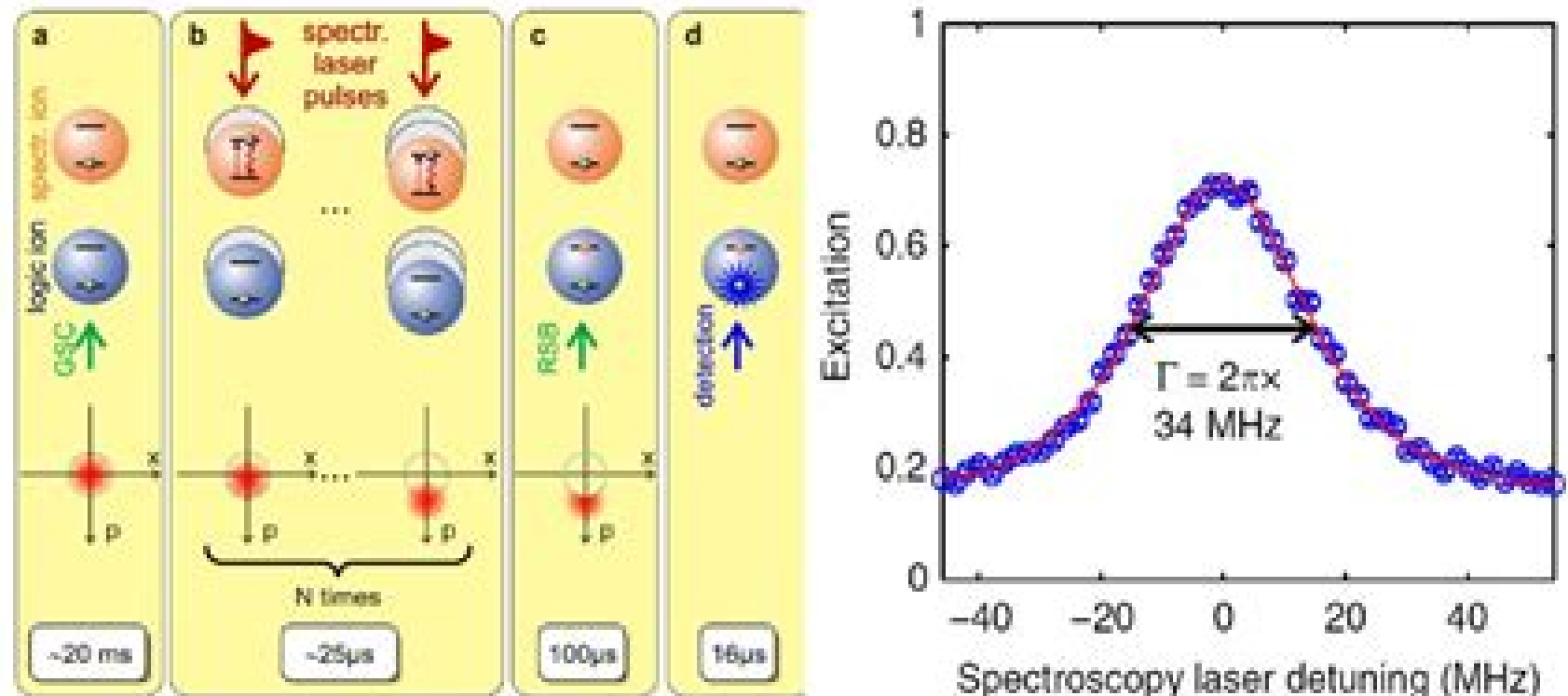


# SPECTROSCOPY OF MOLECULAR IONS

5

## NON-DESTRUCTIVE METHODS

Quantum Sympathetic Heating Spectroscopy (QSHS)  
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# Spectroscopy Of Molecular Ions

**Leonard Edward Duda**



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The Spectroscopy of Molecular Ions A. Carrington, B. A. Thrush, 1987      **Gaseous Molecular Ions** Eugen Illenberger, Jacques Momigny, 2013-03-09

Most of the matter in our solar system and probably within the whole universe exists in the form of ionized particles On the other hand in our natural environment gaseous matter generally consists of neutral atoms and molecules Only under certain conditions such as within the path of lightning or in several technical devices e g gas discharges rocket engines etc will some of the atoms and molecules be ionized It is also believed that the chemistry of the earth's troposphere predominantly proceeds via reactions between neutral particles The complex system of atmospheric chemistry will be treated in one of the forthcoming volumes to this series Why then are ions considered so important that hundreds of laboratories all over the world including some of the most prestigious are involved in research programs on ions covering many different facets from biochemistry to physics One may obtain as many different answers as there are research groups busy in this field There is however one simple common feature which makes it attractive to work with ions since they carry one or more net elementary charges they can easily be guided focused or separated by appropriate electric and magnetic fields and last but not least they can easily be detected Apart from these advantages which are welcome and appreciated by the researcher the study of molecular ions can provide insight into very fundamental aspects of the general behavior of molecules

Highly Sensitive and Efficient Infrared Spectroscopy of Molecular Ions C. Michael Lindsay, 2002

*Laser Spectroscopy of Molecular Ions in an Ion Beam* Jun Li, 1990      **High Resolution Infrared Spectroscopy of Molecular Ions Using a Difference Frequency Laser Spectrometer** Brent David Rehfsuss, 1990      **Infrared Laser Spectroscopy of Molecular Ions** Mark Leon Polak, 1990      *Infrared Spectroscopy of Molecular Ions and Ion-solvent*

*Clusters* Jong-Ho Choi, Mitchio Okumura, California Institute of Technology. Division of Chemistry and Chemical Engineering, 1995      **Emission Spectroscopy of Molecular Ions** Simon Melville Mason, 1988      **Molecular Ions** Joseph Berkowitz, Karl-Ontjes E. Groeneveld, 2012-12-06 The present volume contains contributions presented at the NATO Advanced Study Institute on Molecular Ions held on the island of Kos Greece from September 30 to October 10 1980 The meeting was attended by some 60 participants from 15 different countries It was the first meeting devoted exclusively to the topic of molecular ions Its vitality derived from bringing together experts and students from a wide variety of disciplines whose studies bear upon the structure of molecular ions The aim of the meeting was to assemble these scientists representing many countries in Europe and North America to discuss the advances and capabilities of the various experimental and theoretical approaches and to point out unsolved problems and directions for future research The format involving lecturers and students served as a tutorial Molecular ions play an important role in very diverse fields of nature such as reactions in the ionosphere the processes of formation of molecules in dense interstellar clouds and the magnetohydrodynamics of plasmas used for energy generation Our understanding of the properties of molecular ions their electronic and geometric structures has been developing from a variety of sources as far removed as tickling ions with radiofrequency radiation and smashing them apart at relativistic energies Various laser techniques are described and the queen of structural determination spectroscopy is well represented On the instrumental side older techniques have been perfected and new methods have evolved      *The Spectroscopy of Molecular Ions* A. Carrington, B. A. Thrush, 1988

**Infrared Laser Spectroscopy of Molecular Ions and Clusters** Martin H.W. Gruebele, 1988      **Ab-initio Study of X-ray Spectroscopy of Molecular Ions** Alessandra Puglisi, 2017 Molecular ions cover important roles in study and characterization of astrophysical and laboratory plasma To this purpose different spectroscopic techniques are used among which we found the X-ray photoelectron spectroscopy and the X-ray photoabsorption spectroscopy This PhD work is focused on the calculation of X-ray photoabsorption spectra of molecular ions of silicon carbon and oxygen  $XH_n$   $XSi$   $CO_n$   $n=1, 2, 3$  The former is excited on the L 2p shell while the others on the K 1s shell produced in plasma discharge We developed numerical protocols which permit to compute with reasonable precision the K and L shell photoabsorption spectra combining electronic structure and nuclear wavepacket propagation methods The optimization of the geometries and the calculation of the ionization potentials IP are carried out using the density functional theory DFT The relaxation effects due to the core hole creation are taken into account at the self-consistent field SCF level The potential energy surfaces PES and the dipole moment transitions are computed at the post Hartree Fock configuration interaction CI level The spin-orbit coupling effect are explicitly taken into account through the Breit-Pauli operator The theoretical results have been compared with the experimental data and they allow the interpretation of the experimental bands      *Scientific and Technical Aerospace Reports*, 1980      *Microwave Spectroscopy of Molecular Ions Near Dissociation* Shoe Taylor, 1997      **Spectroscopy of**

**Molecular Ions and Dications** Peter Kreynin, University of Newcastle upon Tyne. School of Natural Sciences, 2005

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