23rd International Conference on Spectral Line Shapes
19-24 June, 2016, Toruń, Poland
The 23rd International Conference on Spectral Line Shapes was organized by Institute of Physics Nicolaus Copernicus University in cooperation with Aleksander Jabłoński Foundation.

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Contact:
Institute of Physics, Nicolaus Copernicus University
Grudziądzka 5/7, Toruń, Poland
e-mail: icsls23@fizyka.umk.pl
webpage: icsls23.fizyka.umk.pl

Aleksander Jabłoński Foundation
Grudziądzka 5/7, Toruń, Poland
e-mail: kontakt@faj.org.pl
webpage: www. faj.org.pl
23rd International Conference on Spectral Line Shapes

Book of Abstracts

19 - 24 June 2016, Toruń, Poland
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Dionisio Bermejo (Spain)
Roman Ciuryło (Poland)
Elisabeth Dalimier (France)
Alexander Devdariani (Russia)
Robert Gamache (USA)
Motoshi Goto (Japan)
Magnus Gustafsson (Sweden)
Carlos Iglesias (USA)
John Kielkopf (USA)
John C. Lewis (Canada)
Valery Lisitsa (Russia)
Eugene Oks (USA)
Christian Parigger (USA)
Gillian Peach (UK)
Luka Popovic (Serbia)
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LOCAL ORGANIZING COMMITTEE

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Piotr Wcisło
Szymon Wójtewicz
Mikołaj Zaborowski

Aleksander Jabłoński Foundation

Ewa Kaszewska
Monika Czajkowska
INVITED SPEAKERS

Annette Calisti
(Aix-Marseille Université, Marseille, France)

Alain Campargue
(LIPhy, Université Grenoble Alpes, Grenoble, France)

Elisabeth Dalimier
(Pierre and Marie Curie University – Paris 6, Paris, France)

Thibault Delahaye
(Université Paris Est Créteil, Paris, France)

Aleksandra Foltynowicz
(Umea Universitet, Umea, Sweden)

Iouli E. Gordon
(Harvard-Smithsonian Center for Astrophysics, Cambridge, USA)

Robab Hashemi
(University of Lethbridge, Alberta, Canada)

Takeshi Higashiguchi
(Utsunomiya University, Utsunomiya, Japan)

Paul Julienne
(University of Maryland, College Park, Maryland, USA)

Daniel Lisak
(Nicolaus Copernicus University, Toruń, Poland)

Valery Lisitsa
(Moscow Institute of Physics and Technology, Moscow, Russia)

Andrew Ludlow
(National Institute of Standards and Technology, Boulder, CO, USA)

Javier Martín-Torres
(LuleåTekniska Universitet, Luleå, Sweden)

Luigi Moretti
(Seconda Universita Degli Studi di Napoli, Napoli, Italy)
Eugene Oks  
(Auburn University, Auburn, Alabama, United States of America)

Christian Parigger  
(University of Tennessee Space Institute, Tullahoma, USA)

Gillian Peach  
(University College London, London, United Kingdom)

Joel Rosato  
(Aix-Marseille Université, Marsille, France)

Stefan A. Schäffer  
(University of Copenhagen, Copenhagen, Denmark)

Uwe Sterr  
(Physikalisch-Technische Bundesanstalt, Braunschweig, Germany)

Satoshi Tojo  
(Chuo University, Japan)

Wim Ubachs  
(VU University, Amsterdam, Netherlands)

Ad van der Avoird  
(Radboud Universiteit, Nijmegen, Netherlands)

Tigran Vartanyan  
(ITMO University, Saint Petersburg, Russia)

Sergey Yurchenko  
(University College London, London, United Kingdom)
CONFERENCE PROGRAMME
SUNDAY JUNE 19, 2016  
Place: Collegium Maximum Nicolaus Copernicus University, Plac Rapackiego 1, Toruń

18:00 – 20:00  Welcome Reception / Registration

MONDAY JUNE 20, 2016  
Place: Culture And Congress Centre Jordanki, Aleja Solidarności 1-3, Toruń

8:00 –  
Registration

8:20 – 10:00  Monday Oral Session 1 (Mo.O.1)  
Chairperson: Roman Ciuryło

8:20 – 8:40  Józef Szudy: Reminiscences and reflections on the history of International Conferences on Spectral Line Shapes  (Mo.O.1.I1)

8:40 – 9:20  Paul S. Julienne: Line shapes in cold atom phenomena  (Mo.O.1.I2)

9:20 – 10:00  Andrew Ludlow: High-resolution optical-clock spectroscopy of ultracold, trapped ytterbium  (Mo.O.1.I3)

10:00 – 10:20  Coffee break

10:20 – 12:00  Monday Oral Session 2 (Mo.O.2)  
Chairperson: Alexander Devdariani

10:20 – 11:00  Stefan A. Schäffer: Towards passive and active laser stabilization using an ensemble of thermal strontium atoms with cavity-enhanced interaction  (Mo.O.2.I1)

11:00 – 11:40  Gillian Peach: Ultracold collisions in metastable helium  (Mo.O.2.I2)

11:40 – 12:00  Goran Pichler: Photoionization bands of Cs2 molecules  (Mo.O.2.C1)

12:00 – 14:00  Lunch

14:00 – 15:00  Monday Oral Session 3 (Mo.O.3)  
Chairperson: Gillian Peach

14:00 – 14:40  Uwe Sterr: Lineshapes in narrow-line one and two-color photoassociation spectroscopy of ultracold calcium  (Mo.O.3.I1)

14:40 – 15:00  Mateusz Borkowski: Limits on non-Newtonian gravity via state-of-the art photoassociation spectroscopy  (Mo.O.3.C1)
15:00 – 18:00  *Special event 1 – Guided tour (group 1) / Business Meeting*

20:00 – 22:00  *Special event 2 - Chivalrous Competition Show*

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**TUESDAY JUNE 21, 2016**

*Place: Culture And Congress Centre Jordanki, Aleja Solidarności 1-3, Toruń*

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**8:20 – 10:00  Tuesday Oral Session 1 (Tu.O.1)**
Chairperson: Eugene Oks

8:20 – 9:00  Takeshi Higashiguchi: *Efficient EUV and soft x-ray sources with unresolved transition array from highly charged ions in high-Z plasmas* (Tu.O.1.I1)

9:00 – 9:40  Elisabeth Dalimier: *X-ray spectroscopy of super-intense laser-produced plasmas for the study of nonlinear processes. Comparison with PIC simulations* (Tu.O.1.I2)

9:40 – 10:00  Veronica Gonzalez-Fernandez: *Optogalvanic spectroscopy applied to the study of hollow cathode discharges devices* (Tu.O.1.C1)

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**10:00 – 10:20  Coffee break**

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**10:20 – 12:00  Tuesday Oral Session 2 (Tu.O.2)**
Chairperson: Roland Stamm

10:20 – 11:00  Valery S. Lisitsa: *Excitation of atoms and ions in plasmas by ultrashort electromagnetic pulses* (Tu.O.2.I1)

11:00 – 11:40  Eugene Oks: *Advances in the semiclassical theory of Stark broadening of hydrogen lines in plasmas* (Tu.O.2.I2)

11:40 – 12:00  Motoshi Goto: *Self-reversal in Lyman-α line profile for diagnosis of fusion plasma* (Tu.O.2.C1)

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**12:00 – 14:00  Lunch**

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**14:00 – 15:20  Tuesday Oral Session 3 (Tu.O.3)**
Chairperson: Magnus Gustafsson

14:00 – 14:40  Ad van der Avoird: *Collision-induced spectra of molecular nitrogen and oxygen* (Tu.O.3.I1)

14:40 – 15:20  Tigran Vartanyan: *Spectroscopic characterization of highly excited atoms colliding with solid surfaces* (Tu.O.3.I2)
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<td>Coffee break</td>
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<td>15:40 – 17:00</td>
<td>Tuesday Oral Session 4 (Tu.O.4)</td>
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<td>16:40 – 17:00</td>
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<td>Patryk Jasik: <em>The electronic structure and photoinduced processes in the diatomic and triatomic alkali molecules</em></td>
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<td>Tuesday Poster Session (Tu.P)</td>
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<td><strong>WEDNESDAY JUNE 22, 2016</strong></td>
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<td>8:20 – 10:00</td>
<td>Wednesday Oral Session 1 (We.O.1)</td>
<td>Wim Ubachs: <em>Physics beyond the Standard Model from molecular hydrogen</em></td>
<td>(We.O.1.I1)</td>
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<td>Daniel Lisak: <em>Molecular line shapes study with cavity-enhanced absorption and dispersion spectroscopy</em></td>
<td>(We.O.1.I2)</td>
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<td>Francesco Cappelli: <em>Study of the frequency stability of a quantum cascade laser frequency comb</em></td>
<td>(We.O.1.C1)</td>
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<td>Coffee break</td>
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<td>10:20 – 12:00</td>
<td>Wednesday Oral Session 2 (We.O.2)</td>
<td>Aleksandra Foltynowicz: <em>High-resolution optical frequency comb spectroscopy</em></td>
<td>(We.O.2.I1)</td>
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<td>Alain Campargue: <em>CRDS and OF-CEAS of water vapor in the near infrared: Spectroscopic database and self-continuum absorption</em></td>
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<td>Marco Marangoni: <em>High-resolution comb-assisted Lamb dip spectroscopy</em></td>
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12:00 – 14:00  

**Lunch**

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14:00 – 15:20  
**Wednesday Oral Session 3 (We.O.3)**  
Chairperson: Robert R. Gamache

14:00 – 14:40  
Luigi Moretti: *The lineshape problem in the vibration-rotation spectrum of water molecule*  
(We.O.3.I1)

14:40 – 15:20  
Robab Hashemi: *Line-shape studies of methane and carbon monoxide*  
(We.O.3.I2)

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15:20 – 15:40  
**Coffee break**

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15:40 – 16:40  
**Wednesday Oral Session 4 (We.O.4)**  
Chairperson: Motoshi Goto

15:40 – 16:20  
Annette Calisti: *Ionization-potential depression study in dense plasmas – Application to spectroscopic diagnostics*  
(We.O.4.I1)

16:20 – 16:40  
Alexander Kouzov: *Shape theory of resonant four-wave mixing signals induced by rotational anisotropy*  
(We.O.4.C1)

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17:00 – 19:00  
**Wednesday Poster Session (We.P)**

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20:00 – 22:00  
**Banquet**  
Place: Old Town Hall, Rynek Staromiejski 1, Toruń

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**THURSDAY JUNE 23, 2016**  
Place: Culture And Congress Centre Jordanki, Aleja Solidarności 1-3, Toruń

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8:20 – 10:00  
**Thursday Oral Session 1 (Th.O.1)**  
Chairperson: Daniel Lisak

8:20 – 9:00  
Sergey Yurchenko: *ExoMol project: Molecular line lists for exoplanet and other hot atmospheres*  
(Th.O.1.I1)

9:00 – 9:40  
Iouli E. Gordon: *Line shape parameters in HITRAN2016 and beyond*  
(Th.O.1.I2)

9:40 – 10:00  
Gang Li: *FTIR based measurements of the 2-0 band of HCl broadened by CO₂ at 1.76 µm*  
(Th.O.1.C1)

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10:00 – 10:20  
**Coffee break**

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Thursday Oral Session 2 (Th.O.2)
Chairperson: Valery S. Lisitsa

10:20 – 11:00 Javier Martin-Torres: *Importance of line-mixing on planetary atmosphere studies* (Th.O.2.I1)

11:00 – 11:40 Thibault Delahaye: *High-resolution spectroscopy for space-based remote sensing missions: example of the MERLIN mission* (Th.O.2.I2)

11:40 – 12:00 Jacek Krelowski: *Diffuse interstellar bands - the oldest standing unsolved problem in all of spectroscopy* (Th.O.2.C1)

12:00 – 14:00 Lunch

FRIDAY JUNE 24, 2016
Place: Culture And Congress Centre Jordanki, Aleja Solidarności 1-3, Toruń

Friday Oral Session 1 (Fr.O.1)
Chairperson: John C. Lewis

8:20 – 9:00 Joël Rosato: *Line shape models for magnetic fusion plasmas* (Fr.O.1.I1)

9:00 – 9:40 Christian G. Parigger: *Self-absorption effects on line shapes in laser-induced plasma* (Fr.O.1.I2)

9:40 – 10:00 John T. Costello: *Stagnation layers in annular laser produced plasma* (Fr.O.1.C1)

10:00 – 10:20 Coffee break

Friday Oral Session 2 (Fr.O.2)
Chairperson: Christian G. Parigger

10:20 – 10:40 Jarosław Koperski: *Interatomic potentials of 12-group van der Waals dimers: Probing discrepancies between theory and experiment* (Fr.O.2.C1)

10:40 – 11:00 Evgeny Stambulchik: *Effects of plasma microfield rotation in Stark broadening* (Fr.O.2.C2)

11:00 – 11:20 Zoran Simić: *On the Stark broadening of Cr VI spectral lines in astrophysical plasma* (Fr.O.2.C3)

11:20 – 12:00 Closing
POSTER SESSIONS
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Monday Oral Session 1
(Mo.O.1)

Chairperson: Roman Ciuryło
Józef Szudy

Józef Szudy was born in Zalesie, Poland in 1939. He received the MSci and PhD degrees in physics from the Nicolaus Copernicus University (NCU) of Toruń in 1962 and 1968, respectively. From 1972 to 1974 he worked at the Department of Physics of the University of Windsor in Canada on pressure broadening of spectral lines. He was Associate Professor at the Institute of Physics of NCU from 1977 to 1987 and became Ordinary Professor in 1987. In 1979, 1981 and 1984 he worked as a Visiting Scientist at the Service de Physique Atomique, Centre d’Etudes Nucleaires de Saclay, France on collision-induced spectra associated with dipole-forbidden transitions in the alkali-rare-gas systems. From 1984 to 2002 he was Director of the Institute of Physics, and from 2002 to 2008 he was a Dean of the Faculty of Physics, Astronomy and Informatics of NCU. In 2004 he was elected as a Corresponding Member of the Polish Academy of Sciences. He is a member of the Optical Society and the Polish Physical Society. As Professor Emeritus he is currently involved in studies on history of physics.
Reminiscences and reflections on the history of International Conferences on Spectral Line Shapes

J Szudy

1 Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziądzka 5, 87-100 Toruń, Poland

A brief account of the history of International Conferences on Spectral Line Shapes (ICSLS) is given. Although in common use the “Europhysics Study Conference on Spectral Line Broadening and Related Topics” held in Meudon in 1973 is referred to as the first in the current sequence of ICSLS meetings, it is noted that five conferences dealing with line shape topics were organized before 1973 both in the USA and in Europe. Some details are given about their format and program. In particular, “The First International Conference on Spectral Lines” held in 1972 at the University of Tennessee at Knoxville is remembered as a meeting fully devoted to line shape problems, and as such should be regarded, in addition to the Meudon conference, as one of the roots of the line-shape community. Some of the highlights of particular ICSLS conferences as well as characteristics of their proceedings are briefly reviewed.
Paul S. Julienne

Paul S. Julienne obtained his Ph. D. in Chemical Physics in 1969 from the University of North Carolina at Chapel Hill. After postdoctoral work at the National Bureau of Standards (NBS), he worked with the Plasma Physics Division at the Naval Research Laboratory before returning to NBS (now called NIST) in 1974, where he has remained ever since. He served as a group leader for the Quantum Processes Group, as a NIST Fellow, and as a founding Fellow of the Joint Quantum Institute (JQI) of NIST and the University of Maryland. After retiring in 2013, he serves as a NIST Scientist Emeritus and an Emeritus Fellow and Adjunct Professor of Physics at the JQI. He is a Fellow of the American Physical Society (APS) and was awarded the 2004 Davisson-Germer Prize of the American Physical Society and the 2015 William F. Meggers Award of the Optical Society of America. Since the mid-1980s, his research has concentrated on the collisions and spectroscopy of cold and ultracold atoms and molecules and their applications in quantum gases and optical lattices.
Line shapes in cold atom phenomena

P S Julienne

1 Joint Quantum Institute, NIST and the University of Maryland, College Park, Maryland 20742 USA

Cold and ultracold atoms and molecules with temperatures ranging from the mK to nK scales have come to play a quite important role in atomic, molecular, and optical physics in recent years. Most of our understanding of the near-threshold bound state and scattering properties has come from analyzing a variety of "spectra" where the response of a cold atomic or molecular gas is measured as some control field is varied, such as a magnetic [1], electric, or oscillatory electromagnetic field [2]. This talk will illustrate how the "line shapes" of such spectra can be used to build an understanding of even quite complex atoms with complex spectra.

Lanthanide atoms like Er or Dy have several isotopes that can be laser cooled to low temperature and evaporatively cooled into the quantum degenerate regime of Bose-Einstein condensation or Fermi degeneracy. These complex atoms with high orbital and spin angular momentum have large magnetic dipole moments. Varying the magnetic field strength generate a dense spectrum of threshold scattering resonances at which loss of atoms occurs through three-body recombination. Furthermore, the spacing of the resonances conforms to a Wigner-Dyson distribution that is indicative of chaotic dynamics [3,4]. We show how the "line shapes" of these three-body loss spectra and the radio-frequency induced loss of atoms can be used to demonstrate the existence of broad "universal" resonances that color the dense spectrum of narrow chaotic ones [5]. These resonances are associated with the "universal" states associated with the mixed van der Waals and dipolar character of the long range potential between the two atoms. The rich few-body physics of cold complex atoms and molecules remains the object of ongoing research.

Figure 1. Spectrum of three-body atom loss versus magnetic field $B$ for the collisions of two $^{164}$Dy atoms in their $J=8$ $M=-8$ magnetic Zeeman ground state at a temperature of 2.4 $\mu$K. The ordinate represents the number of atoms remaining after a fixed hold time at each field value $B$. Several “broad” features sit on a background of narrow “chaotic” resonances. The dense spectrum of such resonances (an average of 5 per Gauss) is not experimental “noise;” each resonance position has a reproducible location in B. From Reference [5].

References:

High-resolution optical-clock spectroscopy of ultracold, trapped ytterbium

A Ludlow\(^1\)

\(^1\) National Institute of Standards and Technology, Boulder, Colorado, USA

Two-valence-electron systems have a simple electronic structure which is well-suited to a variety of ultracold atomic studies and quantum manipulation. Perhaps their most ubiquitous application has been in the development of optical atomic clocks, exploiting spin-forbidden transitions from the ground state to very-long-lived metastable states. Here I will describe high resolution spectroscopy of the intercombination ‘clock’ transition in ultracold ytterbium. Ytterbium is confined in an optical lattice operating at the so-called magic wavelength, where spectroscopic light shifts due to the optical confinement are highly-cancelled. The lattice confinement enables spectroscopy also free from Doppler and atomic recoil effects. Consequently, ultranarrow spectra with linewidths below 1 Hz have been observed, pushing the limits of experimentally-observed line quality factors. This high resolution affords direct observation of spectral line broadening and asymmetries caused by relatively weak atomic interactions within the optical lattice. These interactions occur between ground and excited state atoms occupying the same optical lattice site. Laser-driven motional excitation within the optical lattice also gives rise to motional ‘sideband’ spectra. For the typically employed case of a one-dimensional optical lattice, these sideband spectra have rich structure which, similar to other trapped atom systems, can be used to deduce atomic temperature at the microKelvin level. Finally, I will discuss limits to this high resolution spectroscopy using the Stark-cancellation techniques of a magic-wavelength optical lattice.
MONDAY ORAL SESSION 2  
(Mo.O.2) 
Chairperson: Alexander Devdariani
Stefan A. Schäffer

Stefan Alaric Schäffer is a Ph.D. Fellow from the Niels Bohr Institute at the University of Copenhagen, where he is currently working on cavity-enhanced spectroscopic systems. With a broad interest in laser spectroscopy and quantum optics Stefan's publications reflect his work on molecular clock systems as well as cavity QED systems with ensembles of cold atoms. His thesis work centers on the realization of a continuous superradiant laser of interest in the pursuit of ultrastable atomic clocks. Stefan was previously affiliated with the Université Pierre et Marie Curie in Paris, and has received separate research grants in order to pursue experiments devised in collaboration with JILA at the University of Colorado, Boulder.
Towards Passive and Active Laser Stabilization Using an Ensemble of Thermal Strontium Atoms with Cavity-Enhanced Interaction

S A Schäffer¹, B T R Christensen¹, S M Rathmann¹, M H Appel¹, M R Henriksen¹, J Ye², J W Thomsen¹

¹ The Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, DK-2100, Denmark
² JILA, NIST and University of Colorado, Boulder, Colorado 80309-0440, USA

Quantum metrology and ultra stable optical atomic clocks rely on the frequency stability of reference lasers [1-3]. These lasers have linewidths down to tens of mHz [4], relying heavily on stabilization to ultra stable reference cavities [5] whose fractional frequency stability is currently limited by the Brownian motion in the mirror substrates [6]. The possibility of using cavity-enhanced spectroscopy on narrow transition lines has been studied in [7]. It has also been proposed to use the direct emission of radiation from atoms with such narrow lines instead [8]. It could be possible to use radiation emitted on such narrow lines directly as a reference laser, which, however, requires extremely large samples in order to generate considerate intensity during the long transition relaxation time. This requirement is relaxed significantly if one considers the case of superradiant or superfluorescent emission of light. In this case the photon emission flux can be considerably increased by collective atomic decay, while simultaneously achieving a narrowing of the emitted light compared to the transition linewidth [9,10]. Some advances have already been made in connection with proof-of-principle quasi-continuous superfluorescent systems [9] using atoms loaded into an optical lattice at very low temperatures.

We report the observation of superfluorescent-like behaviour of an ensemble of strontium atoms freely moving at temperatures of about 4 mK. The atoms have a strong collective coupling to a single cavity mode, significantly enhancing their cooperativity, and allowing them to emit a burst of photons into the cavity mode, see Figure 1. In this approach the atoms act as the active part of the laser allowing enhanced emission intensity on a narrow atomic transition. The NICE-OHMS technique for heterodyne detection where the atom-cavity system acts as a passive frequency reference is also presented for the bad cavity regime, with recent results concerning the phase-response and transmission shape at large atom numbers.

Figure 1. a) "Active" system setup. b) Pi-pulse followed by a superfluorescent-like burst in the cavity transmission.

Superfluorescence in the bad cavity regime is an interesting alternative approach towards an ultra narrow continuous laser source. The narrowing of the linewidth in the superfluorescent light means that such a device could significantly increase the stability and accuracy of reference lasers for use in optical atomic clocks (ESA Contract No. 4000108303/13/NL/PA-NPI727-2012).

References:

Gillian Peach

Having completed a Ph.D. degree at Royal Holloway College, University of London, I moved to UCL in October 1960. I joined the theoretical atomic physics group headed by Michael Seaton and worked on photoionization and free-free absorption processes relevant to astrophysics. The year 1965-66 was spent at the University of Maryland where I worked in the group of Hans Griem who introduced me to the theory of spectral line broadening in plasmas. Subsequently I have studied atom-atom collisions for a wide range of temperatures and the connected problems of line broadening by neutral atoms.
Ultracold collisions in metastable helium

G Peach1, D G Cocks2 and I B Whittingham2

1 Department of Physics and Astronomy, University College London, London WC1E 6BT, UK
2 College of Science, Technology and Engineering, James Cook University, Townsville 4811, Australia

Ultracold collisions of metastable helium atoms are widely used to study collision dynamics in dilute quantum gases as the large internal energy can be released during collisions, allowing novel experimental strategies based upon single atom detection to be implemented. The metastable system is usually prepared in its fully stretched spin polarized state from which Penning ionization is strongly suppressed.

One important technique is photoassociation in which two interacting ultracold atoms are resonantly excited by a laser to bound states of the molecule formed during collision. Photoassociation of the ultracold bosonic homonuclear metastable $^4\text{He}^* + ^4\text{He}^*$ system to excited rovibrational bound states that dissociate to the $^4\text{He}(1s\ 2s\ ^3\text{S}) + ^4\text{He}(1s\ 2p\ ^3\text{P}_j)$ limits, where $j = 0, 1, 2$, have been observed by many groups. Our detailed theoretical analysis of this system [1], based upon single channel and multichannel calculations, allowed the role of non-adiabatic and Coriolis couplings to be investigated and permitted criteria to be established for the assignment of the theoretical levels to the experimental observations using the short-range spin character of each level and their couplings to the metastable ground states. Excellent agreement was obtained for the nearly 50 observed levels. Subsequently we have investigated photoassociation in the fermionic metastable homonuclear $^3\text{He}^* + ^3\text{He}^*$ system [2] where the presence of hyperfine structure leads to a very different pattern of energy levels below the $^3\text{He}(1s\ 2s\ ^3\text{S}) + ^3\text{He}(1s\ 2p\ ^3\text{P})$ asymptotes. As no experimental observations are available for this system, we have assessed the observability of the theoretical levels using the above criteria and have identified purely long-range levels and 30 short-range levels suitable for experimental investigation. Very recently we have extended our investigations to photoassociation in the heteronuclear $^3\text{He}^* + ^4\text{He}^*$ system [3]. No purely bound long-range states were found, although several resonances with line widths smaller than 1 MHz were obtained.

Currently we are investigating elastic and ionizing collisions in spin-polarized metastable $^4\text{He}^* + ^4\text{He}^*$, $^3\text{He}^* + ^3\text{He}^*$ and $^3\text{He}^* + ^4\text{He}^*$ systems in the absence of an exciting laser where the spin dipole interaction can induce relaxation from the initial spin polarized state to states from which Penning ionization is highly probable.

References:

There are many spectral phenomena connected with the ionization of the cesium dimers. Since the coexistence of cesium atoms and molecules is precluding easy separation of the two we decided to study absorption spectrum of dense cesium vapor in an all-sapphire cell employing superheating of the vapor, with a special emphasis on the highly structured photoionization continuum. This continuum appears to be composed of atomic and molecular contributions which can be separated by means of additional superheating of cesium vapor in the sapphire cell. This was possible due to the small amount of cesium filling which completely evaporated at temperature of about 450 °C. This enabled the overheating of cesium dimers which greatly reduced its concentration at a temperature of 900 °C leaving almost pure atomic Cs vapor. The analysis of the thermal destruction indicated that the highly structured molecular component of the photoionization continuum can be attributed to cesium dimers. We discuss the possible origin of the structured photoionization continuum as stemming from the absorption process from the ground state of the Cs$_2$ molecule to the doubly excited Cs$_2$$^{**}$ molecule above Cs$_2^+$ limit. The corresponding potential curves are presently unknown, and their calculations will illuminate this interesting phenomenon. At the moment we assume that the relevant potential curves are subjected simultaneously to mutual interactions and autoionization [1]. Thermal emission from the superheated cesium vapor was additionally studied to very high temperatures from 700 °C to 1000 °C. We observed a number of atomic and molecular spectral features simultaneously in emission and absorption, especially peculiar thermal emission of cesium dimer diffuse bands ($2 \ ^3 \Pi_g \leftarrow a \ ^3 \Sigma_u^+$ transitions) around 710 nm coexisting with absorption bands around first resonance lines at 852 nm and 894 nm. The main result is the comparison between the absorption and emission profiles of the above mentioned diffuse bands [2]. A possible application of the observed phenomena will be discussed in terms of the solar energy conversion using dense cesium vapor. Another possibility is to make laser action at the excimer transition of diffuse bands if the superheated vapor is located within an appropriate laser cavity.

References:

MONDAY ORAL SESSION 3
(Mo.O.3)
Chairperson: Gillian Peach
Uwe Sterr

Dr. Uwe Sterr has more than 20 years of professional experience with research in ultracold atoms, precision spectroscopy and the development of ultrastable lasers for applications in fundamental and applied research. He graduated with a PhD in experimental physics from Bonn University, Germany, in 1993 on high-resolution optical Ramsey spectroscopy with laser-cooled magnesium atoms.

In 1994 and 1995 he was a Visiting Scientist with the US National Institute of Standards and Technology, Gaithersburg, MD, in the group of W. D. Phillips, where he was investigating laser-cooled metastable atomic xenon, and in 1995 at the group of R. L. Byer at Stanford University to develop optical parametric oscillators with periodically poled materials.

Then he joined industry for the development of diode-pumped solid-state lasers in collaboration with the Laser-Zentrum Hannover. Since 1997 he is with the German National Metrology Institute, the Physikalisch-Technische Bundesanstalt (PTB) in Braunschweig, now leading the group “Unit of Length”.

In his group the first Bose-Einstein condensate of earth-alkaline atoms was produced in 2009. He is currently engaged in the development of millihertz-linewidth lasers, novel optical cavities with reduced thermal noise, and in the investigation of the properties of ultacold calcium atoms for application in metrology.
Photoassociation of alkaline earth atoms on their narrow intercombination transitions gives valuable information on molecular interaction potentials with unprecedented accuracy and allows a variety of precision experiments. These transitions are also expected to enable manipulation of atomic scattering properties by optical Feshbach resonances with low atomic losses. From alkaline earth atoms investigated so far, calcium offers the narrowest $^{1}S_{0}-^{3}P_{1}$ intercombination line with a natural linewidth of 375 Hz at a wavelength of 657 nm.

In our experiment we trap ensembles of about $10^{5}$ calcium atoms in a crossed dipole trap at temperatures of approximately 1 µK. By one-color photoassociation spectroscopy we previously measured [1] molecular states corrected for quadratic magnetic shifts [2] in the $a^3\Sigma_{u}^{+}, c^3\Pi_{g}$ exited state potential. In recent experiments using two-color photoassociation spectroscopy in both Raman and Autler-Townes configuration, we investigated the three most weakly bound vibrational levels in the $X^1\Sigma_{g}^{+}$ potential of $^{40}$Ca$_2$.

To extract the unperturbed line center with uncertainties of only a few kHz, a detailed analysis of the lineshape is performed. There we have to include the homogenous lineshape of the free-bound transitions [3] and the broadening by the Doppler effect and the thermal collision energy.

From the measured binding energies, improved long range potentials were obtained. In both the excited and ground state, the interaction potential at typical internuclear separations for these weakly bound levels is dominated by the long range coefficients $C_6, C_8$ which have been derived using a quantum calculation including information of the inner potential [4]. Our data also give a precise value for the s-wave ground-state scattering length $a = 308(10)a_0$, being an important step in the implementation of low loss optical Feshbach resonances for alkaline earth metals.

This work is funded by the DFG through the Research Training Group 1729.

References:

Limits on non-Newtonian gravity via state-of-the-art photoassociation spectroscopy

M Borkowski¹, A A Buchachenko²,³, R Ciuryło¹, P S Julienne⁴, H Yamada⁵, K Yuu⁵, K Takahashi⁵, Y Takasu⁵, Y Takahashi⁵,⁶

¹ Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziadzka 5, 87-100 Torun, Poland
² Skolkovo Institute of Science and Technology, 100 Novaya Street, Skolkovo, Moscow Region, 143025, Russia
³ Institute of Problems of Chemical Physics RAS, Chernogolovka, Moscow District 142432, Russia
⁴ Joint Quantum Institute, National Institute of Standards and Technology and the University of Maryland, 100 Bureau Drive, Stop 8423, Gaithersburg, Maryland 20899-8423, USA
⁵ Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan
⁶ CREST, Japan Science and Technology Agency, Chiyoda-ku, Tokyo 102-0075, Japan

We demonstrate a unique approach to test the fundamental law of gravity at the nanometer scale. We utilize a photoassociative measurement of the binding energies of ytterbium dimers of yet unprecedented accuracy of ~500 Hz. Thanks to the variety of isotopes available we are able to investigate the mass-dependent effects in the atomic interactions in the ytterbium dimer. We use four different atomic interaction models to provide constraints on the size of Yukawa-type corrections to the gravitational force. The constraints obtained in this initial experiment are only three orders of magnitude larger than those using other techniques and with further advances in the theoretical interaction models, photoassociation spectroscopy could become one of the leading tools in the investigations of gravitational forces in the nanometer range.
TUESDAY ORAL SESSION 1
(Tu.O.1)

Chairperson: Eugene Oks
Takeshi Higashiguchi

Takeshi Higashiguchi is an associate professor in Utsunomiya University. His research activities have focused on short-wavelength light sources, hybrid short pulse laser system in mid-IR, high average solid-state lasers, x-ray microscope, and advanced optics for vector wave generation.
Efficient EUV and soft x-ray sources with unresolved transition array from highly charged ions in high-Z plasmas

T Higashiguchi

Utsunomiya University

Light sources based on spectral emission from unresolved transition arrays (UTAs), which originate from the highly charged ions (HCIs) in high-Z plasmas are of great interest in fundamental research and for industrial applications, such as extreme ultraviolet (EUV) lithography for future integrated circuits [1], laser-driven water window soft x-ray (SXR) sources for single shot imaging of biological cells in vivo [2], and material sciences [3]. UTA emission can provide high output power with high conversion efficiency of laser input energy to EUV or soft x-ray emission because the transitions responsible, which are of the type \(4p^64d^n - (4p^64d^{n-1}f + 4p^54d^{n+1})\) \(n = 4 - n = 4, \Delta n = 0\) originate from several charge states and appear at almost the same wavelength [4] so that resonance lines from a number of charge states contribute. In fact, such UTA emission at a wavelength of 13.5 nm from LPP EUV sources with high average power and a conversion efficiency greater than 4% based on highly charged tin (Sn) plasmas are currently used for EUV lithography [5].

UTA emission from \(n = 4 - n = 4 (\Delta n = 0)\) transitions in LPPs of other higher-Z elements occurs at wavelengths that can be used for other applications such as soft x-ray microscopy (SXM) in the water window SXR region from 2.3 to 4.4 nm and the carbon window which lies between 4.4 and 5 nm. We have shown that the strong resonance UTAs emitted by Nd:YAG laser-produced plasmas of high-Z elements ranging from \(\text{Sn}\) to \(\text{Bi}\) obey a quasi-Moseley’s law (see Fig. 1) [6]. Laser-produced bismuth (Bi) plasmas are one of the candidates for a water window SXR source [7,8], and consequently their spectrum has been recently analyzed.

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**References:**

Elisabeth Dalimier

As a Full Professor at the University Pierre and Marie Curie (UPMC), I have been teaching atomic-molecular-plasma physics at the level Licence (direction of the UPMC Licence program) and then statistical physics, atomic physics in plasmas, inertial fusion science at the level Master (direction of the Fusion Science Master at UPMC).

As a Senior Researcher I belong to LULI-UPMC (Laboratoire pour l’Utilisation des Lasers Intenses- Ecole Polytechnique and UPMC), I am involved in the theory and simulations for hot dense plasmas, more precisely in atomic physics and spectroscopy. I have been also involved as the head of the team Atomic Physics in Dense Plasmas in collaborative experiments at the LULI laser facility at the Ecole Polytechnique.

I give in the following my topics of interest for the last ten years: Stark effects in dense plasmas, quasi-molecules and charge exchange, colliding plasmas, Stark profiles in the presence of strong oscillating field, Langmuir dips. For the last three years I have been working mostly on the X-ray spectroscopy of super intense laser-produced plasmas for the study of nonlinear processes.

X-ray spectroscopy of super-intense laser-produced plasmas for the study of nonlinear processes. Comparison with PIC simulations

E Dalimier¹, A Faenov²,³, E Oks⁴ et al

¹ LULI - UPMC Univ Paris 06 ; Sorbonne Universités ; CNRS, Ecole Polytechnique, CEA : Université Paris-Saclay - F-75252 Paris cedex 05, France
² Institute for Academic Initiatives, Osaka University, Suita, Osaka, 565-0871, Japan
³ Joint Institute for High Temperatures, Russian Academy of Sciences, Moscow 125412, Russia
⁴ Physics Department, 206 Allison Lab, Auburn University, AL 36849, USA

We present X-ray spectroscopic diagnostics in femtosecond laser-driven experiments revealing nonlinear phenomena, such as parametric decay instabilities PDI, caused by the strong coupling of the laser radiation with the created plasma.

Among those nonlinear phenomena, we found the signatures of the Two Plasmon Decay (TPD) instability in a laser-driven CO\textsubscript{2} cluster-based plasma by analyzing the Langmuir dips in the profile of the O VIII Ly\textsubscript{e} line, caused by the Langmuir waves created at the high laser intensity $3 \times 10^{18}$ W cm\textsuperscript{-2}\textsuperscript{[1]}. The experiments were performed at J-Karen Laser facility (Kansai Photon Science Institute, Japan).

At the same facility J-Karen we revealed the nonlinear phenomenon of the Second Harmonic Generation (SHG) of the laser frequency by analyzing the nonlinear phenomenon of satellites of Lyman delta and epsilon lines of Ar XVII \textsuperscript{[2]}. The efficiency of converting the incident laser shot into the second harmonic was 2% which was in agreement with the 2-Dimensional Particle-In-Cell (2D PIC) simulations.

In the case of relativistic laser-plasma interaction developed at the super intense Vulcan Petawatt laser facility (Rutherford Appleton Laboratory, UK), we discovered the PDI-induced ion acoustic turbulence produced simultaneously with Langmuir waves via irradiation of thin Si foils by laser intensities of $10^{21}$ W cm\textsuperscript{-2}. In agreement with PIC simulations, the ability of this ultra-intense laser radiation to penetrate the regions of the density higher than the critical density was confirmed and both the amplitude of the Langmuir waves and the root-mean-square field of the ion acoustic waves were determined from the shapes of Si XIV Lyman lines.

All these studies involved improvements of the spectral line shape theory necessary for the conditions of the femtosecond laser-driven plasmas; the simultaneous contributions of the high-frequency plasma turbulence (Langmuir waves) and of the Low-frequency Electrostatic Plasma Turbulence LET (ion acoustic wave) were taken into account in addition to the traditional broadenings due to ions and electrons. As concerning the SHG, it was necessary to produce the theory of satellites under the action of a bi-chromatic laser field.

In conclusion we showed that X-ray spectroscopy can be used for the laboratory modeling of nonlinear physical processes in astrophysical objects and a better understanding of intense laser-plasma interactions.

References:

Optogalvanic spectroscopy applied to the study of hollow cathode discharges devices

V González-Fernández¹, K Grützmacher¹, L M Fuentes², C Pérez¹, M I de la Rosa¹

¹Dpto. de Física Teórica, Atómica y Óptica, Universidad de Valladolid, Paseo Belén 7, 47011, Valladolid, Spain
²Dpto. de Física Aplicada, Universidad de Valladolid, Paseo Belén 7, 47011, Valladolid, Spain

In the Plasma Laser Spectroscopy Laboratory (University of Valladolid) electric field strength measurements are done by optogalvanic spectroscopy applied to the 1S-2S Hydrogen transition, in a low-pressure pure Hydrogen plasma, generated in a hollow-cathode discharge (HCD), in glow-discharge regime [1, 2]. The electric field present in the discharge causes the Stark splitting and shifting of the 2S level of Hydrogen, that allows determining the electric field strength value [3].

This HCD device has two anodes and one cathode, placed in between both of them. All the pieces have cylindrical symmetry, with an axial perforation. In order to analyse the electric field dependence with different configurations of the HCD, cathode diameter and cathode material have been varied. All this study has been done also in a wide range of pressures (from 270 Pa to 1350 Pa), and covering different currents (from 25 mA to 300 mA).

Pulsed UV laser radiation centred in 243 nm is generated by a 10 Hz injection-seeded Q-switched Nd:YAG laser (Continuum, Powerlite), and a second laser based in non-linear crystals, that provides a single longitudinal mode radiation, with 3 ns of temporal duration, and 300 MHz bandwidth. For the measurements, the UV radiation is divided in two beams with the same optical path, focusing and overlapping in the cathode fall region (2mm), in a 150 µm focus. The focus quality is controlled at real time by a spectral profile analyser (LaserCam-HR-UV) that gives size and energy distribution information in every measurement [4]. The detection of the 1S-2S Stark components is done in two steps: first, the absorption of two photons circularly polarized; and second, while tuning the laser frequency, the change of the voltage drop between the cathode and one anode is measured, and recorded shot by shot for each scan. At this moment, the optogalvanic measurements are being done with two different cathodes and two different diameters: stainless steel (10 and 15 mm) and tungsten (10 and 15 mm), covering the cathode fall region. The first analysis shows that the electric field strength is much stronger in the hollow cathode made of tungsten than in the stainless steel one.

Acknowledgments
The authors thank DGICYT (Ministerio de Economía y Competitividad) for the project ENE2012-35902, FEDER funds, and the grant BES-2013-063248 given to V. González-Fernández.

References:

TUESDAY ORAL SESSION 2
(Tu.O.2)
Chairperson: Roland Stamm
Valery Lisitsa

The member of International commitee of ICSLS from Russia. Education: Moscow Engeneering Physical Institute (Nuclear State University) - 1968 Ph.D. in theoretical physics from Moscow State University - 1974 DrSc in plasma physics from Kurchatov Institute (National Research Center) - 1979 At present time - the head of Radiation theory laboratory in NRC "Kurchatov Institute", Moscow, Russia Professor of Moscow Institute of Physics and Technology Field of interests: radiative-collisional processes in plasmas and gases, including spectral line broadening, plasma spectroscopy, nonlinear laser spectroscopy, elementary collisional processes
Excitation of atoms and ions in plasmas by ultrashort electromagnetic pulses

V A Astapenko¹, S V Sakhno¹, S Yu Svita¹ and V S Lisitsa¹,²,³

¹ Moscow Institute of Physics and Technology, Dolgoprudnyi, Russia
² Russian Research Center ‘Kurchatov Institute’, Moscow, Russia
³ National Research Nuclear University MEPhI, Moscow, Russia

The problem of atoms and ions diagnostics in rarefied and dense plasmas is under consideration. The application of ultrashort laser pulses is proposed for excitations of ions from ground atomic states. The excitation increases sharply populations of excited atomic states in contrast with standard laser induced spectroscopy based on radiative transitions between excited atomic states. Two cases of highly charged ions excitations by ultrashort pulses are analyzed in details: low density plasmas with domination of Doppler broadening and high density plasmas with domination of Stark (Holtsmark) broadening.

Theoretical study of excitation of highly charged ions in plasma under the action of USP of femto- and attosecond durations is performed. Transitions from the ground state to np-states are considered in view of their fine splitting, characteristic Doppler broadening of lines in plasma, and Gaussian pulses typical for low density plasmas. The same transitions are calculated for high density plasmas with Stark broadening.

The dependence of the excitation probability on the duration and the carrier frequency of a pulse (the main parameters characterizing possibilities to use USP in plasma diagnostics) is of special interest.

The general formula based on perturbation theory makes it possible to find the dependences of transitions probabilities on laser pulses duration and plasma broadening parameters.

On the basis of the general formulas the excitation probability from ground state of hydrogen-like ions broadened by Holtsmark plasma micro-field is calculated. Two cases of ultra-short pulses laser-plasma interaction are considered, namely cold rarefied plasma and hot and dense plasma.

It is shown that the excitation probability is determined by two dimensionless parameters: detuning of carrier frequency from resonance, β, and broadening parameter α = Δτ, where Δ is typical broadening width, and τ is pulse duration.

In the case of hot rarefied plasmas the transition probabilities are calculated taking into account thin structures of excited atomic energy levels.

The detail investigation of transition probabilities dependence on carrier frequency detuning from resonance and pulse durations is presented.

**Figure 1.** The dependence of the normalized probability of excitation of a hydrogen-like ion at the transition 1s → 2p on the pulse duration for different nucleus charges: solid curve - Z = 10, dotted curve - Z = 15, dashed curve - Z = 20, dash-and-dot curve - Z = 25; the carrier frequency of a pulse is \( \omega_c = (\omega_{j=1/2} + \omega_{j=3/2})/2 = \bar{\omega} \).
Eugene Oks

Eugene Oks received his Ph.D. degree from the Moscow Institute of Science and Technology, and later the highest degree of Doctor of Sciences from the Institute of General Physics of the Academy of Sciences of the USSR by the decision of the Scientific Council led by the Nobel Prize winner, academician A.M. Prokhorov. Oks worked in Moscow (USSR) as the head of a research unit at the Center for Studying Surfaces and Vacuum, then – at the Ruhr University in Bochum (Germany) as an invited professor, and for the last 26 years – at the Physics Department of the Auburn University (USA) in the position of Professor. He conducted research in 5 areas: atomic and molecular physics, plasma physics, laser physics, nonlinear dynamics, and astrophysics. He founded/co-founded and developed new research fields, such as intra-Stark spectroscopy (new class of nonlinear optical phenomena in plasmas), masing without inversion (advanced schemes for generating/amplifying coherent microwave radiation), and quantum chaos (nonlinear dynamics in the microscopic world). He also developed a large number of advanced spectroscopic methods for diagnosing various laboratory and astrophysical plasmas – the methods that were then used and are used by many experimental groups around the world. He published over 300 papers and 4 books, the latest one published in 2015 being titled “Breaking Paradigms in Atomic and Molecular Physics”.

He is the Chief Editor of the journal “International Review of Atomic and Molecular Physics”. He is a member of the Editorial Boards of the two other journals: International Journal of Spectroscopy and Open Journal of Microphysics. He is also a member of the International Program Committees of the two conferences: Spectral Line Shapes, as well as Zvenigorod Conference on Plasma Physics and Controlled Fusion.
Advances in the semiclassical theory of stark broadening of hydrogen lines in plasmas

E Oks

1 Physics Department, 206 Allison Lab, Auburn University, Auburn, AL 36849, USA

Hydrogen spectral lines continue to be used as an important practical tool for diagnosing various laboratory and astrophysical plasmas. As experiments move to very high electron densities of plasmas or to strongly magnetized plasmas, new physical phenomena have to be taken into account while calculating Stark broadening of hydrogen spectral lines, as presented in this talk.
Self-reversal in Lyman-α line profile for diagnosis of fusion plasma

M Goto¹, K Sawada², T Oishi¹ and S Morita¹

¹ National Institute for Fusion Science, Toki 509-5292, Japan
² Shinshu University, Nagano 380-8553, Japan

We have observed the Lyman-α line profile for a discharge in the LHD (Large Helical Device), a heliotron-type fusion experimental machine of the magnetic confinement. Figure 1 shows the result with crosses. A salient feature of the spectrum is the dent at the center of the line profile, which is thought to be due to a strong reabsorption effect by low temperature atoms.

![Figure 1. Lyman-α line profile observed (crosses) and synthetic (solid line).](image)

For a quantitative understanding of the line profile we have solved a one-dimensional radiation transport equation which is expressed as

\[
\frac{d}{dx}I(\lambda, x) = \eta(\lambda, x) - \kappa(\lambda, x)I(\lambda, x),
\]

where the coordinate \( x \) is taken along the line-of-sight, \( \eta(\lambda, x) \) is the emission coefficient, and \( \kappa(\lambda, x) \) is the absorption coefficient. The parameters \( \kappa(\lambda, x) \) and \( \eta(\lambda, x) \) depends on the ground state density and \( n = 2 \) level density, respectively, and they are derived from a technique based on the Laplace inversion of the Balmer-α line profile [1] recently developed by our group. The complete synthetic line profile is shown in Fig. 1 with the solid line. The absolute intensity of the measured data is scaled so as to fit the synthetic profile in the wavelength ranges \( |\lambda - \lambda_0| > 0.04 \) nm where an optically thin condition is expected.

The agreement in the tail component of both profiles is satisfactory, which supports our understanding regarding the penetration profile of atoms in the core region. There exists, however, a severe discrepancy in the central part of the line profile, which indicates the accuracy of the parameters derived from the analysis of the Balmer-α line profile is insufficient in the edge region. This result is to a certain extent expected because the condition of equivalent temperature between atoms and protons assumed in the Balmer-α line analysis could be inappropriate in the low temperature or in the plasma boundary region where the molecular processes play an important role instead of the charge exchange processes for the production of atoms.

We have further performed a three-dimensional Monte-Carlo simulation of neutral atom transport and have obtained clues to understand the cause of the disagreement between the measured and synthetic line profiles. Thus, it is shown that the Lyman-α line can be used complementarily to the Balmer-α line analysis in determining the complete neutral density profile.

References:

Tuesday Oral Session 3
(Tu.O.3)

Chairperson: Magnus Gustafsson
Ad van der Avoird

Ad van der Avoird obtained his Ir. and Ph.D. degrees from the Technical University Eindhoven, in 1964 and 1968. He worked at the Battelle Institute in Geneva (1964–1967) and the Unilever Research Laboratory in Vlaardingen (1967–1971). In 1971 he became full professor of Theoretical Chemistry in Nijmegen, and in 2008 emeritus. He held visiting professorships at Yeshiva University, New York (1970), the University of California in Berkeley (1992), and the University of Bielefeld (1996). In 1979 he was elected member of the Netherlands Royal Academy of Arts and Sciences and in 1997 of the International Academy of Quantum Molecular Sciences. In 2007 he received an Alexander von Humboldt Senior Research Award and he regularly worked for shorter periods as a visiting scientist at the Fritz Haber Institute of the Max Planck Society in Berlin and at the Technical University Munich.
Collision-induced spectra of molecular nitrogen and oxygen

T Karman\(^1\), G C Groenenboom\(^1\) and A van der Avoird\(^1\)

\(^1\)Theoretical Chemistry, Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

The collision-induced spectra that we studied for molecular nitrogen and oxygen are quite different in nature. For N\(_2\) we looked at collision-induced absorption (CIA) in the rotation-translation far-infrared region, produced by the dipole moments induced in N\(_2\) during collisions with other N\(_2\) molecules. For O\(_2\) we studied electronic transitions from the ground \(X^3\Sigma_g^-\) state to the excited \(b^1\Sigma_g^+\) and \(a^1\Delta\) states. These transitions in the near IR and visible spectrum are forbidden both by spin and spatial symmetry, but they become allowed during collisions with other ground state O\(_2\) molecules, in the spin-triplet state of the O\(_2\)-O\(_2\) collision complex. Knowledge of the nitrogen CIA spectra is important in the study of planetary atmospheres, the oxygen transitions are used in calibrating satellite instruments that help to determine the atmospheric temperature, pressure, and composition.

In all of the earlier theoretical calculations of the CIA spectrum of N\(_2\) it was assumed that the molecules interact with an isotropic potential and the exchange of identical molecules was neglected. We derived an efficient method for the calculation of CIA spectra from quantum scattering calculations in which the anisotropic interactions and exchange between the colliding molecules are fully taken into account. This method was applied [1,2], with the use of ab initio calculated intermolecular potential and dipole moment surfaces, to compute CIA spectra of N\(_2\) in the frequency range from 0 to 300 cm\(^{-1}\) and temperatures up to 300 K. We found that the exchange effects are generally small, but that the inclusion of anisotropic interactions has a substantial effect on the CIA spectrum of N\(_2\) over the whole rotation-translation far-infrared region. It is also demonstrated that the isotropic potential approximation works well for the CIA spectra at higher temperatures.

The calculation of ab initio potential and transition dipole surfaces for ground \(X^3\Sigma_g^-\) state O\(_2\) molecules interacting with excited \(b^1\Sigma_g^+\) or \(a^1\Delta\) state molecules is not an easy job. For the \(X^3\Sigma_g^- - b^1\Sigma_g^+\) O\(_2\)-O\(_2\) dimer the excitation can occur on either molecule. In the Born-Oppenheimer approximation this gives rise to two adiabatic states in which the excitation is delocalized over the monomers. The two resulting adiabatic potentials are degenerate for specific dimer geometries and non-adiabatic coupling has to be taken into account. Also for the \(X^3\Sigma_g^- - a^1\Delta\) dimer there will be degeneracies in the adiabatic potentials because of the possibility to excite either O\(_2\) molecule, but additionally there are dimer structures for which the two substates of the \(a^1\Delta\) O\(_2\) monomers are degenerate. Hence, there is non-adiabatic coupling between four adiabatic states in this case. Instead of dealing with the non-adiabatic couplings directly, we work with diabatic states in which the excitations remain localized on either one of the monomers. We developed an efficient and rather general multiple-property-based diabatization algorithm in which the transformation between adiabatic and diabatic representations is determined by requiring a set of properties in both representations to be related by a similarity transformation [3]. This set of properties is determined in the adiabatic representation by rigorous electronic structure calculations on the excited O\(_2\)-O\(_2\) dimer. In the diabatic representation, the same properties are determined using model diabatic states defined as products of undistorted rotated monomer wave functions. With the electric quadrupole moment, orbital angular momentum, and spin-orbit coupling of the dimer used as properties, this produced a unique set of diabatic intermolecular potentials for the O\(_2\)-O\(_2\) dimer in both excited electronic states, as well as ground-excited state transition dipole moment surfaces for the diabatic states. Scattering calculations with these coupled potentials and calculations of the CIA spectra are in progress.

References:

Tigran A. Vartanyan

Tigran A. Vartanyan got his Ph.D. degree in 1980 and a scientific degree of Dr. Sc. in 2004. He joined Vavilov State Optical Institute in 1976 and was working there till 2005. His last position was a head of laboratory. Since 2006 he is a professor and a head of laboratory of Surface Photophysics at the Saint Petersburg National Research University of Information Technologies, Mechanics and Optics (ITMO University). Published more than 140 research papers in the peer reviewed scientific journals. He calculated the nonlinear optical effects in reflection of light form the gas-solid interface and predicting unusual spectral features in the light reflection from narrow gas slices. He has initiated and gave theoretical foundations for a new method to measure ultrafast dephasing times of surface plasmons localized in metal nanoparticles. He suggested a new type of a label-free biosensor. His current research interests are in the field of atomic spectroscopy, photoinduced surface processes, nanoplasmonics, and nanotechnology.
Spectroscopic characterization of highly excited atoms colliding with solid surfaces

T Vartanyan¹, P Petrov¹, A Pazgalev², R Drampyan³, N Leonov¹

¹ ITMO University, Kronverkskiy pr. 49, St. Petersburg 197101, Russian Federation
² Division of Plasma Physics, Atomic Physics and Astrophysics, Ioffe Physical-Technical Institute, St. Petersburg, Russian Federation
³ Institute for Physical Research, National Academy of Sciences of Armenia, 0203, Ashtarak-2, Armenia

Steadily increasing importance of atom-wall collisions in modern devices based on micro fabricated spectroscopic cells [1,2] calls for detailed investigation of interaction between atoms in highly excited states with the solid surfaces. It is commonly believed that the probability of quenching of electronic excitation in the aftermaths of collision with the solid surface is very high. For this reason, all computations of the spectroscopic effects in the extremely thin cells are based on the assumption that the atoms leave the surfaces of the cell walls in their ground state [3-6]. On the other hand, there are several evidences of the complex phenomena that take place at the collisions of highly excited atoms with the solid surface, in particular, at least 15% of rubidium atoms that arrive at the surface of sapphire in the $5D_{5/2}$ state leave the surface in the $6P_{3/2}$ state [7,8]. This conclusion follows from the comparison of the measured fluorescence intensity with the model simulations [9,10]. To learn more about these processes we performed time of flight measurements on rubidium atoms adsorbed at the surface of sapphire and excited by the laser pulses produced by the optical parametric oscillator. At the shortest wavelength of 420 nm it was possible to transfer the adsorbed atoms to the higher excited state that correlates with the $6P_{3/2}$ states of the free rubidium atom. Counterintuitive reduction of the mean kinetic energy of the desorbed atoms with the increase of the photon energy supports the conclusion that appreciable amount of atoms leave the surface in an excited electronic state.

This work was supported by the Marie Curie International Research Staff Exchange Scheme Fellowship within the 7th European Community Framework Programme: "Light-Matter Coupling in Composite Nano-Structures"-"LIMACONA" (Grant Agreement No: PIRSES-GA-2013-612600), by the Russian–Armenian bilateral project RFBR 15-52-05030, 15 RF-024; and by the Russian Ministry of Education and Science 2014/190, 074-U01.

References:
Tuesday Oral Session 4
(Tu.O.4)
Chairperson: Elisabeth Dalimier
Satoshi Tojo

Satoshi Tojo has been working in the field of laser spectroscopy of atoms and molecules since 1997 in Graduate School of Engineering at Kyoto University.

He received the Doctor of Engineering degree in engineering science from Kyoto University for his work on reflection spectroscopy of alkali atoms using an electric quadrupole transition in 2003.

He researched ultracold atoms and molecules using laser-cooled Yb cloud with spin-forbidden transition as a Postdoc in Graduate School of Science at Kyoto University from 2004, and multi-component Bose-Einstein condensates of Rb atoms with atom-molecular coupling using magnetic dipole transitions as an Assistant Professor at Gakushuin University from 2006.

He has built up new lab as an Associate Professor at Chuo University since 2012. His present interest is higher order interactions of atoms and molecules with optical near-field using optical forbidden transitions.
Laser spectroscopy of gaseous atoms in local field using optical forbidden transitions

S Tojo

Department of Physics, Chuo University, 1-13-27 Kasuga, Bunkyo, Tokyo 112-8551, Japan

Laser spectroscopy in a local field is one of powerful techniques to investigate interactions among atoms, molecules, and matters: reflection spectroscopy for observation of atom-surface interactions [1], and photoassociation spectroscopy of ultracold atoms for measurement of localized diatomic and molecular interactions [2]. The localized matter can generate large field gradient owing to the considerably localized light filed near the surface and van der Waals potentials between atoms.

Optical forbidden transitions are well-known for application of precision spectroscopy such as atom clocks due to narrow spectra [3]. However, since an interaction area of a local field for atoms is appreciably smaller than that of free space, it is extremely difficult to observe spectra using forbidden transitions with a small transition rate less than $10^{-6}$. Therefore, optical forbidden transitions had been out of target for use in local field measurements. Nevertheless, higher-order interactions such as electric and magnetic multipole moments and spin-orbital interactions in optical forbidden transitions can be of interest because such transitions are sensitive to field inhomogeneity.

We have experimentally investigated optical forbidden transitions of atoms in local fields. We have found enhanced oscillator strength of an electric quadrupole transition of cesium atoms with an evanescent field depending on an angle of incidence of light using attenuated total reflection spectroscopy [4] as shown in Fig. 1(a). In the case of a spin-forbidden transition, we have measured interatomic interactions using laser-cooled ytterbium atoms in photoassociation spectroscopy [5] in Fig. 1(b). Due to its narrow transition line, we have found different diatomic interactions between different isotopes due to different local fields. We will also report on new experimental and calculation results with hot and cold atoms in local fields [6, 7].

Figure 1. (a) Ratio of line strengths of an electric quadrupole transition of $^{133}$Cs atoms in an evanescent field between experiment and calculation with a fixed transition strength depending on relative incident angle $\delta$ from the critical angle. (b) Partial-wave potential as a function of interatomic distance and the reconstructed squared wave functions in ultracold $^{174}$Yb (open circles) and $^{176}$Yb (closed triangles) atoms.

References:

Hydrogen dimer features in low temperature collision-induced spectra

M Gustafsson

1 Applied Physics, Luleå University of Technology, 97187 Luleå, Sweden

Despite the weak attraction between hydrogen molecules, if hydrogen gas is sufficiently cool, a significant fraction of the molecules may form weakly bound van der Waals complexes. The importance of these complexes, which are also called dimers, in the absorption spectrum of hydrogen gas has long been recognized. They have been studied both theoretically and experimentally [1–4], and their influence on Jupiter’s and Saturn’s spectra has been verified [1]. Recently, it has been discovered that a discrepancy on the order of 10% in the absorption coefficient is significant for the analysis of Jupiter’s atmosphere [5]. Therefore, more accurate calculations of absorption data are desired.

The influence of the dimers on the spectrum increases with decreasing temperature. This is illustrated in Fig. 1 where the experimental hydrogen spectrum around the rotational transitions S(0) and S(1) at 20 K is presented. The computed spectrum in the isotropic potential approximation (IPA) excluding all dimer and resonance contributions is also displayed for comparison. This temperature is admittedly lower than what is typically considered in modeling of the atmospheres of the giant planets. However, the measurement provides an excellent testing ground for theoretical treatments of the dimer features, since they are so pronounced at this low temperature.

Figure 1. The measured spectrum of pure hydrogen gas around the rotational transitions S(0) and S(1) are shown in panel (a) and (b), respectively [4]. Spectra calculated in the isotropic potential approximation (IPA) without including dimers are also shown for comparison.

This theoretical study has the purpose to explore ways to compute the dimer contributions to the hydrogen spectrum more accurately than what has been done before. The contributions are of three different characters: (i) The free–free contribution, computed with proper anisotropic potential accounted for, shows resonance features. These are due to quasibound states close to the energy of the higher rotational state of the transition in question. (ii) Although there are only a few bound states, there are some bound–bound contributions in the S(0) case (not for S(1) as it seems). These should also be computed including the anisotropic potential so that the transition energies are accurate. (iii) The bound–free contribution, since it is of quasi-continuous character, may be computed in the isotropic potential approximation.

References:

[5] Fletcher L 2016 private communication
The electronic structure and photoinduced processes in the diatomic and triatomic alkali molecules

P Jasik¹, T Kilich¹, M Wiatr¹, J E Sienkiewicz¹

¹ Department of Theoretical Physics and Quantum Information, Faculty of Applied Physics and Mathematics, Gdansk University of Technology, ul. Gabriela Narutowicza 11/12, 80-233 Gdansk, Poland

In the present work we investigate the electronic structure of some alkali diatomic and triatomic molecules, photoinduced processes: photodissociation, photoassociation, photoionization, photoisomerization, etc. Investigating small alkali molecules (diatomic and triatomic) we are able to consider several asymptotes can be reached from the ground asymptote by PA given the ∆Ω = 0, ±1 selection rule.

In the recent years, scientists are able to precisely investigate structure of molecules using modern laser spectroscopy techniques [1]. Besides, the rapid development of cold molecular physics and chemistry in the past two decades brings alkali molecules into special attention [2]. It is believed that the novel laser techniques, are not limited to the observation of the chemical reactions, but can be used to control them. Investigating small alkali molecules (diatomic and triatomic) we are able to consider several photoinduced processes: photodissociation, photoassociation, photoionization, photoisomerization, etc.

In the present work we investigate the electronic structure of some alkali diatomic and triatomic molecules, which are NaRb [3], LiCs [4], Rb₂ [5] and Li₂Cs [5]. Alkali-metal small molecules are often considered as prototypes of more complex molecules, so knowledge of their structure is the key factor in describing, understanding and predicting properties of photoinduced processes. Adiabatic potential energy curves and surfaces with spin-orbit couplings, radial couplings, spectroscopic parameters, Franck-Condon factors and electronic transition dipole moment functions have been calculated for these molecules. All data have been obtained by the configuration interaction method used with effective core potentials (ECP) and core polarization potentials (CPP). All results have been compared with available theoretical and experimental data.

Following Stwalley [6], we propose an effective photoassociation processess for heteronuclear alkali molecules. In these systems, it is possible to observe states of all symmetries at the Na(3s)+Rb(5p) and Li(2s)+Cs(6p) asymptotes. Within Hund’s coupling case c, every excited state corresponding to above asymptotes can be reached from the ground asymptote by PA given the ∆Ω = 0, ±1 selection rule.

Figure 1. Possible schemes of photoassociation processes in the NaRb molecule.

References:
WEDNESDAY ORAL SESSION 1 (We.O.1)

Chairperson: Ha Tran
Wim Ubachs

Wim Ubachs received his PhD from Nijmegen University (Netherlands). Thereafter he was PostDoc at the Dalian Institute of Chemical Physics (China) and Stanford University (USA). He is full professor at VU University Amsterdam since 2003, where he acted also as Director of the Laser Centre from 2000-2010. His scientific work is in high-resolution laser spectroscopy, non-linear optics and extreme ultraviolet light, with applications in atmospheric physics as well as in astrophysics. In the past decade he has been involved in astronomical observations, using optical telescopes as well as radio telescopes. He has published > 250 scientific papers, and has received an ERC Advanced grant in 2015. Since 2014 he is also a group leader at the Advanced Research Centre for Nanolithography, a public-private partnership institute in Amsterdam.
Physics beyond the Standard Model from molecular hydrogen

W Ubachs

1Department of Physics and Astronomy, Vrije Universiteit Amsterdam, The Netherlands

The spectroscopy of molecular hydrogen can be used for a search into physics beyond the Standard Model. Differences between the absorption spectra of the Lyman and Werner bands of H₂ as observed at high redshift and those measured in the laboratory can be interpreted in terms of possible variations of the proton-electron mass ratio \( \mu = m_p/m_e \) over cosmological history. Investigation of some ten of such absorbers in the redshift range \( z = 2.0 - 4.2 \) yields a constraint of \( \Delta \mu / \mu < 5 \times 10^{-6} \) at 3σ [1]. Similarly, spectra of molecular hydrogen in the photospheres of white dwarf stars reveal that the proton-electron mass ratio does not depend on (strong) gravitational fields [2].

While such astronomical studies aim at finding quintessence in an indirect manner, laboratory precision measurements target such additional quantum fields in a direct manner. Laser-based precision measurements of dissociation energies, vibrational splittings and rotational level energies in H₂ molecules and their deuterated isotopomers HD and D₂ produce values for the rovibrational binding energies fully consistent with quantum ab initio calculations including relativistic and quantum electrodynamical (QED) effects [3]. Similarly, precision measurements of high-overtone vibrational transitions of HD⁺ ions, also result in transition frequencies fully consistent with calculations including QED corrections [4]. These comprehensive results of laboratory precision measurements on neutral and ionic hydrogen molecules can be interpreted to set bounds on the existence of possible fifth forces [5] and of higher dimensions [6], phenomena describing physics beyond the Standard Model.

References:

Daniel Lisak

Daniel Lisak received his Ph.D. from Nicolaus Copernicus University (NCU). He joined the group of Atomic, Molecular and Optical Physics at NCU. He was a visiting researcher at University of Naples, Italy, at NIST, USA and at NMIJ/AIST, Japan and at Universite Paris-Est Creteil, France. He is currently a professor at NCU. His main scientific interest is investigation of atomic and molecular spectral line shapes in a gas phase and development of cavity-enhanced spectroscopic methods. He is also involved in development of optical clocks.
Molecular line shapes study with cavity-enhanced absorption and dispersion spectroscopy

D Lisak

1 Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Grudziądzka 5, 87-100 Toruń, Poland

High-accuracy measurement of spectral line shapes is important in growing number of fields, including basic research, metrology and many gas-sensing applications. This is associated with fast development of new ultra-accurate spectroscopic techniques. For of weak absorption lines cavity-enhanced techniques, such as cavity ring-down spectroscopy (CRDS), proved excellent performance and spectral line shapes with extremely high signal-to-noise ratios [1,2] were demonstrated using the frequency-stabilized cavity ring-down spectroscopy (FS-CRDS) [3]. Recent results of accurate line-shapes investigation using CRDS and other cavity-enhanced spectroscopy methods, described below, will be presented.

The exponential light decays measured in CRDS, is related to the spectral width of the cavity modes. This phenomenon is exploited in the cavity mode-width spectroscopy (CMWS) [4–6] in which absorption spectrum can be retrieved by precise measurements of half-widths of the cavity modes. Analysis of CRDS and CMWS methods reveals their complementarity in terms of achievable accuracies at different levels of intra-cavity absorption [5]. For low absorptions the best precision is expected with the CRDS technique, where the ring-down decays are long. In the opposite case of high absorption and short ring-down time, the cavity modes become broad and the precision of CMWS should be higher.

Measurement of dispersion mode shifts provides another possibility for very accurate quantitative spectroscopy. Since frequency is a physical quantity that can be measured most accurately, direct measurement of absolute or differential mode frequencies to obtain a spectrum in the 1-dimensional cavity mode dispersion spectroscopy (1D-CMDS) [7,8] should eliminate potential problems with nonlinearities of detection system and minimize systematic instrumental errors. Contrary to any absorption spectroscopy, in 1D-CMDS both axes of the spectrum can be linked to the primary frequency standard [9]. Typical mode widths of the cavities used in high-sensitivity absorption spectroscopy are at kHz level. Therefore a used lasers must be extremely narrow spectrally and precisely tunable.

These new cavity-enhanced techniques may be especially useful in applications that require high accuracy of weak absorption measurements, e.g. gas spectroscopy for atmospheric monitoring and gas metrology, Doppler thermometry, as well as fundamental study of spectral line shapes. Direct comparison of spectra obtained with various cavity-enhanced techniques enables identification of potential instrumental errors at sub-percent level of accuracy required in many modern applications.

References:

Study of the frequency stability of a quantum cascade laser frequency comb

F Cappelli1, G Campo1, I Galli1, G Giusfredi1, S Bartalini1, D Mazzotti1, P Cancio1, S Borri1, B Hinkov2, J Faist2 and P De Natale1

1 CNR-INO – Istituto Nazionale di Ottica, Largo Enrico Fermi 6, 50125 Firenze FI, Italy & LENS – European Laboratory for Non-Linear Spectroscopy, Via Nello Carrara 1, 50019 Sesto Fiorentino FI, Italy
2 Institute for Quantum Electronics, ETH Zurich, 8093 Zürich, Switzerland

Recently it has been discovered that quantum cascade lasers (QCLs) can generate optical frequency combs (OFCs) in the mid infrared [1], but a detailed analysis of the possibility of a fine control of the emission to use them for high-resolution spectroscopy and metrology applications is still missing. Here the first attempt of frequency stabilizing a mid-infrared quantum cascade laser comb (QCL-comb) against a metrological mid-infrared intracavity-difference-frequency-generated comb (IC-DFG-comb) through a single phase-locking chain is presented. The result is that the locking essentially reduces the offset fluctuations, but does not sensitively affect the mode spacing. The overall single QCL-comb tooth linewidth is reduced from 500 kHz down to values ranging from 1 to 23 kHz on a 40-ms time scale.

The tested QCL-comb emits around 4.70 µm with a spacing (fs) between the longitudinal modes (QCL-comb teeth) of about 7 GHz. The IC-DFG-comb, generated using an intracavity scheme [2] and characterized by a spacing (fr) of about 1 GHz, is essentially used to convert the MIR QCL-comb spectrum down to the radio frequencies (RF) using a dual-comb-like setup. A properly implemented phase-locked-loop (PLL) locks one QCL-comb tooth to an IC-DFG-comb tooth.

When the QCL-comb operates in free-running regime, the peaks in the HBNS are about 500-kHz wide (FWHM). Once closed the loop and optimized the PLL parameters, the HBNS has been acquired with a spectrum analyzer. In fig. 1 the amplitude of the signal acquired on a 40-ms time scale is shown. The locked peak is resolution-bandwidth-limited, while for the others a linewidth of few kilohertz on a 40-ms time scale is obtained.

![Figure 1. 4 FFT amplitude of the HBNS acquired using spectrum analyzer 1 on a 40-ms time scale. The QCL-comb operates in locking condition.](image)

The QCL-comb modes are about 100, and the residual frequency noise on the modes on the sides of the spectrum is 23 kHz. We can state that the overall single QCL-comb mode linewidth is reduced from 500 kHz to values ranging from 1 to 23 kHz on a 40-ms time scale, depending on the distance from the center of the spectrum. This preliminary study paves the way to a full control of this type of sources, thus dramatically widening the applicability of such miniaturized comb sources.

References:

WEDNESDAY ORAL SESSION 2
(We.O.2)
Chairperson: Piotr Masłowski
Aleksandra Foltynowicz

Aleksandra Foltynowicz is Assistant Professor at the Department of Physics, Umeå University, Sweden. Aleksandra took her master degree in experimental physics at Adam Mickiewicz University in Poznań, Poland. During her PhD in the group of Ove Axner at Umeå University she worked with ultrasensitive cavity-enhanced frequency modulation spectroscopy (NICE-OHMS). After obtaining her PhD degree at Umeå University in 2009 she spent 2 years in Jun Ye’s group at JILA, University of Colorado, Boulder, working with optical frequency comb spectroscopy (OFCS). She is now leading a group at Umeå that works with development and applications of OFCS for precision spectroscopy and sensitive multispecies detection. She co-authored 26 publications and 2 book chapters about NICE-OHMS and OFCS. Aleksandra received a number of grants and awards, most recently the Ingvar Carlsson Award from the Swedish Foundation for Strategic Research, the technical and natural science prize from the Royal Skyttean Society, and the Knut and Alice Wallenberg Academy Fellowship.
High-resolution optical frequency comb spectroscopy

A Foltynowicz¹, L Rutkowski¹, A C Johansson¹, A Khodabakhsh¹

¹ Department of Physics, Umeå University, 901 87 Umeå, Sweden

Fourier transform spectrometers (FTS) based on optical frequency combs allow detection of broadband molecular spectra with high signal-to-noise ratios within acquisition times orders of magnitude shorter than conventional FTS based on thermal sources [1]. Due to the pulsed nature of femtosecond lasers that produce frequency combs, the interferogram consists of a series of bursts separated by an optical path difference (OPD) equal to c/f_{rep} (where c is the speed of light and f_{rep} is the repetition rate of the comb) rather than a single burst at zero OPD. In conventional FTS the resolution is given by the inverse of the OPD; however, in comb-based FTS it is sufficient to acquire an interferogram in a symmetric range around a single burst with length precisely matched to the comb line spacing (i.e. equal to c/f_{rep}) in order to exceed the spectrometer’s nominal (OPD-limited) resolution and precisely measure the intensity change of the individual comb lines [2]. This allows measurements of broadband high-resolution spectra without any influence of the instrumental lineshape function even when the nominal resolution is coarser than the linewidth of the absorption features, and reduces the acquisition time and interferometer length by orders of magnitude compared to conventional high-resolution FTS. Moreover, a frequency comb can be efficiently coupled to an enhancement cavity, which yields high sensitivity to absorption and low concentration detection limits [3].

I will present the principles and experimental implementation of cavity-enhanced optical frequency comb spectroscopy based on a Fourier transform spectrometer. Our system is based on an Er:fiber femtosecond laser locked to an enhancement cavity with a finesse of ~10 000, and a fast-scanning FTS with auto-balancing detector. A single-burst interferogram is acquired in 0.5 s and yields a nominal resolution of 750 MHz (OPD of 40 cm). Figure 1(a) shows a low-pressure CO₂ spectrum obtained by interleaving 5 spectra from single-burst interferograms with different repetition rates, together with a fit of a model spectrum [3] based on line parameters from the HITRAN database and Voigt profile. No influence of the instrumental lineshape function is visible [Fig. 1(b)] even though the CO₂ linewidth at this pressure is 457 MHz, below the nominal resolution of the spectrometer.

Figure 1. (a) Cavity-enhanced spectrum of the $3\nu_1 + \nu_3$ band of 1000 ppm CO₂ in N₂ at 50 Torr (black, 5 averages) together with a fit of the model spectrum (red, inverted for clarity) (b) A zoom of the R24e line with a linewidth of 457 MHz measured with a spectrometer with a nominal resolution of 750 MHz

References:

Alain Campargue

Alain Campargue earned his PhD degree in 1986 at the Grenoble University. Currently, he is CNRS Senior Scientist at LIPhy Laboratory of the University of Grenoble-Alps. He is leading the applications to molecular spectroscopy of the high sensitivity laser techniques developed in the LIPhy group “Lasers, Molecules and Environment” (in particular CW-CRDS). His favorite target species are molecules of atmospheric interest: water vapor (including continuum absorption), methane ozone, carbon dioxide. He is leading the “Laboratoire International Associé “SAMIA” between CNRS and the Institute of Atmospheric Optics in Tomsk (RAS).
CRDS and OF-CEAS of water vapor in the near infrared: Spectroscopic database and self-continuum absorption

A Campargue$^1$, S Kassi$^1$, D Mondelain$^1$, S N Mikhailenko$^2$, D Romanini$^1$

$^1$ Univ. Grenoble Alpes, CNRS France
$^2$ Institute of Atmospheric Optics, RAS, Tomsk (Russia)

During the last years, different cavity enhanced absorption techniques have been developed in our laboratory to improve the knowledge of the absorption spectroscopy of water vapor in the near infrared. Our approach concerns both extensive measurements of rovibrational lines beyond the sensitivity of standard techniques and the determination of the self- and foreign-continua of water vapor in the transparency windows.

The different experimental methods include the CRDS technique with a series of 90 DFB laser diodes and an ECDL allowing for a continuous coverage of the 1.71-1.18 μm range, CRDS and OF-CEAS with DFB laser diodes or VECSEL in the 2.3 μm region, OF-CEAS with a MQW laser near 4.35 μm. As a result a new spectroscopic database [1] has been constructed for natural water vapor in the 5850-8340 cm$^{-1}$ region and accurate measurements of the water vapor continuum at different spectral points of the 4.4, 2.3, 1.6 and 1.2 μm transparency windows are reported for the first time [2].

Fig.1 summarises a part of our results which will be detailed during the presentation.

**Figure 1.** Overview comparison between the HITRAN2012 and our line lists for water vapor between 5850 and 8340 cm$^{-1}$ and spectral dependence of the self-continuum cross-section, $C_s$, derived from the MT_CKD V2.5 model and measured by FTS, CRDS and OF-CEAS.

References:

High-resolution comb-assisted Lamb dip spectroscopy

D Gatti¹, R Gotti², A Gambetta¹², G Galzerano¹, P Laporta¹², M Marangoni¹²

¹ Istituto di Fotonica e Nanotecnologie-CNR, P.za L. da Vinci 32, 20133 Milano, Italy
² Dipartimento di Fisica - Politecnico di Milano, Via Gaetano Previati 1/C, 23900 Lecco, Italy

The advent of frequency combs enabled the acquisition of absorption spectra with an unprecedented level of precision and prompted the investigation of subtler and subtler collisional effects on the shape of absorption profiles. This has been carried out so far mostly in the Doppler broadening regime, the main reason being the technical difficulty to access absorption saturation with a large variety of molecules and to combine this regime with a precise and sensitive acquisition of Lamb dips.

In this work we introduce a novel comb-assisted spectrometer operating over a broad spectral range from 1.5 to 1.63 µm with a detection limit of 2.5·10⁻¹¹ cm⁻¹ over 200 s, a frequency accuracy at the kHz-level and an intra-cavity intensity enhancement up to 1.5 kW/cm², which is shown to be suitable for high-quality measurements of Lamb dip profiles of weak transitions, below 10⁻²³ cm/mol, also in combination with extremely weak Einstein coefficients, down to 5 mHz. Interestingly, the spectrometer relies (see Fig. 1a) on a purely dc detection regime at the output a 100,000-finesse cavity, where noise suppression is achieved by an extremely tight Pound-Drever-Hall locking of the probe laser to the cavity through interposition of a single-sideband modulator.

![Figure 1. a) Lamb-dip spectrometer setup; (b) 100-fold averaged Lamb dip profile of the P(30) line; (c) dispersion of centre frequencies for 25 independent sets of measurements](image)

Precision and accuracy of the spectrometer were tested at a relatively low intra-cavity field intensity on three well-characterized intense lines of the 10100-0000 band of acetylene. Fig. 1 (b) reports, in particular, the Lamb-dip profile of the P(30) line at a pressure of 0.4 Pa, as obtained by averaging 100 spectra made up of 100 spectral points. Panel (c) represents the line–center frequency retrieved from a pure Lorentianz fit of 25 fully independent sets of measurements, everyone encompassing 100 scans. The rms deviation of data amounts to 1.1 kHz only, which accounts for an impressive Type A uncertainty of 5 parts over 10¹². The centre frequency was found to agree within 2.5 kHz with that obtained by metrological institutes [1] on the same lines.

By shifting the intra-cavity intensity to 1.5 kW/cm² it was possible to achieve saturation and acquire spectra with a signal-to-noise ratio up to 100 for the P(15) line of the 01120-0000 band of acetylene, featuring a line-strength below 10⁻²³ cm/mol and an Einstein coefficient of 5 mHz only, among the weakest ever observed in the Doppler-free regime. This result paves the way to highly accurate Lamb-dip surveys over thousands of lines in the telecom spectral region, with full access to both dip shapes and line saturation intensities upon changing the intra-cavity power.

References:
WEDNESDAY ORAL SESSION 3
(We.O.3)

Chairperson: Robert R. Gamache
Luigi Moretti

Luigi Moretti received the Laurea Degree in Physics from the University “Federico II” of Naples in May of 1999. In 2003 he received the PhD title in Electronic Engineering with research activity in silicon optoelectronic devices. From 2004 until to 2008 he has been researcher at University “Mediterranea” of Reggio Calabria and its research activity was focused on the electromagnetic propagation in aperiodic photonic crystals and in the designing of advanced silicon optoelectronics device. Currently, he is associate professor at Second University of Naples where he works in the fields of molecular spectroscopy and modelling of spectral line-shape. He is author or co-author of more than 50 publications on international journals.
The lineshape problem in the vibration-rotation spectrum of water molecule

L. Moretti, A. Castrillo, M. D. DeVizia, E. Fasci, P. Amodio, and L. Gianfrani

1Department of Mathematics and Physics of Second University of Naples

Water vapor is the most important constituent in the Earth’s atmosphere, being responsible for about 70% of the known atmospheric absorption of sunlight and the majority of the greenhouse effect. Highly accurate, in situ measurements of water concentration are absolutely relevant for a full comprehension of atmospheric radiation transport, atmospheric chemistry, cloud formation, and precipitation. The recent efforts in the realization of a spectrometer with a highly accurate, absolute, and repeatable frequency axis in the whole near-infrared range (between 1 and 3 μm), jointly with a sufficiently high signal-to-noise ratio, has led to a deeper line-shape investigations, aimed at a better understanding of the physical mechanisms determining the absorption profile associated to a given vibration-rotation transition. This is particularly interesting for the water vapor molecule, for which the precise knowledge of the molecular spectroscopic parameters is an indispensable prerequisite for the retrieval of molecular densities. In addition to a very well designed experiment, highly accurate measurements of relevant parameters, such as line intensity factors and pressure broadening coefficients, require a very reliable physical understanding of the line shape that may present quite strong departures from usual Voigt profile.

In this talk, we discuss about the recent progress in the line-shape modeling of water near-infrared spectra. Our studies demonstrates that the molecular confinement alone is unable to explain entirely the departures from the Voigt profile and that the speed dependence of pressure-induced broadening and shifting cannot be ignored, even in the case of pure water samples at relatively small pressures. Furthermore, we investigate the dependence of line broadening and shifting parameters on the choice of the line-shape model, putting in evidence that the quadratic approximation, widely employed in the past literature in a variety of classical line-shape models, for a large number of molecules and colliding partners, fails to reproduce the experimental shape, especially at pressure greater than 133 Pa. These works have contributed to the tuning of a sophisticated and refined spectral analysis procedure for the absorption profile of self-colliding H218O molecules in the Doppler Broadening Thermometry (DBT) experiments for the determination of the Boltzmann constant.

Despite their very different physical origin, the Dicke and speed-dependent effects have a similar influence on the line-shape profile providing both to line narrowing. As a matter of fact, the speed dependence of collisional width is difficult to distinguish from Dicke narrowing, especially in the low-pressure limit. In order to overcome this difficulty, a global approach has been implemented to simultaneously fit spectra across a given range of pressures, sharing a number of free parameter at the aim of reducing significantly statistical correlation issues among them. Consequently, we demonstrated the possibility of determining several spectroscopic parameters as collisional broadening and shifting coefficients with high precision and accuracy at the level of 10−3. Finally, we discuss about the theoretical limit of accuracy and precision in the determination of Doppler width by means of a global fitting procedure. We adopt several semiclassical line-shape models to fit a very realistic and sophisticated model, known as partially correlated speed-dependent Keilson-Storer profile. We demonstrate that the Doppler width can be determine with a precision and accuracy of 0.42 and 0.75 part per million respectively.

References:

Robab Hashemi

Robab Hashemi is a second year PhD student in “Earth, Space and Physical Science” in University of Lethbridge, AB, Canada. Her master was in the field of Cosmology and she did a master fellowship in University of Zurich and did research on Dark Matter. Having Studied at University of Lethbridge under supervision of Dr. Predoi-Cross, Robab has obtained knowledge in 'Laser Spectroscopy' with application in Green House Gas monitoring as well as data analyzing using MATLAB and Labview programming. Now, working on environmental applications regards to CO$_2$ fluxes and biomass monitoring using airborne laser scanning. The other ongoing research of her is to obtain more accurate information on the low lying infrared bands of N$_2$O by recording the high resolution far-infrared spectrum of a pure and mixture of N$_2$O with air.
Line-shape studies of methane and carbon monoxide

R Hashemi1, A Predoi-Cross1, A V Nikitin2,3, Vl G Tyuterev4, K Sung5, M A H Smith6, V Malathy Devi7, A S Dudaryonok8, N N Lavrentieva9, A C Vandeae10, J Vander Auwera11

1 Dept. of Physics & Astronomy, University of Lethbridge, Alberta, AB, Canada
2 Laboratory of Theoretical Spectroscopy, V.E. Zuev Institute of Atmospheric Optics, Russian Academy of Sciences, Tomsk State University, Tomsk, Russian Federation
3 QUAMER laboratory, Tomsk State University, Tomsk, Russian Federation
4 Groupe de Spectromtrie Molculaire et Atmosphrique, UMR CNRS 6089
5 Universit de Reims, U.F.R. Sciences, Reims Cedex 2, France
6 Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California, CA, USA
7 Science Directorate, NASA Langley Research Center, Hampton, Virginia, VA, USA
8 Dept. of Physics, College of William & Mary, Williamsburg, Virginia, VA, USA
9 Service de Chimie Quantique et Photophysique, C.P. 16009, Université Libre de Bruxelles, B-1050 Brussels, Belgium
10 V.E. Zuev Institute of Atmospheric Optics, Siberian Branch of the Russian Academy of Sciences, 1 Akademishian Zuev square, 634021 Tomsk, Russia
11 Belgian Institute for Space Aeronomy, Planetary Aeronomy Division, 3 avenue circulaire, B-1180 Brussels, Belgium

The success of planetary atmospheric remote sensing studies often relies on having highly accurate sets of laboratory data to interpret them. Advances in remote sensing instrumentation are pushing the requirements for accuracy of spectroscopic line parameters included in databases such as HITRAN or GEISA. Today’s state of the art line shape models go beyond the Voigt model, to include subtle effects such as line mixing, correlation between collisional narrowing, the velocities of molecules, the ro-vibrational relaxation mechanisms, to mention a few [1-5]. Two atmospheric trace gases, namely methane and carbon monoxide have been considered in our study. Due to the importance of methane as a trace atmospheric gas and a greenhouse gas and its contributions to the terrestrial Carbon Cycle, we have carried out a precise line-shape study to obtain the self- and air half-width coefficients, self- and air shift coefficients and off-diagonal relaxation matrix element coefficients for methane transitions in the spectral range known as the “methane octad”. In addition, the associated temperature dependences of these coefficients have been measured in the 4300-4500 cm⁻¹ region. The high signal to noise ratio spectra of pure methane and of dilute mixtures of methane in dry air with high-resolution, have been recorded at temperatures from 148 K to room temperature using the Bruker IFS 125 HR Fourier transform spectrometer (FTS) at the Jet Propulsion Laboratory, Pasadena, California. The analysis of spectra was done using a multi-spectrum nonlinear least-squares curve fitting technique [6]. Besides being an active greenhouse gas present in the terrestrial atmosphere, carbon monoxide is also present in the atmosphere of Venus [6]. Understanding its sources, sinks and distribution in the Venusian atmosphere can help scientists better understand the dynamics taking place in the mesosphere and the lower thermosphere (from 70 to 120 km). The Venusian atmosphere is probed by the “Solar Occultation in the InfraRed” (SOIR) instrument on board the ESA “Venus Express” spacecraft [7]. The first overtone band of the main isotopologue of Carbon monoxide is located near 4260 cm⁻¹ (2.3 μm) and can be observed in SOIR spectra [8]. Our study is intended to diminish the gap in knowledge for line parameters of CO broadened by CO₂ over a range of temperatures. Fourier transform absorption spectra of the 2–0 band of ¹²C¹⁶O mixed with CO₂ have been recorded at total pressures from 156 to 1212 hPa and at 4 different temperatures between 240 K and 283 K. CO₂ pressure-induced line broadening and line shift coefficients, and the temperature dependence of the former have been measured including line mixing. Measured line-shape parameters were compared with theoretical values, calculated for individual temperatures using a semi-empirical method and the Exponential Power Gap (EPG) law.

References:
WEDNESDAY ORAL SESSION 4
(We.O.4)
Chairperson: Motoshi Goto
Annette Calisti

Dr. Annette Calisti is senior researcher at the French National Center for Scientific Research (CNRS) and Deputy Director of the laboratory of Physics of Ionic and Molecular Interactions (PIIM), in Marseille (France). She received her doctorate from the University of Provence (Marseilles, France) in 1989 working with Professor R. Stamm, on Stark profile studies in plasmas by using numerical simulations. She is, with B. Talin and R. Stamm, at the origin of the line shape code – the PPP code – for complex emitters in hot and dense plasmas. Her main research interests concern the spectroscopic diagnostics of hot dense plasmas. At the interface between atomic and plasma physics, this subject covers fundamental aspects of the understanding of the plasma – radiation interaction mechanisms and their modeling, and applied aspects for the interpretation of experimental results. She shares the I. V. Kurchatov prize for the best scientific research work of the year 2013, on « News effects in kinetic theory of atomic radiative processes in plasmas ». 
Ionization-potential depression study in dense plasmas - Application to spectroscopic diagnostics

A Calisti1, S Ferri1, C Mossé1, B Talin1

1Aix-Marseille Université - CNRS, PIIM UMR7345, Campus Saint-Jérôme, 13397 Marseille, France

The radiative properties of an atom or an ion surrounded by a plasma, are modified through various mechanisms. For instance the line shapes of radiation emitted by bound-bound transitions are broadened and therefore carry information useful for plasma diagnostics. Depending on plasma conditions the electrons supposedly occupying the upper quantum levels of radiators no longer exist as they belong to the plasma free electron population. All the charges present in the radiator environment, electrons and ions, contribute to the lowering of the energy required to free an electron in the fundamental state. This mechanism is known as ionization potential depression (IPD). The knowledge of IPD is useful as it affects both the radiative properties of the various ionic states and their populations. Its evaluation deals with highly complex n-body coupled systems, involving particles with different dynamics and attractive ion-electron forces. A few recent experiments [1, 2] leading to IPD measurements in situ renew interest for this issue. On the other hand some approximate models (e.g. [3, 4]) allow to discuss experiments as they provide a scaling for the IPD.

This interest has motivated the development of an alternative approach. The present work on IPD is carried out using a classical molecular dynamics (MD) code, the BINGO-TCP code [5, 6], developed recently to simulate neutral multi-component (various charge state ions and electrons) plasma. Our simulations involve a mechanism of collisional ionization/recombination necessary to simulate stationary plasmas with a definite temperature and equilibrated populations of ions of various charge states. The study focuses on aluminum plasmas for different ionic densities and several temperatures in order to explore the IPD for different plasma coupling conditions. Results will be compared with experimental data when they exist.

Figure 1. Influence of the ionic structure on the ionization potential depression (IPD) for an aluminum plasma at solid density

References:
Shape theory of resonant four-wave mixing signals induced by rotational anisotropy

A Kouzov\(^1\), P Radi\(^2\), N Filippov\(^1\), T Sinyakova\(^1\)

\(^1\)Faculty of Physics, Saint Petersburg State University, Ulyanovskaya str. 3, Saint Petersburg 198504, Russia

\(^2\)Paul Scherrer Institute, CH-5232 Villigen, Switzerland

Recent experiments [1] at the Paul Scherrer Institute have revealed unique abilities of the Resonant Four-Wave Mixing (RFWM) spectroscopy to study rotational and translational anisotropy of photofragments produced by absorption of plane-polarized photons. Of particular interest are the signals which are solely due to orientational correlations between the rotational momentum \(J\) and the recoil velocity \(v\), the crucial signatures of the photolytic bond rupture mechanism. Here, the RFWM signal shapes are theoretically derived and shown to reduce to a simple functional form in the high-recoil limit. An accent is made on the yet unexplored rotational helicity effect for which \(J\) and \(v\) of a photofragment are either parallel or antiparallel. The helicity manifests itself via characteristic full dips of the Doppler-broadened profiles detected on the OH radicals produced by photolysis of \(\text{H}_2\text{O}_2\) by a plane-polarized 266 nm laser radiation. Figure 1 gives a comparison between the experimental [1] and simulated, helicity-induced profiles of the \(Q_1(6)\) line of the \(A^2\Sigma^+\)-\(X^2\Pi(0,0)\) OH vibronic band.

![Figure 1. Measured (dots, Ref.1) and simulated (red dashed line representing the helicity-induced contribution) shapes of the \(Q_1(6)\) line of the \(A^2\Sigma^+\)-\(X^2\Pi(0,0)\) OH vibronic band](image)

This study was supported by the Swiss National Science Foundation (grant 200021 153170/1), the Russian Foundation for Basic Research (grant 15-03-04997) and by the Saint-Petersburg State University (grant 11.38.265.2014).

References:

Sergey N. Yurchenko

Born in Frunze, USSR, I earned my Physics Diploma with Honours in 1992 from Tomsk State University where I also received my PhD in 1997. I have worked as a research associate in Wuppertal University, Steacy Institute of NRC Canada (NERC Fellowship), Muelheim-an-der Ruhr (Max Planck Fellowship) and TU Dresden. In 2011 I have joined the Physics and Astronomy department at UCL as a manager of the ExoMol project, where I am currently a senior lecturer. I study spectroscopic properties of hot polyatomic molecules, especially those which are found to be important for atmospheres of exoplanets and cool stars. This is also the aim of the ExoMol project (www.exomol.com) which I manage. I am a developer of the computational method TROVE (Theoretical ROVibrational Energies), used for efficient production of molecular line lists of polyatomic molecules. I am active in social media (www.facebook.com/exomol) and like twitting (https://twitter.com/TroveMaster).
ExoMol project: Molecular line lists for exoplanet and other hot atmospheres

S Yurchenko

1 Department of Physics and Astronomy, University College London, Gower Street, WC1E 6BT, London, UK

The fundamental molecular data play principal role for spectral characterization of astrophysical objects cool enough to form molecules in their atmospheres (cool stars, extrasolar planets and planetary discs) as well as in a broad range of terrestrial applications. The ExoMol project aims at providing a comprehensive solution to this problem by generating spectroscopic data for molecules of importance in the atmospheres of exoplanets [1]. These data are widely applicable to other problems such studies on cool stars, brown dwarfs and circumstellar environments as well as industrial and technological problems on Earth.

ExoMol employs a mixture of first principles and empirically tuned quantum mechanical methods to compute comprehensive and very large rotation–vibration and rovibronic line lists. For diatomic molecules we have developed a new flexible, multistate computer program capable of solving a general diatomic problem with arbitrary number and types of couplings. For polyatomic molecules a combination of variational and perturbation theory approaches is used. Critical points of the large-scale production of molecular line lists involving high rotational excitations needed for simulating molecular spectra at temperatures higher than 500 K will be discussed.

Results span a variety of closed (NaH, SiO, PN, NaCl, KCl, CS) and open (BeH, MgH, CaH, AlO, VO) shell diatomics to triatomics (HCN/HNC, SO2, H2S, H3+), tetratomics (H2CO, PH3, SO3, H2O2), plus methane [2] and nitric acid [3]. This has led directly to the detection of new species in the atmospheres of exoplanets [4]. A new comprehensive data release has just been completed [5]. Progress on and future prospects of the project will be summarized.

References:

Iouli Gordon

Dr. Iouli Gordon is a physicist at the Harvard-Smithsonian Center for Astrophysics in Cambridge, USA. He is one of the managers of the HITRAN and HITEMP spectroscopic databases which constitute an international reference standard for spectroscopic parameters needed for atmospheric, but also for other scientific and industrial, applications. He played major role in the development and public release of HITRAN2008, HITRAN2012 and HITEMP2010 databases. He is now spearheading the efforts towards the HITRAN2016 database. Dr. Gordon obtained his Diploma in Engineering Physics at the Moscow Institute of Physics and Technology, Russia (1999), MSc in Physics at the University of Toronto, Canada (2001), and PhD at the University of Waterloo, Canada (2006). His research interests focus on laboratory and theoretical molecular spectroscopy of atmospheric and astrophysical interest, use of available spectroscopic information to construct databases that aid research in diverse areas of science and industry, and development of the tools for enhancing data accessibility and effectiveness of scientific collaborations in the field of molecular spectroscopy.
Line shape parameters in HITRAN2016 and beyond

I E Gordon¹, P Wcisło¹,², J S Wilzewski¹,³, R V Kochanov¹,⁴, C Hill¹,⁵, Y Tan¹, L S Rothman¹

¹ Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, 60 Garden St Cambridge MA 02138, USA
² Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun, Grudziadzka 5, 87-100 Torun, Poland
³ Ludwig-Maximilians-Universität, Faculty of Physics, Munich, Germany and German Aerospace Center (DLR) Oberpfaffenhofen, Germany
⁴ Laboratory of Quantum Mechanics of Molecules and Radiative Processes, Tomsk State University, 36 Lenina Avenue, 634050 Tomsk, Russia
⁵ University College London, Gower Street, London WC1E 6BT, UK

The HITRAN molecular spectroscopic database [1] is a compilation of spectroscopic parameters of dozens of molecules that a variety of computer codes use to predict and simulate the transmission and emission of light in different environments (especially planetary atmospheres). Recently we have replaced the traditional ASCII format of the database with a modern relational database structure accessible through the dynamic user interface HITRANonline [2] available at www.hitran.org. This new structure allows substantial evolution of the database with respect to line shapes. There are two major directions in which this evolution is progressing (although it is not limited to these directions).

The first direction is that, in order to increase the potential of the HITRAN database in planetary sciences, experimental and theoretical line-broadening coefficients, line shifts and temperature-dependence exponents of molecules of planetary interest broadened by H₂; He; and CO₂ are now provided in the database (in addition to air and self broadening that were traditionally provided in HITRAN). So far these data are available for several gases for which we constructed complete datasets [3]. For the construction of these datasets, experimental and theoretical data have been assembled from available peer-reviewed sources. The collected data were evaluated and used to create semi-empirical models for calculating relevant parameters for every line of the studied molecules in HITRAN. Another important development is that apart from the Voigt profile parameters that were traditionally provided in HITRAN, we are able to add parameters associated with many common line profiles, including Galatry, speed-dependent Voigt, and the HT profiles [4]. As a test case, we created a first complete dataset of the HT parameters for every line of molecular hydrogen in the HITRAN database [5]. The database was constructed based on the analyses of the high-resolution experimental data measured in different bands. In this work we also separated the line shape parameters into four temperature regimes to ensure correct calculation of the absorption at different temperatures. Apart of being able to obtain all of these relevant data from HITRANonline users can utilize HITRAN Application Programming Interface (HAPI) that we recently developed. Planned future developments, including implementation of line mixing into the database, will also be discussed.

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References:

FTIR based measurements of the 2-0 band of HCl broadened by CO$_2$

at 1.76 $\mu$m

G Li$^1$, H Tran$^2$, M Gisi$^3$, O Werhahn$^1$ and V Ebert$^{1,3,4}$

1 Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany
2 Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA, UMR CNRS 7583)
3 Physikalisch Chemisches Institut, U Heidelberg, INF 253, 69116 Heidelberg
4 Center of Smart Interfaces, TU Darmstadt, Petersenstraße 32, Darmstadt 64287, Germany

Fourier transform absorption spectra of the 2–0 band of HCl mixed with CO$_2$ have been measured at room temperature for total pressures ranging from 1 bar to 10 bar at an interval of 0.5 bar. For the first time, reliable and complete CO2-induced broadening and shift coefficients have been retrieved for the entire 2-0 band of H$^{35}$Cl and H$^{37}$Cl, respectively. Voigt line shapes and subclasses of the Hartmann-Tran profile were adopted to retrieve spectral line data (e.g. broadening parameters), employing conventional single-spectrum regression analysis as well as simultaneous multi-spectrum fits. A super-Lorentzian effect on the far wings was observed in the recorded spectra at high pressures, when the recorded spectra were compared with pure Lorentzian simulations.
THURSDAY ORAL SESSION 2
(Th.O.2)
Chairperson: Valery S. Lisitsa
Javier Martin-Torres

Javier Martin-Torres is the Chair Professor in Atmospheric Science at the Luleå University of Technology in Kiruna, Sweden. He graduated in Theoretical Physics and doctorated “Cum Laude” with a thesis on radiative transfer that was the starting point of a long research career throughout which he has developed the topic for its application to different research projects, from atmospheric studies to planetary exploration. In this line, he has developed and validated radiative transfer algorithms for Earth observation missions from space, namely, SABER/TIMED and CLARREO among others, and he is the author of the code FUTBOLIN (FULL Transfer By Optimized LIne by line), which has been adapted to the modelling of the atmosphere of the Earth as well as other planets.

He has worked for Institut für Meteorologie und Klimaforschung and Universität Karlsruhe, Germany; AS&M, Inc. at NASA/Langley Research Center, Hampton, USA; Jet Propulsion Laboratory, Pasadena, USA; Lunar and Planetary Institute, University of Arizona, Tucson, USA; California Institute of Technology (CalTech), Pasadena, USA, and Spanish Research Council, having participated in numerous research projects, both as Co-investigator and as Principal Investigator. He is Fellow at the School of Physics and Astronomy, College of Science and Engineering of the University of Edinburgh. He has received several NASA awards as a member of the MSL team, the NASA Achievement Award as part of the Space Shuttle Columbia Investigation Team, the NASA/Langley Group Achievement award as part of the SABER experiment team, the NASA/Langley Award for “Outstanding contributions to Space Shuttle Columbia Investigation Team”, and the AS&M at NASA/Langley Special Award 2002, 2005, 2006, 2007.

He is author of co-author of more than 80 peer-reviewed papers and several white books of reference within planetary exploration, and has been invited editor of the Journal of Quantitative Spectroscopy and Radiative Transfer.
Importance of line-mixing on planetary atmosphere studies

J Martín-Torres¹,² and T Mendaza¹

¹ Division of Space Technology, Department of Computer Science, Electrical and Space Engineering, Luleå University of Technology, Kiruna, Sweden
² Instituto Andaluz de Ciencias de la Tierra (IACT), Avenida de las Palmeras 4, Armilla (Granada), Spain

Line-mixing occurs when collisions between a radiating molecule and broadening gas leads to a population transfer between the ro-vibrational molecular states and a redistribution of spectral intensity within a band. The intensity of the effect increases with pressure since it is proportional to the broadening gas intensity.

A good knowledge of the spectral lines shapes for the infrared active atmospheric molecules is very important for an accurate radiative transfer modelling, with implications for the retrieval from remotely sensed infrared spectra, and energetic balance studies.

Within the impact approximation, the absorption coefficient taking account of line-mixing depends on the frequency-independent complex Relaxation Matrix introduced by Ben-Reuven in 1966. Its diagonal elements are related to pressure broadening, while non-diagonal elements are related to line mixing.

In this work we:

1. Review the existing line-mixing literature;
2. Present a new generic model to compute: (i) the Line Mixing Relaxation Matrix, which is easily adaptable to any linear molecule using spectroscopic voigt-lines, for any band under non-reactive molecule collisions regimes; and (ii) the dipole moment of every transition and level population of the selected molecule. The model is based on the Energy-Corrected Sudden (ECS) approximation/theory introduced by DePristo (1980) [1], and on previous Relaxation Matrix studies for the interaction between molecular ro-vibrational levels [2], atoms [3], linear molecules [4,5,6]. The model is open source, and it is user-friendly: the user only has to select the wished molecule and vibrational band to perform the calculations. It reads the needed spectroscopic data from the HIgh-resolution TRANsmission molecular absorption (HITRAN) [7] and ExoMol [8].
3. Present examples affecting Earth and planetary atmospheres where the impact of line-mixing effects is non-negligible.

References:

Thibault Delahaye

Dr. Thibault Delahaye is currently working as a Postdoctoral Fellow at LISA laboratory in Paris-Est Créteil University (Paris 12) and CNRS. He received his PhD from Faculty of Physic at Reims University in 2014 with a specialization in theoretical modelisation of molecular spectra and first principles calculation from ab initio surfaces at GSMA laboratory. His research topics include small molecules of atmospherical and planetological interest such as methane or ethylene. Since late 2014 he joined the Franco-German climate mission MERLIN conducted by respective national space research centers (CNES and DLR). More specifically, his work examines the precise modeling of collisional effects involving methane and various perturber (air, H2O) to improve the remote sensing of methane total column from the MERLIN satellite, with the very challenging goal of detecting sources and sinks, which requires to model the absorption with an extremely high (sub-percent) accuracy.
High-resolution spectroscopy for space-based remote sensing missions: example of the MERLIN mission

T Delahaye¹, H Tran¹

¹ Laboratoire Interuniversitaire des Systèmes Atmosphériques, UMR CNRS 7583, Créteil, France

Climate change is one of the greatest challenges presently facing mankind, and methane is one of the most powerful anthropogenic greenhouse gases. For a better understanding of future climate trends, it is necessary to apply precise space-based measurements in order to obtain a global view on the complex processes that control atmospheric methane concentration. In this context, a satellite dedicated to the measurements of atmospheric methane is under joint development by the French and German space research centers (CNES and DLR). The so-called MERLIN mission (Methane Remote Sensing Lidar Mission, 2020) aims at providing global information on atmospheric methane concentration (methane column density) with a relative uncertainty less than 1% and with a spatial resolution of 50 km along the measurement track under cloudy and variable-solar illumination conditions [1,2]. The main data product will be the column-weighted dry-air mixing ratio of CH₄, which will be used to characterize natural (flood zones, notably due to the thawing of permafrost in the Arctic) and anthropogenic (transport and transformation of coal and natural gas, ruminant livestock, etc.) sources of the gas.

Such spectroscopic monitoring of gases in the atmosphere of the Earth requires a precise description of absorption lines shapes that goes beyond the usual Voigt profile (VP). In the case of methane, the differences between the measured profiles and those given by the VP can be very important [3,4], making the VP completely incompatible with the reliable detection of sources and sinks from space. These differences are due to various collisional effects between molecules that are neglected by the VP (line-mixing, Dicke narrowing effect and speed dependence of the collisional broadening and shifting). The consideration of the recently recommended line-shape model, the Hartmann-Tran profile (HTP) [5], along with line-mixing, is then particularly relevant in this context.

This lecture reviews our latest results on the modeling of methane lines broadened by air in the 1.64 µm region and the associated spectroscopic parameters, taking into account the latter collisional effects and their temperature dependence. These results were obtained by simultaneously fitting the model parameters to high sensitivity and high-resolution cavity ring-down spectroscopy (CRDS) spectra recorded at the National Institute of Standards and Technology (NIST) and high-resolution tunable diode laser spectra recorded at the Groupe de Spectroscopie Moléculaire et Atmosphérique (GSMA, Reims), over a wide pressure and temperature range. The influence of collisions involving water vapor will also be discussed. The use of these spectroscopic data and the associated model to calculate the spectrum absorption coefficient to analyze ground-based atmospheric TCCON will finally be presented.

References:

Diffuse interstellar bands - the oldest standing unsolved problem in all of spectroscopy

J Krełowski

Centre for Astronomy, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziadzka 5, 87-100 Torun, Poland

The story of diffuse interstellar bands (DIBs) started in 1922 when Mary Lea Heger discovered the first two such features, centered near 5780 and 5797 Å, using then modern panchromatic emulsion. Since that time the list of known DIBs expanded to nearly 500 entries but their carriers remain as puzzling as they were at the beginning. Such a big set of spectral features cannot be carried by a single species; moreover their strength ratios are heavily variable. This is why it is now commonly believed that DIBs are carried by relatively complex molecular species present practically everywhere in the interstellar clouds. However, none of these hypothetical molecules was identified until now. Among the proposed species popular ones are chain molecules based on carbon skeleton, polycyclic aromatic hydrocarbons and, possibly, fuleranes. The talk gives a short description of basic observational facts and their comparison with laboratory spectra of suspect molecules.
FRIDAY ORAL SESSION 1
(Fr.O.1)
Chairperson: John C. Lewis
Joël Rosato

Joël Rosato is working in the field of plasma spectroscopy, with a special emphasis on applications to magnetic fusion plasmas. After obtaining his PhD in Marseille, France, in 2007, he has got a postdoctoral researcher position at the Jülich Research Center, in Germany, where he contributed to the development of a spectroscopic database for the magnetic fusion community. Joël is now associate professor in France at Aix-Marseille University. He is in charge of a 2nd year master degree training in the field of spectroscopy and radiation physics. He continues to work on spectral line shape modeling in collaboration with the magnetic fusion community, including ITER and other European research institutes. His research fields of interest include atomic physics with Stark and Zeeman effects, radiation transport, and plasma turbulence.
Line shapes in the presence of nonlinear wave collapse in a plasma

J Rosato¹, Y Marandet¹, R Stamm¹

¹ PIIM, UMR 7345 Aix-Marseille Université / CNRS, Centre de St-Jérôme Case 232, F-13397 Marseille Cedex 20, France

The ITER tokamak (www.iter.org) under construction in France will be equipped with an extensive set of diagnostics. As in current machines, passive spectroscopy will be used. In this talk, a review of modeling techniques is presented with a special emphasis on the description of hydrogen line shapes. Specific issues relevant to magnetic fusion plasmas (e.g. turbulence) are also examined.
Christian Parigger

The research interests of Dr. Christian Parigger include fundamental and applied spectroscopy, nonlinear optics, quantum optics, ultrafast phenomena, ultrasensitive diagnostics, lasers, combustion and plasma Physics, optical diagnostics, biomedical applications, and in general, atomic and molecular and optical (AMO) Physics. His Mag. rer. nat. degree shows work on optical bistability at the University of Innsbruck, Austria, with guidance by Dr. Peter Zoller. The PhD degree studies are on the subject of polarization spectroscopy and magnetically induced switching at the University of Otago, Dunedin, New Zealand, with guidance by Drs. Wes Sandle and Rob Ballagh. He also holds the Dr. rer. nat. degree in Physics from the University of Innsbruck, Austria. Since 1987, his work encompasses experimental, theoretical and computational research together with teaching, service, and outreach at the Center for Laser Applications at The University of Tennessee Space Institute, Tullahoma, Tennessee, USA.
Self-absorption effects on line shapes in laser-induced plasma

C G Parigger¹, D M Surmick¹, G Gautam¹

¹University of Tennessee Space Institute, 411 B.H. Goethert Parkway, Tullahoma, TN 37388, USA

Laser-induced breakdown spectroscopy facilitates the characterization of laboratory scale micro-plasma. This plasma is generated for a variety of applications to include determination of elemental composition in laser ablation experiments or investigation of physics processes associated with optical breakdown. During early expansion, atomic lines dominate the spectroscopic signatures although molecular bands occur frequently when femtosecond laser radiation is used. In this work, self-absorption and/or line-reversal is of interest [1-4]. In the experiments, 13 ns, 190 mJ, Q-switched Nd:YAG radiation is focused to create micro-plasma in standard ambient temperature and pressure (SATP) air [5, 6], in ultra-high-pure (UHP) hydrogen gas contained in a cell [7, 8], and at or near an ice surface [9, 10]. Figure 1 illustrates time-resolved spectroscopy results using 10 ns gate widths to record spatially-resolved spectral snapshots of the plasma kernels at a time delay, τ, of 400 ns and 150 ns for SATP air and UHP hydrogen, respectively. Abel inversion is utilized to explore the nearly radially symmetric plasma. A slight asymmetry is caused by the nature of focusing radiation to obtain plasma. The spatial and temporal variations of the plasma kernel however can be influenced by the specific irradiance distribution of the laser pulses.

Figure 1. (a) SATP air, τ = 400 ns, Hα: Nₑ = 2 × 10¹⁷ cm⁻³. (b) Nₑ after Abel inversion. (c) UHP hydrogen, 1.08 × 10⁵ Pa (810 Torr), τ = 150 ns, Hα: Nₑ = 8.4 × 10¹⁷ cm⁻³. (d) Nₑ from Hα and Hβ lines.

The Hα line shapes indicate distortions, contributions to line-widths primarily due to Stark broadening, spectroscopic red shifts, and evidence of self-absorption. In view of the error bars associated with analyses of Hα and Hβ lines, self-absorption of the Hα line can affect determination of electron density, Nₑ. This is supported by experiments in air from comparisons with N⁺ lines, and in hydrogen gas from comparisons of the results obtained after Abel inversion of line-of-sight Hα and Hβ line profiles.

References:
Stagnation Layers in Annular Laser Produced Plasmas

B Delaney¹, T J Kelly¹, E T Kennedy¹ and J T Costello¹

¹ School of Physical Sciences and National Centre for Plasma Science and Technology, Dublin City University, Glasnevin, Dublin 9, Ireland

When two laser plasmas are formed adjacent to each other, in an ambient pressure of less than $10^{-3}$ mbar, the plasmas will expand not normal to the target but also laterally. The plasmas will decelerate at the collision plane, with their kinetic energy being converted into excitation energy, forming what is known as a stagnation layer while the two initial plasmas are known as ‘seed plasmas’ [1].

Current interest in stagnation layers comes from the ability to manipulate their physical characteristics; density, temperature, shape, etc. by varying target geometry or laser-target interaction characteristics [2]. The traditional set up for generating stagnation layers involves using a wedge prism to split a laser beam into two parts; these beams are then focused onto the target with a lens. This system while useful for quickly and easily generating stagnation layers does have some drawbacks, principally the inherent asymmetry of the set up. When the upper half of the laser beam is passed over the wedge prism the lower half passes through the prism and is deflected downwards. The deflected beam gives rise to a focal spot with a somewhat elliptical footprint and consequently a seed plasma with potentially different characteristics than the one formed by the undeflected portion of the laser beam. Hence the resulting stagnation layer which can also become asymmetrical.

To generate a symmetrical stagnation layer the wedge prism in the above set up was replaced with an axicon which can be either a plano-conical lens or a rotationally symmetric prism [3]. A Gaussian laser beam, passed through an axicon, is first transformed into a Bessel-Gauss beam, while beyond the depth of field of the axicon, it diverges to form an annular beam profile. This annular beam is then focused onto a target to produce an annular plasma, an example of an annular plasma is shown in figure 1.

![Figure 1. Time resolved broadband emission imaging of a copper plasma with a 5ns exposure time taken 5ns after plasma formation with a viewing angle of (a) 0° and (b) 90°.](image)

Time-resolved broadband emission imaging has been employed to investigate the evolution of an annular laser produced plasma. To date it has been shown that a stagnation layer forms at the centre of an annular copper plasma formed at an ambient pressure below $1x10^{-3}$ mbar. Stagnation layers formed with an axicon or a wedge prism on an aluminium target will be compared in terms of expansion dynamics, electron temperature and electron density measurements. Expansion dynamics will be monitored using both broadband and filtered time resolved imaging while electron temperatures and densities will be extracted from time resolved spectroscopic measurements of selected emission line intensities and profiles. The results of these comparisons will be presented at the conference.

References:

FRIDAY ORAL SESSION 2
(Fr.O.2)
Chairperson: Christian Parigger
Interatomic potentials of 12-group van der Waals dimers: Probing discrepancies between theory and experiment

T Urbańczyk1, M Krośnicki2, M Strojecki3, A Pashov4, A Kędziorcki5, J Koperski1

1 Smoluchowski Institute of Physics, Jagiellonian University, prof. S. Łojasiewicza 11, 30-348 Kraków, Poland
2 Institute of Theoretical Physics and Astrophysics, University of Gdaňsk, Wita Stwosza 57, 80-952 Gdaňsk, Poland
3 Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Niezapominajek 8, 30-239 Kraków, Poland
4 Department of Physics, Sofia University, 5 James Bourchier Boulevard, 1164 Sofia, Bulgaria
5 Institute of Physics, Nicolaus Copernicus University, Grudziądzka 5/7, 87-100 Toruń, Poland

Results of new all-electron \textit{ab initio} calculations and revisit of experimental studies of the interatomic potentials of lower-lying \textit{ungerade} excited and ground electronic energy states of the Hg$_2$ and Cd$_2$ van der Waals complexes are used as probes of discrepancies between theory and experiment. From simulations of the previously and presently measured LIF excitation and dispersed emission spectra new analytical representations of the excited- and the ground-state interatomic potentials are proposed. An inverted perturbation approach was also used to improve the studied interatomic potentials. The comparison of the new \textit{ab-initio} calculated potentials with the results of the analyses illustrates an improve theory-to-experiment agreement for such a demanding system like Hg$_2$ or Cd$_2$.

![Figure 1](image)

**Figure 1.** (a) LIF excitation spectrum recorded previously [1] using the A$^1\Omega_u^+ (6^{1}P_1) \leftrightarrow X^1\Omega_u^+$ transition in Cd$_2$. (b) Simulation [2,3] performed assuming for the A$^1\Omega_u^+$- and X$^1\Omega_u^+$-state representations a Morse and L-J($n$−6)-Morse functions, respectively. Vicinity of the $\nu'=36-38$ is shown in inset.

Support by the National Science Centre Poland: UMO-2015/17/B/ST4/04016 is acknowledged.

References:

[3] Western C M, PGOPHER 8.0, University of Bristol
Effects of plasma microfield rotation in Stark broadening

E Stambulchik¹ and A V Demura²

¹ Faculty of Physics, Weizmann Institute of Science, Rehovot 7610001, Israel
² National Research Centre “Kurchatov Institute”, Kurchatov Square 1, Moscow 123182, Russia

Lineshapes of atomic radiative transitions broadened by plasma is a complex problem lacking a general analytic solution. Indeed, several models have been suggested to treat it, but paradoxically, calculating the spectral line broadening even of the simplest—Lyman-alpha—transition in plasma results in a significant spread between results of different models. Here, we argue that for the hydrogen spectral lines with the central Stark components, the quasistatic broadening regime is never realized for the line core in a one-component plasma (OCP). Instead, the broadening due to either electrons or ions alone evolves from the impact regime to another regime, also dynamical in nature. In the latter (referred to here as “rotational” broadening), the line width only depends on the typical frequency of the plasma microfields and is independent of both the microfield magnitudes and the atomic properties of the transition. We also demonstrate that the rotational broadening is asymptotically reached in the high-density/low-temperature limit by other transitions with an unshifted central component, such as the Balmer-alpha line. A simple expression is suggested interpolating between the two asymptotic regimes, applicable to broadening due to electrons and ions alike. The treatment is further extended to realistic two-component plasmas. Comparison to results of accurate computer simulations shows a good agreement over a very large range of plasma parameters, both for the case of one- and two-component plasmas [1].

Figure 1. Lyman-alpha FWHM versus \( Z_p \) in an OCP, assuming \( N_p = 10^{17} \text{ cm}^{-3} \) and \( T_p = 1 \text{ eV} \)

The obtained results are illustrated in Figure 1 by OCP computer simulations [2] of the Lyman-alpha FWHM as a function of the charge \( Z_p \) of the proton-mass perturbing particles, with the density \( N_p = 10^{17} \text{ cm}^{-3} \) and temperature \( T_p = 1 \text{ eV} \) being fixed. It is seen that starting from some critical values of the perturber charge, the FWHM does not depend on \( Z_p \) and becomes constant, approximately equal to \( v_p N_p^{1/3} \) (\( v_p \) is the thermal perturber velocity defined with the reduced mass of the perturber-radiator pair), that demonstrates one of the essentialities of the rotational regime of Stark broadening [1].

References:

On the Stark broadening of Cr VI spectral lines in astrophysical plasma

M S Dimitrijević1, Z Simić1, S Sahal-Bréchot2

1 Astronomical observatory, Volgina 7, 11060 Belgrade, Serbia
1 LERMA, Observatoire de Paris, PSL Research University, CNRS, Sorbonne Universities, UPMC Univ. Paris 06, France

Rauch et al. [1] have found Cr V, Cr VI and Cr VII lines in the spectrum of LS V +46°21 white dwarf, which is the central star of planetary nebula Sh 2-216. High-resolution, high-signal to noise ratio ultraviolet spectra obtained by FUSE (Far Ultraviolet Spectroscopic Explorer) and HST/STIS (Space Telescope Imaging Spectrograph aboard the Hubble Space Telescope) have been used. Rauch et al. [1] stated that: „Theoretical should provide data which covers the astrophysical relevant temperature and density space. Better atomic and line-broadening data will then strongly improve future spectral analyses and thus, make determinations of photospheric properties more reliable.”

Since the Stark broadening is usually the most important line/broadening mechanism in white dwarf atmospheres (see e.g. [2]), in this work we will present results of semiclassical perturbation [3,4] calculations of Stark broadening parameters of Cr VI spectral lines, due to collisions with electrons, protons and doubly charged helium ions, the main perturbers in white dwarfs. Calculation are performed in function of perturber density and temperature, for plasma conditions of interest for white dwarfs.

Obtained results are used to demonstrate the importance of Stark broadening of Cr VI lines for analysis and synthesis of spectra of white dwarfs, using a theoretical model of DB white dwarf atmosphere and comparing Stark and Doppler widths in function of optical depth. It is demonstrated that for majority of relevant plasma conditions Stark broadening is dominant in comparison with Doppler broadening.

The obtained Stark broadening parameters of spectral lines, broadened by electron-, proton-, and He III-impacts with Cr VI emitter / absorber will be also implemented in the STARK-B database (http://stark-b.observ.fr – [5]), a part of Virtual Atomic and Molecular Data Center (VAMDC - http://www.vamdc.org – [6]).

References:

TUESDAY POSTER SESSION
(Tu.P)
Analysis of The collision-induced A absorption spectra of H$_2$- H$_2$ complexes in the second overtone band of H$_2$ at temperature 77 and 298 K

M Abu-KHarma

1 Department of Physics and Basic Sciences, Al-Balqa Applied University, P.O. Box 15008, Amman 11134, Jordan

The second overtone band ($\delta v = 3$ 0) of H$_2$-H$_2$ spectra at different temperatures were analyzed using the Birnbaum-Cohen (BC) line shape function for the quadrupolar transitions and the Levine-Birnbaum (LB) line shape function for the overlap transitions. The observed spectra were modeled with synthetic profiles which are composed of the superposition of an overlap-induced and a quadrupolar-induced profile. Satisfactory agreement of the measurements with the synthetic profiles is observed.

References:

H-like ions with penetrating collisions

S Alexiou

1 University of Crete, TETY, 71409 Heraklion, TK 2208, Greece

In impact calculations one needs to evaluate the collisional term:

\[ \{ 1 - S_a S_b^\dagger \} = Q_a I_b + Q_b I_a + Q_{ab} \]  

with

\[ \langle n_a lm | Q_a | n_a l' m' \rangle = \frac{2}{\omega_{n_0}^2} I(n_a, l, n_a, l') \]  

\[ \langle n_a lm | n_a l'' m'' \rangle \cdot \langle n_a l'' m'' | r | n_a l' m' \rangle, \]  

\[ I(n, l, l', n') = \frac{1}{2} \int_{-\infty}^{\infty} du C_1 (R(t); n, l, l', n') \frac{\epsilon (\epsilon - \cosh u)}{(\cosh \epsilon - 1)^2} \]  

and \( C_1 \) is given by[1]:

\[ C_1 = 1 - e^{-a R(t)} P_{2n+1} (a R(t)) \]  

with \( P(x) \) a polynomial, \( a R(t) = \xi (\cosh u - 1) \) and \( \xi = \frac{2 Z_s n_0}{n_0} = Z (Z - 1) e^2 \), \( Z \) the spectroscopic charge number, \( n \) the principal quantum number of the upper or lower level and \( n_0 \) the Bohr radius. I essentially includes the atomic collision physics, while the eccentricity \( \epsilon \) and velocity integrations represent the plasma parameter phase space average. We recover the standard behavior \( I = 1 \) if \( C_1 = 1 \), i.e. in the case of no penetration.

The effect of penetration is expected to soften the interaction and hence result in a reduction of broadening compared to not taking this effect into account. However this is not always the case. As illustrated in [1], the relevant collisional integral involves both positive (small \( u \)) and negative (large \( u \)) contributions. Without penetration, the positive contributions win and the result is a value of 1. With penetration, the small \( u \) contributions are damped and the negative contributions may win, resulting in possibly large negative values. This is illustrated in Fig.[1].

![Figure 1](image_url)

Figure 1. The integrand of \( I \) with and without penetration for small \( \epsilon = 1.00001 \) and large \( \xi \).

I can be expressed in terms of the modified Bessel functions \( K_0 \) and \( K_1 \). However, this is numerically very inaccurate and instead a robust method was devised that employs a recursion relation and asymptotics for a related function

\[ N_k = \int_0^\infty du (\cosh u - 1)^k e^{\xi (1 - \cosh u)} \]  

References:

Blue line wings of resonance lines of potassium and sodium perturbed by molecular hydrogen and rare gases

J F Kielkopf¹, N F Allard ², V A Alekseev⁴, F Spiegelman⁵ and G Guillon⁶

We report on work now in progress that compares unified line shape calculations based on a priori potentials with experiments to determine the wings of the sodium and potassium resonance lines broadened by H₂, He, and other rare gases. The spectra of ultra-cool brown dwarf stars, such as the type T ϵ Indi Bab, and inflated hot Jupiter type exoplanets such as HD209458b, show absorption due to neutral Na and K. The strength and shape of these resonance lines is diagnostic of atmospheric conditions, chemistry, and history. In the coolest and densest of such atmospheres, radiative transfer in the visible and near-IR spectrum may be dominated by far wings of the lines broadened by neutral H₂ and He. Similarly, DZ class white dwarfs are low temperature Earth-sized degenerate stars of solar mass lacking atomic H lines but showing heavier elements. Detected through recent observations with the Spitzer and Hubble Space Telescopes, these surprising key spectral signatures are attributed to accreted material and have informed us about the star’s planetary environment. As a consequence, in these astrophysical cases, accurate pressure broadened profiles that are valid at high densities of H₂ and He should be incorporated into spectral models. The theory of spectral line shapes, especially the unified approach we have developed [1], makes possible accurate models of stellar spectra that account both for the centers of spectral lines and their extreme wings in one consistent treatment. This approach to calculating the spectral line profile requires the knowledge of molecular potentials with high accuracy because the shape and strength of the line profile are very sensitive to the details of the molecular potential curves describing the Na/K – H₂/He collisions. Under some circumstances it is possible to test the line shape theories in the laboratory, if not under conditions exactly the same as those in stars, at least under closely similar conditions. A comparison of laboratory experimental data with theoretical profiles establishes the accuracy of the interaction potentials, which remain difficult to compute a priori precisely in most cases.

The laboratory spectra of both Na and K alkalis with H₂, He, and other rare gases are shown in our work to exhibit a systematic pattern of satellites in the blue wing. Xe and Kr produce the strongest satellites closest to the parent line, as expected from the longer range interactions for these highly polarizable noble gases. By contrast, H₂ and He produce satellites farthest from the line. We compare the line satellite positions for H₂, He and other rare gases in order to assess the accuracy of the potentials and ultimately to guide refinement of their computation. The general properties of the full line profiles predicted by the unified line shape theory are confirmed by these comparisons, even where the specifics of the satellite positions set by the details of the potentials may differ between theory and experiment. Very recently we have shown that the laboratory results also confirm the theory identifying a brown dwarf spectral feature as due to K-H₂ [2]. Because the K₂ molecular spectrum overlaps the atomic line wing of interest, it is necessary to remove that contribution for laboratory measurements made under conditions favoring dimer formation. In that analysis we rely on using the far wing of K broadened by Kr as a reference, because with it the dimer contribution can be measured and removed from the experimental absorption coefficient for other gases. The observations and theory reported here add to our understanding of the spectra of the far wings of the alkali resonance lines where in some cases the radiation can only be correctly modeled by a comprehensive spectral line broadening theory.

References:

Measurement of oxygen B-band line center frequency in reference to strontium atomic clock

K Bielska¹, Sz Wójtewicz¹, P Morzyński¹, P Ablewski¹, A Cygan¹, M Bober¹, M Zawada¹, R Ciuryło¹, P Masłowski¹, D Lisak¹

¹ Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Grudziądzka 5, 87-100 Toruń, Poland

We determined unperturbed frequency of the P7P7 transition in the oxygen B-band with respect to the strontium optical atomic clock. The use of the clock laser stabilized to atomic transition as optical frequency reference enabled us to avoid systematic errors occurring in previous measurements and associated with inaccuracy of frequency standard, whereas long term averaging of spectra reduced random errors. Preliminary data analysis indicates that the uncertainty of unperturbed transition frequency is below 30 kHz.

In order to achieve such accuracy and precision, we recorded spectra with the frequency stabilized, Pound-Drever-Hall locked cavity ring-down spectrometer (PDH-locked FS-CRDS), see details in [1] and references therein. The $^{88}\text{Sr} \ ^{1}\text{S}_0-^{3}\text{P}_0$ clock transition served as a frequency reference [2,3]. The link between them was made with Er:fibre optical frequency comb (OFC). The OFC was frequency shifted to 1390 nm range and doubled. Two heterodyne beat-note signals were simultaneously measured at each point of spectra: the first one between the spectrometer’s probe laser and the OFC, and the other one between the OFC and the strontium clock laser. All frequency counters and signal generators were referenced to the same, stable 10 MHz signal from the hydrogen maser [4] transferred from Borowiec near Poznań to our Institute by 330 km fibre link [3,5]. Such procedure enabled us to refer frequency corresponding to each point on the spectrum to the frequency of the clock transition. This is a proof-of-principle experiment which demonstrates application of optical atomic clock in the molecular spectroscopy.

References:

Comparison IR spectra of alanine CH₃CH(NH₂)COOH and alanine CD₃CH(NH₂)COOH

Sz Brym¹

¹ University of Warmia and Mazury, Faculty of Mathematics and Computer Science, Słoneczna 54 street, 10-710 Olsztyn, Poland

Alanine is the optically active amino acid. Comparison of spectra by ATR FTIR technique was obtained. For comparison the fingerprint region i.e. below 1500cm⁻¹ was chosen. After replacement of hydrogen to deuterium in side chain in FTIR spectrum frequency shift of most of the bands to lower values was observed. Because the vibrations are complex, the frequency ratio of comparative bands did not exceed 1,1. The spectrum of alanine in this field consists of separate single bands. After deuteration complex and double bands of diverse intensity were observed. The profiles of these bands were examined.

References:

Cavity enhanced complex refractive index spectroscopy

A Cygan1, Sz Wójtewicz1, P Wcisło1, M Zaborowski1, G Kowzan1, J T Hodges2, R Guo3, J Nawrocki4, P Krehlik5, Ł Śliwczyński5 M Lipiński5, P Masłowski1, R Ciuryło1 and D Lisak1

1 Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Grudziądzka 5, 87-100 Toruń, Poland
2 PRIMALAB, Faculty of Sciences, University of Batna, Batna, Algeria
3 Division of Energy and Environmental Measurement, National Institute of Metrology, Beijing, China, 100013
4 Time and Frequency Department, Astrogeodynamic Observatory of Space Research Center, Borowiec, Drapałka 4, 62-035 Kórnik, Poland
5 Department of Electronics, AGH University of Science and Technology, al. Mickiewicza 30, 30-059, Kraków, Poland

The resonance feature related to atomic and molecular transitions can be observed in absorption as well as in dispersion. The frequency-stabilized cavity ring-down spectroscopy (FS-CRDS) [1] is currently recognized as one of the most accurate absorptive tools for high-resolution measurements of weak molecular spectra which can provide reference spectroscopic data at the sub-percent level of uncertainty. On the other hand, achieving 0.1% agreement between line intensities determined independently in different laboratories is very challenging. Apart from determination of sample physical conditions, the accuracy of the most often used absorptive intensity-based spectroscopic techniques is limited by the linearity and repeatability of the detection system.

Recently we developed two cavity enhanced spectroscopy techniques called cavity mode-width spectroscopy (CMWS) [2-4] and one-dimensional cavity mode-dispersion spectroscopy (1D-CMDS) [5]. They are based on frequency measurement of absorptive broadening and dispersive shift of resonance modes of the high-finesse optical cavity, respectively, and their main feature is negligible susceptibility to systematic instrumental errors of the detection system. Moreover, the 1D-CMDS method is the only one that provides one-dimensional spectra by measurement of only one physical quantity - frequency. Such a light intensity-independent method, with accuracy warranted by the best frequency standards, can be considered as a tool of the future in the field of high-accuracy line shape study as well as a reference for testing the accuracy of other spectroscopic techniques.

A unique experimental setup enabling the simultaneous measurement of the spectra by three cavity enhanced techniques: FS-CRDS, CMWS and 1D-CMDS will be presented. The accuracy of the FS-CRDS method was tested for the first time by comparison to the reference 1D-CMDS method [6]. A complex-fit line shape analysis was used for simultaneously recorded absorptive (FS-CRDS) and dispersive (1D-CMDS) spectra. Limitations of FS-CRDS will be indicated. Moreover, absolute frequencies of unperturbed $^{12}$C$^{16}$O transitions from the near-infrared (3-0) band measured with uncertainties five-fold lower than previously available data will be presented [7]. The frequency axis of spectra was linked to the primary frequency standard. Three techniques (FS-CRDS, CMWS, 1D-CMDS) and various approaches to data analysis were used to estimate potential systematic instrumental errors. Absorptive and dispersive line shapes with quality of the fit higher than 10000:1 are demonstrated [7].

References:

Bound-free transitions in quasi-molecules: $\text{H}^+\text{H}^-\hbar\omega$ collisions

A Dadonova$^2$, A Devdariani$^{1,2}$, E Dalimier$^3$, P Angelo$^3$

1. St. Petersburg State University, Peterhof, Ul’janovskaja St. 3, 198504, St. Petersburg, Russia
2. The Herzen State Pedagogical University of Russia, nab. reki Moiki, 48, 191186, St. Petersburg, Russia
3. LULI - UPMC Univ Paris 06 : Sorbonne Universités ; CNRS, Ecole Polytechnique, CEA :
   Université Paris-Saclay - F-75252 Paris cedex 05, France

The study of radiative transitions in collisional quasi-molecules, that is temporary molecules formed during atom or ion collisions, is one of the traditional areas in plasma spectroscopy. Until recently the study has mainly been limited to bound-bound transitions between quasi-molecular states. In particular, the spectral profiles produced by the reaction of charge exchange $\text{H} + \text{H}^- \rightarrow \text{H}^- + \text{H} + \hbar\omega$ was regarded in [1] as an example of asymptotically forbidden transition in quasi-molecules. The aim of the present work is to highlight the case of the bound-free transitions in quasi-molecules having in mind the recent progress in the study of the photo-effect in atoms and stable molecules, e.g. [2]. The specific reaction $\text{H} + \text{H}^- + \hbar\omega \rightarrow \text{H} + \text{H} + e$ has been taken into account as a typical example of quasi-molecular photo-detachment or photo-ionization processes.

The main characteristics of the photo-detachment are dipole moments for transitions from bound gerade and ungerade states to proper electronic continua $X_{bc}$. They have been calculated within the frame of the zero range potential model [3] that is well adopted to the description of the processes with negative ions. The results for $X_{bc}^2$, which is proportional to the detachment cross-section of the electron from the ungerade state, is shown in Fig.1 in atomic units for two photon energies verses the free electron momentum $k$.

![Figure 1. Square value of the dipole moment depending on k](image)

The ungerade energy term is repulsive and then the collision results in a lowering of the threshold of the electron detachment when compared to that one, $a_0^2/2$, for a single ion. Roots of $X_{bc}^2$ are the result of the sign change of the matrix elements in the transition from mainly detachment in a single ion case to that one in a molecule.

References:
Radiative transitions in quasi-molecules Hg(6^3P_1 – 6^1S_0)+Xe.
The influence of buffer gas atom density on spectral line shape

A Z Devdariani$^{1,2}$, N A Kryukov$^1$, M G Lednev$^3$, A L Zagrebin$^3$

$^1$St. Petersburg State University, Peterhof, Ul’janovskaja St. 3, 198504, St.Petersburg, Russia
$^2$The Herzen State Pedagogical University of Russia, nab. reki Moiki, 48, 191186, St.Petersburg, Russia
$^3$Baltic State Technical University «VOENMEH», Krasnoarmeiskaya St. 1, 190005, St.Petersburg, Russia

The present work is aimed at the explanation of discrepancies in emission spectral profiles obtained in Ref.[1-3] for the excimer band HgXe(A^3O+) – HgXe(X^1O+) at $T \approx 300 K$ and presented in Fig.1, dotted lines 1-4.

![Figure 1. Emission spectral profiles depending on wave length](image)

We suggest that the discrepancies are mainly caused by the recombination and relaxation processes leading to the population ro-vibrational states of the HgXe(A^3O+) excimer. Our suggestion has been backing up by the calculations of the profiles in two limiting cases for the high density and low density of buffer gas atoms, full curves 5,6 and dashed curve 7 correspondingly on Fig.1. The calculations for the of high densities were performed in the frame of quasi-static approach. The calculations for the case of low densities followed the approach proposed in [6]. In both cases potential energy curves determined in [4,5] were used. The comparison leads to the preliminary conclusion that the experimental data obtained in [1-3] can be attributed to the case of intermediate densities.

References:

Quasimolecular emission near the Xe (5p<sup>5</sup>6s<sup>1,3P<sub>1</sub></sup> – 5p<sup>6</sup> 1S<sub>-</sub>) and Kr (4p<sup>5</sup>5s<sup>1,3P<sub>1</sub></sup> – 4p<sup>6</sup> 1S<sub>0</sub>) resonance lines induced by collisions with He atoms

O S Alekseeva<sup>1</sup>, A Z Devdariani<sup>2,3</sup>, M G Lednev<sup>1</sup>, A L Zagrebin<sup>1</sup>

<sup>1</sup>Baltic State Technical University, Krasnoarmeiskaya St. 1, 190005, St. Petersburg, Russia
<sup>2</sup>St. Petersburg State University, Peterhof, Ul'janovskaja St. 3, 198504, St. Petersburg, Russia
<sup>3</sup>The Herzen State Pedagogical University of Russia, nab. reki Moiki, 48, 191186, St. Petersburg, Russia

This study is devoted to the theoretical investigation of the quasimolecular emission of Xe*-He and Kr*-He collision pairs near the Xe (5p<sup>5</sup>6s<sup>1,3P<sub>1</sub></sup> – 5p<sup>6</sup> 1S<sub>-</sub>) and Kr (4p<sup>5</sup>5s<sup>1,3P<sub>1</sub></sup> – 4p<sup>6</sup> 1S<sub>0</sub>) resonance atomic lines. With the use of the pseudopotential method and the effective Hamiltonian method in the formulation [1] the interaction potential curves of the quasimolecules Xe (5p<sup>5</sup>6s) + He and Kr (4p<sup>5</sup>5s) + He were calculated. For the ground states the interaction potential curves determined in [2] have been used.

Based on these potential curves the processes of quasimolecular emission of Xe*+He and Kr*+He mixtures have been considered and the spectral distributions I(\hbar\Delta\omega, \text{cm}^{-5}) of photons emitted have been obtained in the framework of quasistatic approximation [3]. The calculated emission spectra \text{lg}(I/I_0), where I_0 = 10^{-35} \text{cm}^2, for T = 300 K are presented on Figure 1.

Figure 1. The emission spectra of the Xe* + He and Kr* + He collision pairs near the resonance atomic lines for T = 300 K

References:

Speed-dependent Voigt profile parameters for oxygen B-band measured by cavity ring-down spectrometer referenced to the optical frequency comb.

J Domysławska¹, Sz Wójtewicz¹, P Masłowski¹, A Cygan¹, K Bielska¹, R S Trawiński¹, R Ciuryło¹, D Lisak¹

¹Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Grudziądzka 5, 87-100 Toruń, Poland

We present a line-shape parameters data set including the absolute positions, line intensities, pressure broadening and other line-shape parameters for the weak oxygen B-band spectral lines arising from $b^1\Sigma_g^+ - X^3\Sigma_g^-(1 \leftarrow 0)$ transitions. Self-broadened oxygen spectrum was measured at low pressure range by the Pound-Drever-Hall-locked frequency-stabilized cavity ring-down spectrometer (PDH-locked FS-CRDS). The CRD spectrometer was linked to the optical frequency comb (OFC) to ensure the absolute frequency measurement at every point of measured spectrum. The experimental data were analyzed by means of the multispectrum fitting technique which reduces the numerical correlations between fitted line-shape parameters. Data were analyzed using several line profiles. Line intensities, pressure width and shift coefficients and the speed-dependent parameters are determined with subpercent accuracy. The absolute transitions frequencies are determined with accuracy reaching 150 kHz. We compare results for different profiles with the data available in the literature and HITRAN database.

The speed-dependent Voigt profile was chosen for the consistent line-shape parameters data set presentation. The results already published [1-4] are accompanied by unpublished data. Our results show that for the high signal-to-noise ratio laboratory data the Voigt profile is not sufficient to provide the satisfactory description of measured spectra. The use of the VP leads to systematic errors, even several percent, in the line intensities determination as well as collisional broadening and other coefficients. We show also that tests of more advanced profiles including Dicke narrowing and speed-dependent effects are not conclusive for stronger lines of the B band due to limitations of cavity ring-down spectrometer regarding the accessible pressure range for self broadened transitions.

References:

Benchmark comparison of quantum and classical molecular dynamics calculations of collision-induced absorption

W Fakhardji¹, M Gustafsson ¹

¹ Luleå tekniska universitet

Collision-induced absorption (CIA) occurs when two interacting molecules acquire a dipole moment. In a such case, the system can absorb an incoming photon in the infrared region of the electromagnetic spectrum. Therefore, even a gas made of non polar molecule such as CH₄ – N₂ can play a role in absorption, especially in a stellar or planetary atmosphere. Indeed, the description of this process and the computation of the absorption coefficient have an importance in the modelling of the planetary atmospheres containing such molecules.

Due to their difficulties experimental measurements have been done only for a few temperatures for each molecular system. This technical limitation bring us to use numerical methods to compute absorption coefficients over a large range of temperatures.

For gas mixtures composed by low mass molecules, quantum mechanical computations are feasible in order to obtain a collision-induced spectrum. However, for a higher mass molecular system, like the CH₄ – N₂ pair, quantum modelling is forbiddingly cpu-intensive. In this context, a classical approach [1] of the problem is more suitable.

Since for atomic systems quantum and classical computations are both possible, we can pursue both methods for the Ar-Xe pair. Moreover, the Ar-Xe potential has a depth of about 189K [2] which is comparable to that of CH₄ – N₂ [3]. Therefore, the argon-xenon system is a perfect test case for the classical method. This study has the purpose to estimate the relevance of the classical method in a such case.

References:

Modified Complex Robert-Bonamy (MCRB) calculations of H$_2$O transitions broadened by H$_2$ for applications to planetary and exoplanet atmospheres

R R Gamache$^1$ and C L Renaud$^1$

$^1$ Department of Environmental, Earth, and Atmospheric Sciences, University of Massachusetts Lowell, Lowell, MA, USA

Line shape parameters for hydrogen broadening of water vapor are needed to understand remote sensing measurements of planetary and exoplanet atmospheres. In order to address these needs, semiclassical calculations based on the Modified Complex Robert-Bonamy (MCRB) formalism were made. The intermolecular potential for the calculation is comprised of electrostatic, atom-atom (expanded to order 16 and rank 4), induction, and London dispersion terms. The trajectories were determined by numerical integration of the Hamilton’s equations. The average over the Maxwell–Boltzmann distribution of velocities was performed by integration over 35 velocities corresponding to the temperature range 75K – 27000K. The formalism is complex valued yielding the half-width and line shift from a single calculation. The calculations are reported at 7 temperatures from 200 to 700 K. The half-width temperature dependence coefficient $n$ was determined using the relation $\gamma(T) = \gamma(T_0)[T_0/T]^n$ with $T_0=296$K. The calculations are compared with a database of measured H$_2$O-H$_2$ line shape parameters. The rotational, vibrational, and temperature structure are discussed.
A comparison of measured and modified complex Robert-Bonamy (MCRB) calculations of line shape parameters for ν₁, ν₂, and ν₃ transitions of HDO broadened by CO₂

R R Gamache¹, C L Renaud¹, V Malathy Devi², D Chris Benner², K Sung³, T J Crawford³, A W Mantz⁴, M A H Smith⁵, G L Villanueva⁶

1 Department of Environmental, Earth, and Atmospheric Sciences, University of Massachusetts Lowell, Lowell, MA, USA
2 Department of Physics, College of William and Mary, Williamsburg, VA, USA
3 Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, USA
4 Department of Physics, Astronomy and Geophysics, Connecticut College, New London, CT, USA
5 Science Directorate, NASA Langley Research Center, Hampton, VA, USA
6 Astrochemistry, NASA Goddard Space Flight Center, Greenbelt, MD, USA

Precise data including line shape parameters and their temperature dependences will be needed to reduce the remote sensing measurements to be made by the ExoMars Trace Gas Orbiter. For that, high-resolution laboratory absorption spectra of HDO in mixture with CO₂ were recorded in the ν₁, ν₂, and ν₃ fundamental bands between the 2.7 and 7 mm regions. The spectra were obtained with the Bruker IFS-125HR Fourier transform spectrometer at the Jet Propulsion Laboratory along with two specially built coolable absorption cells with path lengths of 0.2038 m and 20.941 m at various sample gas temperatures (230 - 296 K), pressures and volume mixing ratios. To aid in the analysis of these spectra modified complex Robert-Bonamy calculations were made. The intermolecular potential was comprised of electrostatic, atom-atom (expanded to 20th order and rank 4) induction, and London dispersion terms. The trajectories were obtained by solving Hamilton’s equations. The Lorentz half-width and pressure-shift coefficients were determined at 7 temperatures between 200 and 700 K. These calculations are compared with the measured parameters determined by a multispectrum nonlinear least squares technique[1]

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References:
A Study of atmospheric aerosol optical properties over Alexandria city- Egypt

E E Kohil¹, I H Saleh¹, Z F Ghatass¹

¹ Department of Environmental Studies Institute of Graduate Studies and research, Alexandria University-Egypt

Atmospheric aerosols play an important role in global and regional climate change. The spectral aerosol optical depth (AOD) was measurement over Alexandria city (31° 12’ N, 29° 55’ E and 43 above sea level) by using MICROTOPS-II sunphotometer. AOD is studied at five different wavelengths 380, 440, 500, 936 and 1020 nm during the period from August 2015 to February 2016. Water vapor is estimated from the measurements of solar intensity at 936 nm. The AOD shows seasonal variation with high values in the summer while the low values in the winter. The changes in the column water vapor have been found and correlated with changes in AOD. This is supported by the observed increase of AOD with relative humidity RH values. Monthly variation of relative humidity was from August 2015 to February 2016. The monthly mean of RH was 58.2% in October 2015, when the summer monsoon is active over Alexandria, RH value starts decreasing after October 2015 and continuously decreases till January 2016 to become 48.8%.

References:

Collisional shift and broadening of hyperfine lines for heavy atoms in an atmosphere of the buffer inert gas

A Glushkov¹, V Mansariysky¹, O Khetselius¹, V Buyadzhi¹ and T Florko¹

¹ Odessa State University – OSENU, Lvovskaya str. 15, Odessa, 65016, Ukraine

Studying collisional shifts and broadening the hyperfine lines for heavy elements (alkali, alkali-earth, lanthanides and others) in an atmosphere of inert gases is one of the important and actual topics of collision theory and spectral lines theory. Special interest attracts the corresponding phenomenon for alkali and lanthanides atom [1,2]. Besides, these atoms are very interested from the point of view of studying a role of the weak interactions in an atomic physics. At last, calculating the hyperfine line shift allows to detect an quality of the wave functions and study a contribution of the relativistic and correlation effects. To calculate the hyperfine spectral lines collision shift one should use the expression from kinetical theory of the spectral lines [1]:

\[ f_p = \frac{D}{p} = \frac{4\pi w_0}{kT} \int_{0}^{\infty} dw(R) \exp(-U(R)/kT) R^2 dR \]

where \( U(R) \) is an effective potential of the inter atomic interaction, which has a central symmetry in a case of the pairs A-B (for example, A=Rb; B=He); \( T \) is temperature, \( w_0 \) is a frequency of the hyperfine transition in the isolated active atom; \( d\omega(R)=D\omega(R)/w_0 \) is the relative local shift of the hyperfine lines, which is arisen due to the disposition of atoms of the A and B on a distance \( R \). The relativistic many-body perturbation theory [3] is used to determine the relativistic Dirac functions for studied atoms.

We present new data on the local and observed collisional \( f_p \) shifts and widths for pairs: A-B (A=Cs,Fr,Tl,Tm; B=He,Ar, Kr,Xe) in dependence on temperature \( T \). Our results are compared with the available experimental data and other theoretical results (see Refs. in [1, 2]), which are obtained within a perturbation theory with the Hartree-Fock or Dirac-Fock zeroth approximation. The feature of our scheme is a precise accounting for the correlation effects with using effective potentials [2]. Analysis shows that our data for studied systems are in the reasonable agreement with available experimental data (at least for available \( T \)). Very interesting features are found for the collisional broadening \( \Gamma_a \) parameter, namely, violation of the known Folly law (\( \Gamma_a \sim f_p \)) for lines in optical part of a spectrum.

References:

Fourier transform VIS and VUV spectroscopy of $^{13}$C$^{17}$O and deperturbation analysis of the $A^1Π$, $v = 0 \rightarrow 3$ levels

R Hakalla$^1$, M L Niu$^2$, R W Field$^3$, E J Salumbides$^{2,4}$, A N Heays$^5$, M Zachwieja$^1$, G Stark$^6$, J R Lyons$^7$, M Eidsberg$^8$, J L Lemaire$^9$, S R Federman$^{10}$, N de Oliveira$^{11}$ and W Ubachs$^2$

$^1$Materials Spectroscopy Laboratory, Department of Experimental Physics, Faculty of Mathematics and Natural Science, University of Rzeszów, ul. Prof. S. Pigonia 1, 35-959 Rzeszów, Poland.
$^2$Department of Physics and Astronomy, and LaserLaB, Vrije Universiteit, De Boelelaan 1081, 1081 HV Amsterdam, Netherlands.
$^3$Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, USA.
$^4$Department of Physics, University of San Carlos, Cebu City 6000, Philippines.
$^5$Leiden Observatory, Leiden University, PO Box 9513, 2300 RA Leiden, Netherlands.
$^6$Department of Physics, Wellesley College, Wellesley, MA 02481, USA.
$^7$School of Earth and Space Exploration, Arizona State University, PO Box 871404, Tempe, AZ 85287, USA.
$^8$Observatoire de Paris, LERMA, UMR 8112 du CNRS, 92195 Meudon, France.
$^9$Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS - Université Paris-Sud, UMR 8214, 1405 Orsay, France (previously at Paris Observatory, LERMA).
$^{10}$Department of Physics and Astronomy, University of Toledo, Toledo, OH 43606, USA.
$^{11}$Synchrotron SOLEIL, Orme de Merisiers, St. Aubin, BP 48, F-91192 Gif sur Yvette Cedex, France.

The high-resolution $B^1Σ^+ \rightarrow A^1Π$ (0, 0) and (0, 3) emission bands of the lesser-abundant $^{13}$C$^{17}$O isotopologue have been investigated by Fourier Transform Spectroscopy in the visible (VIS) region using Bruker IFS-125HR spectrometer located in the Materials Spectroscopy Laboratory in Rzeszów. These are combined with high resolution photoabsorption measurement of the $B^1Σ^+ \rightarrow X^1Σ^+$ (0, 0) and $C^1Σ^+ \rightarrow X^1Σ^+$ (0, 0) bands recorded with the vacuum ultraviolet (VUV) Fourier-transform spectrometer, installed on the DESIRS beamline at the SOLEIL synchrotron. In the studied 17,950 – 22,450 cm$^{-1}$ and 86,800 – 92,100 cm$^{-1}$ regions, 292 transitions have been determined with an absolute accuracy of up to 0.002 cm$^{-1}$. These new experimental data were combined with data from the previously analysed $C \rightarrow A$ and $B \rightarrow A$ systems [1-3]. The comprehensive data set, 885 spectral lines belonging to 11 bands, was used to perform a deperturbation analysis of the $A^1Π$, $v = 0 \rightarrow 3$ levels of $^{13}$C$^{17}$O, taking into account interactions with levels in the $d^3Δ$, $e^3Σ^+$, $a'^3Σ^+$, $I^1Σ^-$, and $D^1Δ$ states. Deperturbed molecular constants were obtained for the $A^1Π$ state and the perturbing levels. The term values for the main and extra levels are presented. Spin-orbit and $L$-uncoupling interaction parameters as well as isotopologue–independent spin-orbit and rotation–electronic perturbation parameters were also derived.

Figure 1. High resolution emission spectra of the $^{13}$C$^{17}$O $B^1Σ^+ \rightarrow A^1Π$ (0, 0) band and its extra-lines (asterisked) recorded by Fourier transform spectroscopy at an instrumental resolution of 0.018 cm$^{-1}$.

References:
Optical frequency comb spectroscopy of H$_2$O and OH in a flame

L Rutkowski$^1$, A Khodabakhsh$^1$, A C Johansson$^1$, D M Valiev$^2$, L Lodi$^3$, Z Qu$^2$, R Ghorbani$^2$, O L Polyansky$^3$, J Tennyson$^3$, F M Schmidt$^2$ and A Foltynowicz$^1$

$^1$Department of Physics, Umeå University, 901 87 Umeå, Sweden
$^2$Department of Applied Physics and Electronics, Umeå University, 901 87 Umeå, Sweden
$^3$Department of Physics and Astronomy, University College London, London WC1E 6BT, UK

Absorption spectroscopy techniques based on continuous wave lasers are often used as a non-intrusive tool for combustion diagnostics, but the limited probed spectral range restricts the number of detected species and the choice of line pairs for thermometry. We employ near-infrared cavity-enhanced optical frequency comb spectroscopy for simultaneous detection of H$_2$O and OH in a premixed methane/air flat flame. We compare H$_2$O spectra to a line list that is more accurate than the HITEMP database and we retrieve concentration and flame temperature from the OH spectra.

The system is based on an Er:fiber femtosecond laser locked to an enhancement cavity with a finesse of ~150. The burner is placed in the center of the cavity and mounted on a vertical translation stage to allow changing the height above the burner (HAB). The cavity transmission is analyzed using a fast-scanning Fourier transform spectrometer equipped with an auto-balancing detector, which acquires one spectrum with 1 GHz resolution in 0.4 s [1]. Figure 1(a) shows a normalized flame spectrum compared with the transition frequencies and line strengths of H$_2$O and OH. Figure 1(b) shows the improvement in accuracy of the new H$_2$O line list compared to the HITEMP line list [2]. By taking ratios between spectra measured at different HABs, we isolate the OH lines from H$_2$O [black, Fig. 1(c)]. Using one HAB as reference, we fit (red) the relative change of OH concentration and temperature between the two HABs involved in the ratio. The results obtained for different ratios are plotted in Fig.1(d) (markers), where they compare well with the theoretical behavior obtained from 1D Cantera calculations for stoichiometric ratio and a methane/air flow of 10 L/min (solid curves).

Figure 1. (a) Normalized flame spectrum at HAB of 2.5mm (black) together with a stick spectrum of transitions from the new H$_2$O list (blue) and OH from HITRAN (orange, divided by 100) calculated at 1950 K. (b) A zoom of the spectrum compared to the new H$_2$O line list (blue) and the HITEMP line list (red). (c) Ratio of two spectra taken at HABs of 5 and 2.5 mm (black) together with a fit (red, inverted) and the residual. (d) Flame temperature and OH concentration obtained from fits at different HABs (markers) compared to the 1D methane/air flame calculations (solid curves).

References:
Noise-immune cavity-enhanced optical frequency comb spectroscopy

A C Johansson¹, L Rutkowski¹, A Khodabakhsh¹, A. Foltynowicz¹

¹Department of Physics, Umeå University, 901 87 Umeå, Sweden

Cavity-enhanced optical frequency comb spectroscopy (CE-OFCS) combines broad spectral coverage and high resolution provided by an optical frequency comb with high sensitivity enabled by the enhancement cavity [1]. The comb lines can be efficiently coupled into the cavity modes by matching the repetition rate of the comb to the free spectral range of the cavity and adjusting the carrier-envelope offset frequency. This effectively enhances the interaction length with the analyte and thus improves the absorption sensitivity and enables measurements of weak transitions and low gas concentrations.

We will present a near-infrared CE-OFCS system for highly sensitive broadband spectroscopy based on noise-immune cavity-enhanced optical frequency comb spectroscopy (NICE-OFCS) [2, 3]. The system is based on an Er-fiber femtosecond laser locked to an enhancement cavity with a finesse of ~11000 using the two-point Pound-Drever-Hall technique [4]. To reduce frequency to amplitude (FM-AM) noise conversion caused by the cavity we utilize phase-sensitive detection of the entire comb in a way similar to continuous wave noise-immune cavity-enhanced optical heterodyne molecular spectroscopy (NICE-OHMS) [5]. In NICE-OFCS the comb is phase-modulated at a frequency equal to (a multiple) of the free spectral range of the cavity to transmit comb lines and sidebands through individual cavity modes. The transmitted light is analyzed using a fast-scanning Fourier transform spectrometer which enables measurement of the entire comb spectrum at acquisition times in the order of a second. The measured interferogram is demodulated at the modulation frequency which effectively cancels the FM-AM noise in the optical domain allowing for measurements at concentrations down to ppb levels. The measured NICE-OFCS spectra are obtained by Fast Fourier transform of the interferogram. Figure 1 shows a normalized NICE-OFCS spectrum of room-temperature CO₂ with 750 MHz resolution, together with a fit of the NICE-OFCS model [3] based on line parameters from the HITRAN database and a Voigt profile. We will present the principles of the technique, its experimental implementation and lineshape model.

![Figure 1. Normalized NICE-OFCS spectrum of the 3v₁+v₃ band of 1000 ppm CO₂ in N₂ at 350 Torr (black) together with a fit (red, inverted for clarity) and residual (bottom panel).](image)

References:

Traceable line strength measurements in carbon dioxide in the spectral region around 1.6 µm using cavity ring down spectroscopy

M Kiseleva¹, J Mandon¹, S Persijn², J Petersen³, L Nielsen³, R Pearce⁴and F Harren¹

¹Institute for Molecules and Materials, Radboud University, Heyendaalseweg 135, 6525 AJ, Nijmegen, the Netherlands
²Dutch Metrology Institute (VSL), Thijsseweg 11, 2629 JA, Delft, the Netherlands
³Danish Fundamental Metrology Institute (DFM), Matematiktorvet 307, DK-2800 Lyngby, Copenhagen, Denmark
⁴National Physical Laboratory (NPL), Hampton Road, Teddington, Middlesex, TW11 0LW, United Kingdom

Accurate measurements of greenhouse gases in the atmosphere are of great importance for understanding changes in the Earth’s climate. Next to concentration measurements, isotopic ratio measurements of stable isotopes allow to trace the origin or sink of such gases as carbon dioxide and methane. Spectroscopic methods play an important role in the accurate determination of those greenhouse gases; its spectroscopic measurements are based on spectral reference databases. Unfortunately the accuracy in the spectral line data provided in the reference databases is not sufficient for modern environmental studies and accurate traceable line data for greenhouse gases are needed.

To obtain accurate line data we used laser-based spectroscopy known by its main advantages – high selectivity and high sensitivity. A dedicated cavity ring down spectrometer was built for traceable line strength measurements in carbon dioxide and methane at the Radboud University. As a light source an external cavity diode laser was used operating in the spectral region 5800 – 6250 cm⁻¹. The mirrors of the cavity ring down cell have at this wavelength a reflectivity of 99.97%, which in combination with a 50 cm cell gives an optical path length of 1.6 kilometers. This allows measuring the values of the line strength of the order of 10⁻²⁶ cm/molecule. To obtain traceable values of the line strength a calibrated pressure meter and the temperature isolated cavity ring down cell were used. Spectral measurements were performed with carbon dioxide mixtures with well-known amount ratio ¹³CO₂/¹²CO₂ that were previously determined gravimetrically at the National Physical Laboratory.

Here, we present the results of the line strength measurements in ¹²CO₂ and ¹³CO₂. For every spectral line of carbon dioxide spectra were recorded at room temperature at three different pressures between 10 and 50 mbar. The analysis of the measured absorption lines was performed using the software that allows adjusting different line profiles to the measured spectra taking into account uncertainty in the measured values of the wavenumber and the decay time. The uncertainty budget of the obtained line strength values is discussed. These data can be used for isotopic ratio measurements in carbon dioxide.

Acknowledgement

This work was performed within the Researcher Excellence Grant associated with the European Metrology Research Project ENV52 HIGHGAS. EMRP is jointly funded by the EMRP participating countries within EURAMET and the European Union.
VIPA spectrometer calibration and comb-cavity locking schemes comparison for sensitive and accurate frequency comb spectroscopy

G Kowzan¹, K F Lee², M Borkowski³, P Ablewski⁴, Sz Wójtewicz⁴, K Stec⁴, D Lisak⁴, M E Fermann³, RS Trawiński³, P Masłowski¹

¹Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Grudziądzka 5, 87–100 Toruń, Poland
²IMRA America, Inc., 1044 Woodridge Ave., Ann Arbor, MI, USA 48105

Direct frequency comb spectroscopy combines the sensitivity and resolution of laser spectroscopy with the speed of broadband spectroscopy, replacing single-line wavelength scanning with a parallel measurement over a large frequency bandwidth. For emerging applications such as human breath analysis and industrial process monitoring, exceptional sensitivity and accuracy are required. Here, we demonstrate a measurement system based on an Er:fiber laser with the repetition rate of 250 MHz, operating in the 1.5–1.6 μm range. Comb teeth are locked to a high-finesse cavity (F = 8500) either by a low bandwidth (~20 Hz) swept locking scheme [2] or a two-point Pound-Drever-Hall scheme [3]. The transmission spectrum is resolved by a VIPA etalon and a diffraction grating, which results in 38-nm wide spectrum (~20 Hz) swept locking scheme [2] or a two-point Pound-Drever-Hall scheme [3]. The transmission spectrum is based on an Er:fiber laser with the repetition rate of 250 MHz, operating in the 1.5–1.6 μm range. Comb teeth are locked to a high-finesse cavity (F = 8500) either by a low bandwidth (~20 Hz) swept locking scheme [2] or a two-point Pound-Drever-Hall scheme [3]. The transmission spectrum is resolved by a VIPA etalon and a diffraction grating, which results in 38-nm wide spectrum (~20 Hz) swept locking scheme [2] or a two-point Pound-Drever-Hall scheme [3]. The transmission spectrum is resolved by a VIPA etalon and a diffraction grating, which results in 38-nm wide spectrum (~20 Hz) swept locking scheme [2] or a two-point Pound-Drever-Hall scheme [3]. The transmission spectrum is resolved by a VIPA etalon and a diffraction grating, which results in 38-nm wide spectrum (~20 Hz) swept locking scheme [2] or a two-point Pound-Drever-Hall scheme [3]. The transmission spectrum is resolved by a VIPA etalon and a diffraction grating, which results in 38-nm wide spectrum (~20 Hz) swept locking scheme [2] or a two-point Pound-Drever-Hall scheme [3]. The transmission spectrum is resolved by a VIPA etalon and a diffraction grating, which results in 38-nm wide spectrum (~20 Hz) swept locking scheme [2] or a two-point Pound-Drever-Hall scheme [3]. The transmission spectrum is resolved by a VIPA etalon and a diffraction grating, which results in 38-nm wide spectrum (~20 Hz) swept locking scheme [2] or a two-point Pound-Drever-Hall scheme [3]. The transmission spectrum is resolved by a VIPA etalon and a diffraction grating, which results in 38-nm wide spectrum (~20 Hz) swept locking scheme [2] or a two-point Pound-Drever-Hall scheme [3]. The transmission spectrum is resolved by a VIPA etalon and a diffraction grating, which results in 38-nm wide spectrum (~20 Hz) swept locking scheme [2] or a two-point Pound-Drever-Hall scheme [3].

The measurement system is based on the HITRAN database [5]. The spectral line shapes distortions caused by interplay of molecular dispersion and cavity resonances are clearly visible. Panel (b): Fractional Allan deviation of single spectral element intensity for two locking schemes, laser beam bypassing the cavity and photodetector array noise.

We present a careful comparison and analysis of the performance of both locking schemes with obtained absorption enhancement, noise averaging and noise-equivalent absorption included. For the PDH scheme we obtain NEA of $9.9 \times 10^{-10}$ cm$^{-1}$ and $7.4 \times 10^{-11}$ cm$^{-1}$ per spectral element. For the swept locking we obtain $5.3 \times 10^{-9}$ cm$^{-1}$ and $1.5 \times 10^{-9}$ cm$^{-1}$ per spectral element. A calibration scheme based on known VIPA dispersion formulas [6] and data points with precisely known frequencies (obtained through the Vernier scheme) is shown. Comparison with other calibration schemes is presented and it is verified that the calibration scheme is limited only by the camera pixel size.

References:

Mid-infrared absorption cross-sections of perfluorodecalin (C$_{10}$F$_{18}$)  
K Le Bris 1, J DeZeeuw 1, P Godin 2, K Strong 2

1 Department of Physics, St Francis Xavier University, Antigonish, Nova Scotia, Canada  
2 Department of Physics, University of Toronto, Toronto, Ontario, Canada

Perfluorodecalin is a chemically inert fluorocarbon and a very efficient gas dissolver. Those properties make this molecule particularly interesting in medical applications such as blood substitutes, wound healing, storage of organ and tissues, oxygen carrier, contrast agent in diagnostic imaging, etc.

Because of its C-F bonds, perfluorodecalin is a potent greenhouse gas regulated by the Kyoto Protocol. Its lifetime is estimated to be in the order of 2000 years. Only one cross-section spectrum of this molecule has been published at a resolution of 0.5 cm$^{-1}$ and a temperature of 296 K [1].

We present pure absorption cross-section of perfluorodecalin in a range of temperature at a resolution of 0.1 cm$^{-1}$. The radiative efficiency and global warming potential have been calculated from the laboratory absorption cross-section spectra and compared with the current accepted values. Acquisitions have been performed in the 550-4000 cm$^{-1}$ spectral range using Fourier transform spectroscopy.

References:

Improved argon-induced shift and broadening coefficients for the 2-0 band of HCl

G Li¹, H Tran², M Gisi³, O Werhahn¹ and V Ebert¹,³,⁴

¹ Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany
² Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA, UMR CNRS 7583)
³ Physikalisch Chemisches Institut, U Heidelberg, INF 253, 69116 Heidelberg
⁴ Center of Smart Interfaces, TU Darmstadt, Petersenstraße 32, Darmstadt 64287, Germany

FTIR absorption spectra of the 2–0 band of HCl in argon have been recorded at room temperature for total pressures ranging from 1 bar to 10 bar. Improved and more complete Ar-induced broadening and shift coefficients have been retrieved from regression analysis of the fitted line widths and positions, respectively. Our newly fitted broadening coefficients are in excellent agreement with values from classical trajectory calculations by Boulet et al. [1] and recent laser based measurements by De Rosa et al. [2], but provide higher accuracy and better consistency. Also, a super-Lorentzian effect on the far wings was observed at high pressures.

Figure 1.

References:

Optical Frequency Comb Fourier Transform Spectroscopy for broadband lineshape parameters retrieval

P Masłowski¹, K F Lee², A C Johansson³, A Khodabakhsh³, G Kowzan¹, L Rutkowski³, A A Mills², C Mohr², J Jiang², M E Fermann² and A Foltynowicz³

¹ Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, ul. Grudziądzka 5/7, 87-100 Toruń, Poland
² IMRA America, Inc., 1044 Woodridge Avenue, Ann Arbor, Michigan 48105, USA
³ Department of Physics, Umeå University, 901 87 Umeå, Sweden

Fourier transform spectrometers (FTS) based on optical frequency combs (OFC) allow detection of broadband molecular spectra with high signal-to-noise ratios within acquisition times orders of magnitude shorter than traditional FTIRs based on thermal sources [1]. Moreover, high absorption sensitivity can be obtained using optical enhancement cavities [2]. Due to the pulsed nature of OFCs the interferogram consists of a series of bursts rather than a single burst at zero optical path difference (OPD). The comb mode structure can be resolved by acquiring multiple bursts [3]. However, the measurement of molecular lines narrower than the resolution limited by the maximum OPD has not been demonstrated.

We show that it is sufficient to acquire an interferogram in a symmetric range around a single burst with length precisely matched to the comb line spacing in order to exceed the spectrometer’s OPD-limited resolution and measure accurately the intensity change of the individual comb lines. Our method allows measurements of broadband spectra with absorption lines narrower than the OPD-limited resolution without any loss of accuracy due to the instrumental lineshape function. Therefore it can be applied for broadband retrieval of lineshape parameters of tens of molecular lines simultaneously, in wide range of pressures, not limited by the OPD of the interferometer. With truly simultaneous detection the influence of the long-term changes in the sample composition and the experimental setup are minimized.

As a demonstration we show the measurements of undistorted low pressure CO₂ and CO absorption lines with linewidths narrower than the OPD-limited resolution using OFC-based mechanical FTS in the near- and mid-infrared wavelength ranges [4]. The near-infrared system is based on an Er:fiber femtosecond laser locked to a high finesse cavity, while the mid-infrared system is based on a fully-stabilized Tm:fiber-laser-pumped optical parametric oscillator coupled to a multi-pass cell. The mid-infrared measurements of fundamental band of CO perturbed by Ar are analyzed in terms of pressure dependence of pressure broadening and shifting and compared with data available in the literature.

References:

Cavity ring-down spectroscopy and cavity-enhanced frequency comb spectroscopy of the second overtone, P branch carbon monoxide transitions in argon

K Stec1, V Silva de Oliveira2, M Zaborowski3, A Cygan1, G Kowzan4, Sz Wójtewicz1, P Wcisło1, R Ciuryło5, D Lisak4, A Ruehl2, I Hartíček2, R S Trawiński1, P Masłowski1

1Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun, Grudziadzka 5, 87–100 Torun, Poland
2Deutsches Elektronen-Synchrotron (DESY), Notkestrasse 85, 22607 Hamburg, Germany

Cavity ring-down spectroscopy (CRDS) is an established technique based on measurements of dependence of light decay time constant on the absorption of the gas sample inside the optical cavity. Its insensitivity to laser power fluctuations and negligible instrumental line shape function makes it a powerful tool for sensitive trace gas detection and detailed spectral line shape analysis.

Absorption spectroscopy based on direct interaction of optical frequency comb (OFC) beam with a gas sample, called direct frequency comb spectroscopy (DFCS), allows for measurements of molecular absorption spectra in wide spectral range and with high signal-to-noise ratio. It removes the limitations of cw-laser spectroscopy caused by time consuming tuning and limited frequency range. Fourier transform spectrometers (FTS) coupled with OFC provide broadband spectral bandwidth and acquisition times orders of magnitude shorter than traditional with FTS coupled with thermal sources [1]. The resolution of FTS with OFC is not limited by the maximum optical path difference between the interferometer arms [2], which makes it suitable for simultaneous acquisition of tens of molecular lines in wide pressure range.

We present measurements of the second overtone, P branch CO band transitions in wide pressure range, performed with both CRDS and OFC-FTS systems. The first setup is a Pound-Drever-Hall-locked frequency-stabilized CRDS spectrometer [3], linked to an optical frequency comb. The enhancement cavity with finesse of 13000 and high signal-to-noise ratio of the spectra allows to reach noise-equivalent absorption of $7 \times 10^{-11}$ cm$^{-1}$. The frequency accuracy of the system is 30 kHz. The broadband system is based on an Er:fiber frequency comb, locked with two-point PDH locking scheme [4] to an enhancement cavity with finesse of 8500. The lines measured with the CRDS system are: P2, P4, P6, P9 and P14 in five pressures from 10 to 700 Torr. Line centers, line shifting and broadening parameters were retrieved, with line center position uncertainties from 130 kHz to 330 kHz. We obtained for the first time line shifting coefficients of the second overtone CO transitions in argon. We also report line broadening coefficients of these transitions with significantly lower uncertainties than previously [5] and provide fitted coefficients of an empirical formula allowing to calculate line broadening of lines not measured in this work. The results of measurements of the same gas sample with OFC-FTS spectrometer will be presented and will include a comparison of the accuracy of the mixing ratio determination as well as the accuracy and precision of retrieved absolute line positions.

References:

CRDS measurements of Acetone concentration

G Revalde¹, J Alnis¹,², E Nitišs³, K Blušs², K Grundšteins¹

¹ Ventspils University College, Inzenieru str. 101, Ventspils, Latvia
² Institute of Atomic Physics and Spectroscopy, University of Latvia, Sknu 4, Riga, Latvia
³ Institute of Solid State Physics, Kengaraga str., Riga, Latvia

The Cavity Ring-Down Spectroscopy (CRDS) system for medical applications is created and first results for detection of acetone are shown. The acetone concentration was measured in the air. In the system a pulsed 1 kHz 266 nm DPSS laser with pulse length of 10 ns is coupled in a gas cell with high reflectivity mirror. The cell operates as a resonator in which the laser pulse decays with a specific decay rates. The decay rate is determined by the distance between the mirrors, mirror reflectivity coefficient and absorptivity of the gas at 266 nm. The light intensity is captured using a high-speed avalanche photodiode. Afterwards an exponential fit in the form \( f(t) = A \cdot e^{-t/\tau} + B \) is done, where the \( A \) is the amplitude of the signal, \( B \) is the intercept and \( \tau \) is the decay rate.

The decay rate was captured as the cell was consecutively filled to 1000 mbar with air with low amount of acetone (30 ppm and 5 ppm respectively), high purity nitrogen gas as well as vacuumed (air pressure of around 0.3 mbar) cell. The obtained experimental data for acetone at the level of 5 ppm are evident in Fig. 1.

![Figure 1. The ringdown decay rate captured in time.](image)

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References:

A modified new expression for the Voigt spectral line profile
G D Roston1, M F Ahmed1, M S Helmi1 and O S Mahran1

1 Department of Physics, Faculty of Science, Alexandria University-Egypt

A modified formula for the Voigt spectral line profile has been obtained. This formula has been transferred from the integral formula to a second order differential equation. The results of the obtained formula are in a perfect agreement with the corresponding published results which are obtained by different numerical calculation methods for a wide range of the line damping parameter (a) for (0 ≤ a ≤ 200). Beside this, there are also four special formulas obtained at different ranges of the line profile [at very small values of a (a → 0) (Gaussian profile), at very large values of a (a → ∞) (Lorentzian profile), (x → 0) (line center) and at (x → ∞) (line wings)].

The A obtained modified formula for the Voigt spectral line profile is given by:

\[ V(x,a) = e^{-x^2} \frac{1}{\sqrt{\pi a}} \sum_{n=0}^{\infty} \frac{(-1)^n(2n)!}{n!(2a)^n} \cos(2ax) + \frac{1}{2a} (- \cos(2ax)) \sum_{n=1}^{\infty} \frac{a^{-n}}{n!} (\cosh(na) - \cos(2a)) \]

\[ \frac{d^2V}{dx^2} = -\frac{2}{a} V + \frac{1}{a^2} \frac{dV}{dx} + \frac{1}{a^3} \sum_{n=0}^{\infty} \frac{(-1)^n(2n)!}{n!(2a)^n} \cos(2ax) + \frac{1}{2a} (- \cos(2ax)) \sum_{n=1}^{\infty} \frac{a^{-n}}{n!} (\cosh(na) - \cos(2a)) \]

Figure 1. The Voigt profiles at the smallest values of (n) for different values of the damping parameter a (●) with the numerical calculations (–).

Figure 1. The relation between the values of (n) at different damping parameter (a) [0.01 – 4] using the polynomial equation \( n = 6.02 + 8.214a - 1.179a^2 \)

References:
Frequency comb based spectrometer continuously tunable from 3 µm to 5 µm

V Silva de Oliveira¹, P Masłowski², A Ruehl¹, I Hartl¹

¹ Deutsches Elektronen-Synchrotron, Notkestrasse 85, Hamburg, Germany
² Institute of Physiscs, Faculty of Physiscs, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, ul. Grudziadzka 5, 87-100 Toruń, Poland

In a frequency comb (FC), a train of phase-stabilized pulses results in a set of equally spaced narrow spectral “comb” modes, whose absolute position can be controlled by reference oscillators. FC sources can be utilized to overcome the frequency resolution limit set by the optical path delay (OPD) in a Fourier-transform spectrometer (FTS) [1,2].

Here, we report on a FC based FTS operating in the mid-infrared (MIR) spectral region. A schematic of the setup is shown in Fig. 1 (a). The MIR FC is based on a phase-stabilized 2 W Yb:fiber laser and difference frequency generation. The laser output is split into two branches whereas a signal field is generated in a highly-nonlinear fiber [3]. The idler field is generated in a periodically-poled lithium niobate crystal with fan-out structure. Its optical spectrum can be continuously tuned from 1900 to 3300 cm⁻¹ (3 µm to 5 µm) as shown in the inset of Fig. 1 (a). Details of the FC source and the possibility to extend its spectral coverage to 1000 cm⁻¹ can be found in Ref. [4]. The spectral readout was realized by a home-built scanning FTS with an optical path delay sufficient to resolve individual FC lines at 150 MHz or 0.005 cm⁻¹ spacing.

Figure 1. (a) Schematic of the frequency comb spectrometer together with the tunable MIR spectrum. (b) Measured CO spectrum (0.61% at 758 Torr in N₂) and comparison with HITRAN database. (c) Zoom on CO R6 line at 2169.19 cm⁻¹. The source was tuned to 4.6 µm to measure the fundamental absorption band of CO. Fig. 1(b) shows the R-branch spectrum measured with 0.008 cm⁻¹ resolution (125 cm OPD in 4 s) together with simulations based on the HITRAN database. The excellent match with HITRAN is highlighted in Fig. 1 (c) showing a zoom to the R6 line at 2169.19 cm⁻¹. The measurement was performed at 758 Torr in a 45 mm long gas cell filled with a mixture of nitrogen and CO (0.61 % concentration). We achieved signal-to-noise ratios of up to 800 by averaging 20 spectra.

The presented spectroscopy setup is suited for wide set of applications for example trace gas detection and is compatible with massively parallel lineshape analysis. It can be used throughout the important MIR spectral region to probe the fundamental vibration bands of molecules with ultrahigh resolution.

Vinicio Silva de Oliveira is a fellow of the CNPq - Brasil

References:
Search for possible laser cooling schemes in terbium atom

D Stefańska¹, B Furmann¹

¹Division of Quantum Engineering and Metrology, Institute for Material Research and Quantum Engineering, Faculty of Technical Physics, Poznań University of Technology, Piotrowo 3, 60-965 Poznań, Poland

The knowledge of the electronic levels structure of the terbium atom has been very scarce until recently; our previous works [1, 2] yielded already some new results. Within the present work, further laser-spectroscopic investigations have been performed for a series of optical transitions in Tb I; these allowed the assignment of a number of energy levels and the rough assessment of transitions strengths (in some cases – also their classification).

Terbium atom is very interesting from the point of view of the hyperfine structure of its electronic levels, e.g. inconclusive results concerning the value of $a_{6s}^{10}$ radial integral [2], not fully consistent with the overall tendency along the lanthanides series, requires further verification. Terbium can also be considered a favorable candidate for laser cooling and trapping, in the context of recent achievements in this field for some other elements in the lanthanides series.

The possibility of repumper-less laser cooling of some lanthanides atoms was demonstrated within the last decade. The idea of Doppler cooling [3] was to apply a strong (but non-cycling) optical $4f^26s^2 \rightarrow 4f^26s6p\ J \rightarrow J + 1$ transition from the ground state, usually in the blue-violet region; the above change in $J$ quantum number allows magneto-optical trapping, as well as possible further polarization-gradient cooling. This scheme was already demonstrated on Er, Tm, Dy and Ho atoms, and proved surprisingly efficient. Some sub-Doppler cooling schemes were also proposed. Of course the most favorable situation occurs in the case of low branching ratios for the leaking transitions, which compete with the cooling transition.

Atomic terbium may present a particularly interesting case, since its odd-parity ground level ($J = 15/2$) is followed by a very low-lying (below 300 cm⁻¹) even-parity level ($J = 13/2$), which exhibits a high thermal population and thus can also be considered as the lower level of a possible cooling transition. Some of the levels investigated within this work might be potentially interesting from the point of view of laser cooling. The results should also allow an analysis of the possible leaking transitions.

References:

An algorithm for calculating the contour Voigt and its improvement and refinement for some ranges of parameters

A Ya Sukhanov¹

¹Laboratory of Lidar Methods, V.E. Zuev Institute of Atmospheric Optics SB RAS, 1 Academician Zuev square, 634021 Tomsk, Russia

In [1] was presented the method for calculating the Voigt contour, in this, it refined and improved. Voigt profile contour used for calculations of the absorption lines and takes into account the effect of Doppler broadening and collision effects [2], this intractable integral with infinite boundaries of integration: \[ \chi(x,y) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\exp\left(-t^2\right)}{y^2 + x^2 - t^2} dt, \]

where \(x, y \geq 0\) - parameters of Voigt conotour depending on wavelength and broadening effects. Different algorithmic approaches to calculate the integral in (1) are used, some of them described in [3-7]. Here it offers improved relative error for \(|x|<1.6\) and \(y<0.02\) range with an error of less than 0.1% compared with the error <0.5% at first algorithm realization and for \(y<0.001\) less than 0.001%

by approximation given:

\[ f(x,y) = \frac{\exp\left(-x^2\right)}{0.351y + 0.3183y - (1.4x^2 - 0.38x^2)y^2 - 0.093} \]  (2)

Approximation based on orthogonal polynomials Hermite, \(f(x,y) = \sum_{i=1}^{10} \frac{A_i}{y^2 + |x-Ax_i|^2}\), for \(y \geq 1.0\) or \((|x|>3.55 \text{ and } y>0.01) \text{ or } |x|>5.000001\), where \(A_i, Ax_i\) - precalculated weight Hermite quadrature. \(Ax = (3.4361583, 2.5327307, 1.7566830, 1.0366104, 0.3429013, -0.3429013, -1.0366104, -1.7566830, -2.5327307, -3.4361583), A = (7.641e-6, 1.344e-3, 0.034, 0.240, 0.611, 0.611, 0.240, 0.034, 3.444e-3, 7.641e-6)\)

For \(|x|>5.000001\) error is less than 0.001%, for \(y \geq 0.7\) and \(y \leq 1.0\) and \(|x|<3.55\) error less than 0.5%, for \(y \geq 1.0\) and \(|x|<3.55\) less than 0.1%, and for \(|x|>3.55\) less than 0.01%.

For the intervals \(y<0.01\) and \(|x|>3.55\) and \(|x|<5.000001\) is recommended to use direct calculation using recursive procedure dividing each grid spacing if necessary and check the relative error of calculation in the division of the interval for calculating the integral for 2, 4 and 8 parts, unfortunately this algorithm with a small stack size for small \(y<0.000001\) can not enough memory, this range has features in which, for example, a standard Mathcad integration algorithm is not working properly. It is suggested to use a linear approximation of integral in expression (1) on a uniform \(x\) and \(y\) grid for the other cases, the accuracy will depend on the amount of memory allocated for the approximation coefficients. Computation speed does not depend on grid spacing, as the respective numbers of coefficients are linear based on it, but it requires estimation and preservation of the approximation coefficients and a large amount of memory for them (for example if \(|x|<1.6\) and \(y>0.02\) and \(y<0.7\) it is need more 100 points for \(x\) and more than 2000 points for \(y\) with relative error <0.01%).

References:

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Measurements of H$_2$O broadening and shifting coefficients of CO$_2$, CH$_4$ and O$_2$ lines

T Delahaye$^1$, X Landsheere$^1$, E Pangui$^1$, F Huet$^1$, J-M Hartmann$^1$, H Tran$^1$

$^1$ Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA, CNRS UMR 7583), Université Paris Est Créteil, Université Paris Diderot, Institut Pierre-Simon Laplace, 94010 Créteil

Atmospheric observation is mainly based on the solar radiation transmitted by the atmosphere or on the thermal radiation emitted by the Earth surface and by the atmosphere. The analysis of the measured data, mostly done through the so-called "inversion" procedures, requires the knowledge of the intrinsic spectroscopic parameters of absorption lines (positions, intensities,...). The collisions between the molecules also have to be considered as their effects yield a modification of the line shape for most of the atmospheric physical conditions (pressure, temperature). Since the amount of water vapor in our atmosphere can be significant at low altitude, spectral line broadening by collisions with water vapor must be taken into account in order to meet the objective of precision of current satellite missions. In this study, H$_2$O-broadening and shifting coefficients of many lines of methane, carbon dioxide and oxygen in the mid- and near- infrared region were measured. For that, spectra of CH$_4$, CO$_2$ and O$_2$ diluted in water vapor were recorded with a high resolution Fourier Transform spectrometer for various pressures and at 50 and 95°C. Line broadening and shifting were retrieved from the measured spectra through fits using Voigt profiles. Values at room temperature and their temperature dependences were then deduced and compared with those of dry air. The results show that H$_2$O-broadenings of methane lines are, on average, 34% larger than those for dry air [1]. For CO$_2$, our result are about 4% lower than the values recommended in a previous study but they confirm the relative variations of the line broadening on the rotational quantum numbers. We also provide the first determination of H$_2$O-induced line shifts of CO$_2$ lines [2].

References:

Super-Lorentzian effects on the line wings of self-broadening HCl and of HCl diluted in Ar

H Tran¹, J-M Hartmann¹, Gang Li², V Ebert²,³,⁴

¹ Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA, UMR CNRS 7583)
² Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany
³ Physikalisch Chemisches Institut, U Heidelberg, INF 253, 69116 Heidelberg
⁴ Center of Smart Interfaces, TU Darmstadt, Petersenstraße 32, Darmstadt 64287, Germany

Super-Lorentzian effects on the line wings of self-broadening HCl and of HCl diluted in Ar are investigated for the first time using classical molecular dynamics simulations (CMDS). Using reliable intermolecular potentials taken from the literature, these CMDS provide the time evolution of the auto-correlation function of the dipole moment, whose Fourier-Laplace transform leads to the absorption spectrum. For each collision-partner, calculations were performed at room temperature and at 1 and 10 atm. Super-Lorentzian effect is quantified by computing the ratios of CMDS-calculated and pure Lorentz line wings. The obtained results are then compared with values deduced from spectra measured in the 1-0 and 2-0 bands using Fourier transform spectrometers. Very good agreement is observed for all considered perturbers showing that CMDS are able to predict the observed super-Lorentzian behaviour of the HCl far line wings.
Transition dipole moment and the ambiguity of determination of interatomic potential in diatomic molecule

T Urbańczyk¹, J Koperski¹, A Pashov²

¹Smoluchowski Institute of Physics, Jagiellonian University, prof. S. Łojasiewicza 11, 30-348 Kraków, Poland
²Department of Physics, Sofia University, 5 James Bourchier Boulevard, 1164 Sofia, Bulgaria

We will show the influence of the distribution of molecular transition dipole moments on the unequivocalness of determination of analytical representation of interatomic potential (especially a Morse potential) based on experimental spectra with unresolved rotational structure. Assuming that the lower state of molecular transition is properly defined, we show, that in case of the spectra, there are many different combination of equilibrium distance in the upper state \( R' \) and transition dipole moments (TDM), which provide correct simulation of the experimental spectrum. We prove, that this ambiguity is significantly reduced for spectra with resolved rotational structure.

![Graph](image.png)

**Figure 1.** (A,C) Reference spectra (red) and simulations (black) performed under an assumption that the \( B^1 \)-state interatomic potential of is represented with a Morse function with parameters \( R'_e = 5.05[\text{Å}], \quad D'_e = 55.0[\text{cm}^{-1}], \quad \beta'_e = 0.988 \text{ Å}^{-1} \) and TDM determined for the following points: \( 2[\text{Å}]= 2.0, \quad 3[\text{Å}]= 2.0, \quad 5[\text{Å}]= 1.0, \quad 8[\text{Å}]= 1.0 \). (B,D) Reference spectra (red) and simulations (black) performed under the same assumption as in (A,C) but with the following parameters \( R'_e = 5.1[\text{Å}], \quad D'_e = 54.97[\text{cm}^{-1}], \quad \beta'_e = 0.988 \text{ Å}^{-1} \) and for TDM determined for points: \( 2[\text{Å}]= 2.0, \quad 3[\text{Å}]= 2.2, \quad 5[\text{Å}]= 3.0, \quad 8[\text{Å}]= 1.0 \). Pairs of the experimental spectra (A,B) and (C,D) were recorded for different experimental conditions: \( T_{\text{rot}} = 3[\text{K}] \) and \( \Delta_{\text{Lorentz}} = 2.5[\text{cm}^{-1}] \) for spectra (A,B); \( T_{\text{rot}} = 15[\text{K}] \) and \( \Delta_{\text{Lorentz}} = 0.3[\text{cm}^{-1}] \) for spectra (C,D). For all simulations, parameters for the \( X^3 \) state were as in [1].

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**References:**

Influence of spontaneous emission on the linear and nonlinear resonances of alkali atoms confined in an extremely thin cell

T Vartanyan\textsuperscript{1}, A Sargsyan\textsuperscript{2}, V Polischuk\textsuperscript{1}, A Krasteva\textsuperscript{3}, St Cartaleva\textsuperscript{3}, G Todorov\textsuperscript{3}

\textsuperscript{1}ITMO University, Kronverkskiy pr. 49, St. Petersburg 197101, Russian Federation
\textsuperscript{2}Institute for Physical Research, National Academy of Sciences of Armenia, Ashtarak-2, Armenia
\textsuperscript{3}Institute of Electronics, Bulgarian Academy of Sciences, Tzarigradsko shosse 72, 1784 Sofia, Bulgaria

The sub-Doppler spectroscopy of alkali atom vapour was strongly advanced by the invention of the Extremely Thin Cells (ETC) \cite{1}. Using the conventional spectroscopic methods of registration, a number of peculiarities in the absorption, reflection and fluorescence spectra were observed in these cells, which are not present in commonly used (cm-size) cells. The main reason for the formation of the sub-Doppler structures in the spectra is the strong spatial anisotropy in the ETC environment. Collisions with the cell walls induce loss of atomic phase memory and excitation quenching. Hence, the atoms departing from the cell walls undergo a transient regime of excitation before they acquire the steady state polarization that corresponds to their velocity as well as to the laser field intensity and detuning. Nonlinear resonances in absorption and fluorescence are also influenced by velocity selective optical pumping \cite{2}. The present work gives a description of the interaction of resonant laser fields with alkali atoms in an ETC with the full account of the hyperfine sublevel degeneracy using iteration procedure over the laser field.

The problem of determination of the nonlinear atomic polarization was solved for arbitrary values of the total angular momenta of the resonance levels for excitation with linearly polarized laser light. Using the previously developed methodology \cite{3-6}, the equations of motion for the statistical operator $\hat{\rho}$ in the irreducible tensor operator (ITO) representation were solved, taking into account the transient processes started by the atomic collisions with the cell walls. Analytical solutions are obtained for the spatial part of the tensor components, $\rho^\kappa_{\rho} (\rho = f, \phi, \xi)$, which characterize the population and longitudinal alignment of the upper ($f^\kappa$), and lower ($\phi^\kappa$) resonance levels and the optical coherence ($\xi^\kappa$), with accuracy up to the third-order terms with respect to the laser field. Taking into account the spontaneous population transfer from the excited levels, it was possible to relate the sign reversal of the nonlinear resonance at the closed transition with a corresponding reversal of the sign of the lower level alignment. In contrast to other works, the decay constants of the upper level and that of the optical coherences are not assumed to be equal. The numerical calculation results show excellent agreement with experimental data obtained for the D\textsubscript{2} lines of $^{133}$Cs confined in an ETC.

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Ab initio line-shape calculations

P Wcisło1, F Thibault2, H Cybulski1, R Ciuryło1

1 Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziądzka 5, 87-100 Toruń, Poland
2 Institut de Physique de Rennes, UMR CNRS 6251, Université de Rennes 1, Campus de Beaulieu, Bât.11B, F-35042 Rennes, France

We present ab initio calculations of spectral line shapes for foreign-perturbed hydrogen molecule and its validation against experimental data. Two collisional effects substantially influencing the shape of optical resonance have to be considered: the phase- or state-changing collisions and the velocity-changing collisions. We calculate these two contributions originating from the interaction potential.

We consider two opposite cases of perturbers: heavy Ar atoms [1] and light He atoms [2]. Both systems are physically interesting due to a strong Dicke narrowing and a strong speed dependence of broadening and shifting. However, the essential difference in their perturber-to-emitter mass ratios considerably discriminates the properties of the internal and translational motions of the H₂ molecule upon a collision. On one hand we performed quantum dynamical close coupling calculations [3] on full-dimensional PESs [1, 4]. On the other hand we handled the velocity-changing collisions by approximating the PESs with a hard-sphere potential [5]. The line-shape originating from this approach is called speed-dependent billiard ball profile (SDBBP) [6].

This approach allowed us to explain an intriguing puzzle that had remained unresolved for 25 years [1]. The previous calculations of the width of Ar-perturbed Raman 1-0 Q(1) line of H₂ resulted in fundamental discrepancy with experiment [7]. We demonstrated that this discrepancy was not caused by the imperfections of the used PESs (as stated in the previous works), but by oversimplified model of the velocity-changing collisions [1].

This approach allowed us also to validate PESs for the H₂-He system. We demonstrated that to test reliably the H₂-He PESs against spectroscopic experimental data, not only the quantum mechanical calculations of the phase- or state-changing collisions are needed (as it was done before), but also a proper description of the velocity-changing collisions is required. This allowed us to show that among the available PESs the most recent state-of-the-art PES [4] best reproduces experimental data [8-10]. We also observed that the range of applicability of this PES (and all the earlier PESs) is limited to pure rotational and fundamental bands, therefore it has to be extended to larger H-H distances to cover overtones. A proper representation of the H₂-He spectra is needed for modeling the atmospheres of gas giants and in long-term perspective it may also be required for exoplanets studies. Moreover the H₂-He system is a good candidate for constructing the first full ab initio line-by-line dataset of molecular spectra line-shape parameters.

References:

Non-Voigt line-shape parameters of H$_2$ spectra for the HITRAN database

P Wcisło$^{1,2}$, I E Gordon$^1$, H Tran$^3$, Y Tan$^{1,4}$, S-M Hu$^4$, A Campargue$^{5,6}$, S Kassi$^{5,6}$, D Romanini$^{5,6}$, C Hill$^{1,7}$, R V Kochanov$^{1,8}$, L S Rothman$^1$

1 Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge, MA, USA
2 Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziądzka 5, 87-100 Toruń, Poland
3 Laboratoire Inter-universitaire des Systèmes Atmosphériques (LISA), CNRS UMR 7583, Université Paris Est Créteil, Université Paris Diderot, Institut Pierre-Simon Laplace, 94010 Créteil Cedex, France
4 Hefei National Laboratory for Physical Sciences at Microscale, iChem center, University of Science and Technology of China, Hefei, 230026 China
5 University of Grenoble Alpes, LIPhy, F-38000 Grenoble, France
6 CNRS, LIPhy, F-38000 Grenoble, France
7 Department of Physics and Astronomy, University College London, Gower Street, WC1E6BT London, UK
8 Laboratory of Quantum Mechanics of Molecules and Radiative Processes, Tomsk State University, Russia

Reliable representation of the shapes of optical resonances in molecular spectra databases requires non-Voigt effects, such as Dicke narrowing and speed-dependent effects, to be considered. We demonstrate how the line-shape parameters for the case of self-perturbed molecular hydrogen, for which the non-Voigt effects are especially pronounced, can be determined. This work was used as a test case [1] for introducing Hartmann-Tran profile [2] parametrization into the HITRAN database [3] taking advantage of its new relational structure and interface [4, 5].

We performed a detailed analysis of the shapes of the recent high-quality H$_2$ spectra recorded with cavity ring-down spectrometers [6, 7] and optical feedback cavity-enhanced absorption spectrometer [8]. We showed the possible solutions to the problems of strong numerical correlations between the parameters and their temperature dependences. Due to computational inefficiency of the previous line-shapes models, which reproduce the H$_2$ spectra better than the simple phenomenological profiles, we developed, for the purpose of the HITRAN database, a new technique allowing the Hartmann-Tran profile [2] to be adopted for the H$_2$ spectra analysis. In order to increase reliability of spectra representation over wide thermodynamic conditions, we introduced four temperature ranges over which all the line-shape parameters are stored separately. Finally we demonstrate the use of the new relational structure of the HITRAN database [4, 5] and the HITRAN Application Programming Interface (HAPI) [9] for the case of H$_2$ spectra.

References:

Photoassociation spectroscopy of ultracold Rb and Hg mixture

M Witkowski¹, B Nagórny², R Munoz-Rodriguez², P Morzyński², P Żuchowski², R Ciuryło², M Zawada²

¹ Institute of Physics, University of Opole, Oleska 48, PL-45-052 Opole, Poland
² Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziądzka 5, PL-87-100 Toruń, Poland

We present an experimental set-up of two species mercury-rubidium magneto-optical trap (MOT). Rubidium atoms are very convenient for variety of experiments with ultracold samples including BEC, magnetic Feshbach resonances, photoassociation and many more [1]. The experimental methods for cooling and trapping rubidium atoms are well developed and commonly used in many laboratories. On the other hand mercury atoms have a rare combination of features that makes them very interesting for cooling and trapping experiments: diversity of bosonic and fermionic isotopes, no hyperfine or fine structure in ground state, meta-stable states with extremely long life times, low Doppler and recoil temperatures. Moreover, due to very high weight mercury atom is a very good candidate for experimental tests of fundamental physics [2,3]. Because of small black body radiation shift and relatively high frequency of the clock transition it is also attractive for optically based metrology of time [5]. Nevertheless, experiments with cold mercury atoms are challenging due to very inconvenient wavelength (254 nm) of the cooling transition.

In bosons with the $s^2$ configuration the clock transition $^1S_0 - ^3P_1$ is strictly forbidden. The commonly used method to overcome this problem is to induce a coupling with $^5P_0$ state which is optically accessible. In the mercury-rubidium MOT, the presence of cold rubidium atoms can be used to broaden the $^1S_0 - ^3P_0$ clock transition in mercury. It was recently demonstrated [4] in an analogical SrRb system that the molecular states supported by the clock transition are dipole allowed at short range. Therefore, also the shifts and widths of the atomic transitions might be modified by a presence of the cold rubidium atoms.

The preliminary results of photoassociation spectroscopy measurements in Hg-Rb mixture are presented. The particular attention is given to the position of photoassociation lines. Moreover, results of measurements of the scattering properties in various isotopes of the mercury atoms are also presented. The results can provide information about the interaction potential, essential to predict the collisional shift of the mercury $^1S_0 - ^3P_3$ clock transition [5–7]. The information about the interaction potential can also be obtained from loading curves of the MOT and from a photoassociation spectroscopy close to the $^1S_0 - ^3P_3$ trapping transition.

One of the goals of the presented experimental set-up is controlled production of ultracold homo- and heteronuclear molecules by the light-assisted photoassociation. We plan to take advantage of the rubidium $5S - 7S$ two-photon line at 760 nm as the photoassociation transition. The absolute frequency of this transition was measured recently by our group with the highest accuracy [8].

References:

Collisional effects in pure D₂. Ultra accurate measurements and \textit{ab initio} calculations.

M Zaborowski¹, P Wcisło¹, F Thibault², Sz Wójtewicz¹, A Cygan¹, G Kowzan¹, P Masłowski¹, D Lisak¹ and R Ciuryło¹

¹Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Grudziądzka 5, 87-100 Toruń, Poland
²Institut de Physique de Rennes, UMR CNRS 6251, Université de Rennes 1, Campus de Beaulieu, Bât.11B, F-35042 Rennes, France

With recent development in theoretical calculations of molecular states energies of H₂ and its isotopologues [1–2] come calculations of the transition frequencies with uncertainty exceeding the level of 10⁻³ cm⁻¹ for the first overtone band (2–0) [3]. Such predictions create an opportunity for testing relativistic and quantum electrodynamics corrections. Moreover, this also opens a way for searching for new physics like additional long-range hadron-hadron interactions [4]. At this level of accuracy, the line-shape effects, including asymmetry, affects the uncertainty of the H₂, HD and D₂ line position determination in the Doppler limit [5]. Spectral line shapes of D₂ transitions are atypical and difficult to describe. Two approaches are available to overcome this problem. In the first strategy, the spectra may be measured at low pressures, where collisional effects are negligible [3]. Nonetheless, it is experimentally challenging due to extremely low intensities of the quadrupole transitions. Another possibility is to record them at higher pressures and concomitantly describe the collisional influence on the spectral line shapes in a more advanced way. Here we present an example of applying this strategy, for the very weak S(2) transition of deuterium in the 2-0 band, using \textit{ab initio} calculations to take into account the collisional effects on the line shape. This line has been measured with the well established frequency-stabilized cavity ring-down spectroscopy (FS-CRDS) method assisted by an optical-frequency comb (OFC) [6,7]. We used the experimental setup described in Ref. [8]. The line positions at high pressures, up to 1000 Torr, were measured with sub-MHz accuracy.

In addition, we extended our measurements to a wide range of temperatures to validate our \textit{ab initio} model. We compare results from the experiment with \textit{ab initio} quantum scattering calculations, where the generalized spectroscopic cross sections are obtained. The real and imaginary parts allow for calculation of the speed-dependent collisional broadening γ(ν) and shifting δ(ν). The velocity-changing collisions are described by the hard-sphere approximation of the \textit{ab initio} potential. The line shape derived from this approach leads to the speed-dependent billiard-ball profile (SDBBP) [9].

References:

Absolute measurement of the $^1S_0 - ^3P_0$ clock transition frequency in neutral $^{88}\text{Sr}$

P Morzyński¹, M Bober¹, D Bartoszek-Bober¹, J Nawrocki², P Krehlik³, Ł Śliwczyński³, M Lipiński³, P Masłowski³, A Cygan¹, P Dunst², M Garus¹, D Lisak¹, J Zachorowski⁴, W Gawlik⁴, Cz Radzewicz⁵, R Ciuryło¹, M Zawada¹

1 Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grużdżdżaka 5, PL-87-100 Toruń, Poland
2 Time and Frequency Department, Astrogeodynamic Observatory of Space Research Center, Borowiec, Drapałka 4, PL-62-035 Kórnik, Poland
3 Department of Electronics, AGH University of Science and Technology, al. Mickiewicza 30, PL-30-059, Kraków, Poland
4 M. Smoluchowski Institute of Physics, Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University, St. Łojasiewicza 11, PL-30-348 Kraków, Poland
5 Institute of Experimental Physics, Faculty of Physics, University of Warsaw, Pasteura 5, PL-02-093 Warsaw, Poland

We report a stability below $7 \times 10^{-17}$ of two independent optical lattice clocks (Sr1 and Sr2) operating with bosonic $^{88}\text{Sr}$ isotope. The value $(429 228 066 418 008.3(1.9)_{stat}(0.9)_{syst}\text{ Hz})$ of the absolute frequency of the $^1S_0 - ^3P_0$ transition was measured with an optical frequency comb referenced to the local representation of the UTC by the 330 km-long stabilized fibre optical link [1]. The result was verified by series of measurements on two independent optical lattice clocks and agrees with recommendation of Bureau International des Poids et Mesures [2].

Figure 1. Frequencies of the $^1S_0 - ^3P_0$ clock transition in bosonic $^{88}\text{Sr}$ recorded in Sr1 and Sr2 at the indicated MJD (top and bottom panels, respectively). In the left panels each solid circle represent 100 s of averaged data, the light and dark-green regions represent $1\sigma$ standard deviation and standard deviation of the mean, respectively. The offset frequency $\nu_{BIPM}$ is the BIPM recommended frequency value [2]. The right panels show a histogram of the frequency measurements with fitted Gaussian function.

References:

[2] Bureau International des Poids et Mesures (BIPM) Recommended Values Of Standard Frequencies For Applications Including The Practical Realization Of The Metre And Secondary Representations Of The Definition Of The Second, Strontium 88 Atom ($f \approx 429 \text{ THz}$) (BIPM, Sèvres, France, 2009)
Wednesday Poster Session
(We.P)
The problem of numerical precision in spectral line shapes calculations

P Ablewski¹, P Wcisło¹, R Ciuryło¹

¹Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziądzka 5, 87-100 Toruń, Poland

Shapes of spectral lines emitted or absorbed by atoms and molecules in gaseous media can be described by profiles which take into account many physical effects such as finite excited state life time, Doppler effect and interactions between atoms or molecules. In some cases analytical formula is well known [1]. For simple models it is possible to perform calculations leading to exact solution. In more complicated situations this approach fails due to simplifications in physical models describing line shapes. For this reason method based on solution of transport-relaxation equation [2] is being commonly used. This approach allows us to combine interactions between atoms and molecules in single collisional operator which is a sum of internal state-changing and velocity-changing collisional operator [3]. In general these operators can depend on velocity and consist expressions describing correlations between internal-state changing and velocity-changing collisions.

For few simple cases it is possible to find exact solution of transport-relaxation equation analytically, but for real physical systems, solution can be found only numerically. Method based on matrix inversion[4, 5] fails for calculations at low pressures. Remedy for that is an iterative approach proposed in [6], which gives correct solutions for a wide range of input parameters, including the low-pressure limit. It was shown that more complicated physical models of spectral line shapes are needed not only in high precision spectroscopy data analysis for basic research [7], but also in application of spectroscopy, for example in Doppler-broadening thermometry [8].

Our aim was numerical analysis of the iterative method of solving transport-relaxation equation describing spectral line shapes and numerical optimization of used approach. During our work we are looking for optimal dimensions of function base in which calculations are being performed and values of non-physical parameters of numerical method which lead us to find optimal solution of problem in finite number of iterative steps.

Our researches resulted to the conclusions about numerical precision which is main problem in solving transport-relaxation equation for complicated physical line shapes models. We have made a complex analysis of ill-conditioned numerical problem and found solution which can be used to perform accurate and precise calculations in real-time with use of any modern CPU or GPU without need of using supercomputers. We have used couple of programming tricks and tools to be able to optimize calculations for multiprocessor, multicore and multithreaded computer systems.

In this poster results of calculations in numerical precisions corresponding to IEEE754 [9] and IEEE854 [10] standards and conclusions of them are being shown.

References:

Computer simulation and experimental studies of the NI 3p$^2$S$^o$–3d$^2$P spectral line Stark broadening

W Olchawa$^1$, A Barteka$^1$ and A Bacławski$^1$

$^1$University of Opole, Institute of Physics, ul. Oleska 48, 45-052 Opole, Poland

The computer simulation method [1] is successfully used for calculation of Stark broadening of spectral lines by plasmas, mainly for hydrogen, hydrogen-like and helium transitions. The new kind of such computer simulation, dedicated to lines, which energy levels are influenced only by the quadratic Stark effect, is introduced and tested in this paper. The electronic width of the well isolated NI multiplet 3p$^2$S$^o$–3d$^2$P obtained from computer simulation is compared with results of our measurement and with the result taken from Griem [2].

The model of the plasma is essentially the same as in commonly used by computer simulation methods, e.g. [3]. The symmetrical splitting formula (Strang [4]) was applied to solve the Schrödinger equation of evolution of the emitter perturbed by ions and electrons. Our new method, based on application of the symmetrical formula, leads to unitary evolution of time. The universal spectral decomposition, recasting the matrix of the electric dipole emitter-plasma interaction in terms of its eigenvalues and eigenvectors, is presented. The decomposition is specific due to block form of the matrix, corresponding to the quadratic Stark effect. An example of results obtained by computer simulation is shown in Figure 1.

Figure 1. Real and imaginary parts of the autocorrelation function (circles) fitted by the inverse Fourier transformation of the $j(x)$ function (solid lines) are presented. The simulated profile is shown in the inset.

Measurements were performed using a wall-stabilized arc, operated at atmospheric pressure. The radiation of the plasma, emitted from homogeneous plasma layers in end-on direction, was measured using a grating-spectrometer with a two-dimensional CCD detector. Experimental values of Stark broadening parameters have been obtained from the best fit procedures applying the Griem-like profile $j(x)$ [2], convoluted with the corresponding Doppler and apparatus profiles.

Results of the tests show that the new computer simulation method provides promising results and can be very useful in calculations of Stark broadening parameters.

References:

EUV induced photoionized plasma, a new medium for spectral investigation

A Bartnik¹, P Wachulak¹, H Fiedorowicz¹, W Skrzczanowski¹, T Fok¹, R Jarocki¹, L Wegrzynski¹

¹Institute of Optoelectronics, Military University of Technology, Warsaw, Poland

Photoionized plasmas are not produced in normal conditions on Earth, but are common in Space. Most of the matter in the Universe is ionized due to heating by gravitational compression or exposure to intense EUV or X-ray radiation. Photoionization of gases is a key process in formation of different kinds of astrophysical plasmas, especially located close to strongly radiating compact objects. Spectral investigations of these plasmas can provide information about astrophysical objects emitting X-ray radiation that irradiate surrounding gases. Interpretation of the observed spectra require constructing of physical models and performing laboratory experiments [1,2] that support the accuracy of the models. Parameters of low temperature photoionized plasmas created in laboratory can be easy controlled and adjusted for specific conditions that can be encountered in Space. It concerns for example hydrogen plasmas with parameters similar to photospheres of white dwarfs. The corresponding experiments allowing for investigation of hydrogen Balmer emission and absorption line profiles were performed at the Z Pulsed Power Facility at Sandia National Laboratories [3].

Low temperature photoionized plasmas can be also produced using laser produced plasma (LPP) extreme ultraviolet (EUV) sources. In this work the corresponding investigations were performed using LPP EUV sources with different parameters. The sources were based on two different laser systems with pulse energies ranging from 0.8 J to 10J and pulse duration 4-10 ns. Laser plasmas were produced by irradiation of double stream gas puff targets with Xe or KrXe mixture as the working gas. EUV or SXR radiation was focused using grazing incidence collectors of different types. The focusing collectors were based on multifoil, ellipsoidal or paraboloidal mirrors optimized for specific wavelength ranges. Different gases were injected into the interaction region, perpendicularly to an optical axis of the irradiation system, using an auxiliary gas puff valve. Irradiation of the gases resulted in ionization and excitation of atoms and molecules forming photoionized plasmas. Spectra in EUV and UV/Vis ranges were measured using a grazing incidence, flat-field spectrograph (McPherson Model 251), equipped with a 450 lines/mm toroidal grating and an Echelle Spectra Analyzer ESA 4000 respectively. In most cases the emission lines were assigned to singly charged atomic or molecular ions. For some ions spectral lines corresponding to inner shell transitions were detected. Spectral intensities and widths were used for estimation of electron temperature and density respectively.

References:


A very large aperture spectrometer for low light OES

R Baude\(^1\), A Escarguel\(^1\), P David\(^1\)

\(^1\) PIIM, Avenue Escadrille Normandie-Niemen, 13397 Marseille cedex 20, France

In low light experiments such as low temperature plasma or astronomical spectroscopy usual tools such as Czerny Turner based spectrometer (CTS) may have a limited efficiency [1]. The spectrometer brightness limitation is due to the fact that a large entrance slit implies a large broadening of the instruments profile. Thus most spectrometers are used with an aperture of a few tens of micrometers.

In the early seventies the CERCO (the French center for optical research and computation) under the supervision of Prof. Lesage designed the so-called Bowen Chamber spectrometer (BCS). The BCS has the particularity to accept a large aperture slit, up to 1000 µm, without significant degradation of the spectrum. Figure 1a) shows the schematic view of the spectrometer. The spherical collimating mirror reflects the light from the entrance slit on a flat reflecting mirror. The collimated beam is reflected toward the holographic grating. Then, the dispersed light enters the Bowen chamber. The chamber is composed of two concentric mirrors, the primary mirror is convex and the secondary is concave.

\[\text{Figure 1. a) Schematic view of the BCS. b) Luminosity (L), resolving power (Rp) and product L.Rp as a function of the entrance slit aperture for the BCS (red) and the CTS (blue).}\]

Figure 1b) presents the comparison of the product (L.Rp) of the luminosity (L) and the resolving power (Rp) for the BCS (bold red) and a classical CTS, the CHROMEX 500is (bold blue). We see that for the CTS the L.Rp is maximum at 100µm aperture due to an exponential decrease of the Rp. The BCS L.Rp increases up to the maximum aperture mainly due to the slow linear decreasing Rp.

Despite the interesting characteristics of the BCS only a few traces are found in the literature [2]. The authors wish to discuss the specifications of the BCS with spectroscopists before prototyping a reasonable size spectrometer based on the BCS. Recent design modifications on the 1972 BCS model have shown promising results with an improvement of 4 times the luminosity with constant L.Rp.

References:

Multi-photon spectroscopy of the many-electron atoms and ions of the Debye plasma a laser field

V Buyadzhi

1 Odessa State University – OSENU, Lvovskaya str. 15, Odessa, 65016, Ukraine

The interaction of a high intensity laser field with an atomic system results in multi-photon excitation, ionization and shifts of the energy levels [1]. A great number of physically different effects occur in atomic systems (ensembles) in dependence upon an intensity, frequency, multi-colority of laser field, energy spectrum structure of an atomic system etc. In the last decade a considerable interest has attracted studying of the elementary atomic processes in plasma environments because of the plasma screening effect on the plasma-embedded atomic systems. In this paper one-and two-color multi-photon spectroscopy of a number of transitions in a hydrogen, lithium and caesium atoms and ions (free and immersed in a Debye plasmas) is studied theoretically. The theoretical approach is based on the relativistic operator perturbation theory (PT) and relativistic energy approach [2]. The energy shift and width of the multiphoton resonances are calculated within an energy approach, which is based on the Gell-Mann and Low adiabatic formalism and formalism of the relativistic Green function for the Dirac equation [2]. The plasmas medium effects are taken into account by introducing the Yukawa-type electron-nuclear attraction and electron-electron repulsion potentials into the electronic Hamiltonian for N-electron atom (ion) in a plasma [3]. There is studied a plasmas with typical corresponding parameters: the Debye lengths $\lambda_D=5$ a.u. (solar core: temperature $T=10^{7}$K; density $10^{32}$ m$^{-3}$) and 25 a.u. (inertial confinement: temperature $T=10^{4}$K; density $10^{28}$ m$^{-3}$). It has been quantitatively determined a variation of the multi-photon resonance enhancement frequencies in dependence upon the plasmas parameters (the Debye length). For example, the corresponding values for the resonance enhancement frequencies $\omega_{r1}$, $\omega_{r2}$ and $\omega_{r3}$ for the $1s$–$4f$ transition in the hydrogen for different Debye lengths ($\lambda_D=5$-50 a.u.) are between 0.009 and 0.023a.u. The obtained results reveal the plasma effects on the multi-photon transition amplitudes for the plasma-embedded atoms (ions). The hydrogen plasma results are compared with the similar data, presented in [4].

References:

Spectroscopy of Rydberg atoms in a black-body radiation field: Relativistic theory of excitation and ionization

V Buyadzhi\textsuperscript{1}, P Zaichko\textsuperscript{1}, O Khetselius\textsuperscript{1}, A Ignatenko\textsuperscript{1}, A Svinarenko\textsuperscript{1}

\textsuperscript{1}Odessa State University – OSENU, Lvovskaya str. 15, Odessa, 65016, Ukraine

The accurate radiative transitions probabilities, ionization rates are needed in astrophysics, plasma diagnostics etc. In the last years an especial interest attracts a diagnostics of the ultracold plasma. Here we present an advanced relativistic quantum defect and model potential method to calculation of the spectra, radiation amplitudes for the Rydberg Na, K, Rb, Cs atoms, their ionization rates of states with \( n = 10-100 \) in the field of blackbody radiation (BBR). The starting master method is the combined energy approach \([1a]\) and relativistic many-body perturbation theory with the zeroth model potential and quantum defect approximation \([1b]\). It provides sufficiently correct and simultaneously simplified numerical procedure to determination of the corresponding radiative transition and ionization properties.

Interaction of the Rydberg atom \( A(nL) \) with the BBR induces transitions to the bound states and states of continuum: \( A(nL)+\hbar \omega_{\text{BBR}} \rightarrow A^+ + e^- \), where \( \hbar \omega_{\text{BBR}} \) - an energy of the BBR photon; \( A^+ \) is the corresponding atomic ion and \( e^- \) is a free electron, which is emitted during the Rydberg atom ionization. Probability of induced BBR transition between the \( nlj \) and \( n'lj' \) states is determined by the standard radiative matrix element and number of photons for \( \omega_{\text{BBR}} \),

\[
W(nlj \rightarrow n'l'j') = \frac{i}{\exp(\omega_{\text{BBR}}/kT)-1} \sum_{\omega} \sigma_{nlj}^{(\omega)} \rho(\omega,T) \omega \]

A rate of ionization in the initial bound Rydberg state \( nL \) is determined by an integral (integration is carrying out on the BBR frequency) of the kind:

\[
\int_{\omega_{\text{el}}}^{\infty} \sigma_{nlj}^{(\omega)} \rho(\omega,T) d\omega,
\]

where, \( \sigma_{nlj}^{(\omega)} \sim e^2 M^2_{nl \rightarrow \omega} + (l+1)M^2_{\omega \rightarrow \omega+1} \), \( \omega_{\text{el}} \) —is the threshold frequency of ionization of the atom in the Rydberg state \( nL \) with the corresponding quantum defect. The calculated data (as example in table 1 there are our data on the BBR rates for Na) on the energy parameters, radiation amplitudes for RA Na, K, Rb, Cs, their ionization rates of states with \( n = 10-100 \) in the BBR field (\( T=300-600K \)) are presented and compared with available experimental data (Kleppner et al; Burkhardt et al) and some results of the alternative theories (Glukhov-Ovsiannikov; Lehman; Dyachkov-Pankratov, Beterov et al) \([2]\).
Advanced relativistic model potential approach to computing the radiation transition and autoionization characteristics for atoms and multicharged ions

V Buyadzhi\textsuperscript{1}, O Khetselius\textsuperscript{1}, A Glushkov\textsuperscript{1}, O Antoshkina\textsuperscript{1} and T Kulakli\textsuperscript{1}

\textsuperscript{1} Odessa State University – OSENU, Lvovskaya str. 15, Odessa, 65016, Ukraine

Accurate radiative decay widths and probabilities, oscillator strengths of atomic transitions are needed for example in astrophysics, thermonuclear plasma diagnostics, in fusion research and laser physics. Traditionally, advanced modeling is important and of current interest in the theory of atomic spectra and associated spectral lines. In our work we present an advanced relativistic model potential approach to compute radiation transition and ionization probabilities and oscillator strengths for alkali atoms and multicharhed ions. The starting master method includes the combined relativistic energy approach and relativistic many-body perturbation theory (PT) with the zeroth order, optimized one-particle approximation [1]. The key feature of the presented fundamental theory is an implementation of the relativistic model potential (one version) or quantum defect (second version) approximation into the framework of the S-matrix energy formalism, applicable to multi-electron atomic system. It provides sufficiently correct, and equally, simplified numerical procedure to evaluate the corresponding radiative transition and ionization properties. This approach appears significantly more advantageous when compared to the standard Hartree-Fock and Dirac-Fock methods. As illustration we computed energies and probabilities of the radiative transitions and ionization characteristics for Li-, Cs-, Fr-like multi-charged ions and neutral atoms (see some data for Fr table 1). Our approach provides reasonable agreement with experiment. We evaluated that all results for oscillator strengths, obtained within our approach in different photon propagator gauges: G1-Coulomb, G2-Feynman; G3-Babushkin are practically equal that is provided by using an effective QED energy procedure.

Table 1. Theoretical reduced dipole matrix elements for a number of transitions of Fr: relativistic Hartree-Fock (RHF; Dzuba-Flambaum); relativistic PT with the Dirac–Fock approximation (Safronova-Johnson-Derevianko), empirical relativistic model potential method (ERMP) by Marinescu et al and our data (experiment: 7p_{1/2}-7s=4.277; 7p_{3/2}-7s=5.898);

<table>
<thead>
<tr>
<th>Transition</th>
<th>PT-DF</th>
<th>ERMP</th>
<th>RHF</th>
<th>Our data</th>
</tr>
</thead>
<tbody>
<tr>
<td>7p_{1/2}-7s</td>
<td>4.256</td>
<td>-</td>
<td>4.279</td>
<td>4.272 (G1)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>4.304</td>
<td>4.274 (G2)</td>
</tr>
<tr>
<td>8p_{1/2}-7s</td>
<td>0.327</td>
<td>0.304</td>
<td>0.291</td>
<td>0.301</td>
</tr>
<tr>
<td></td>
<td>0.306</td>
<td></td>
<td></td>
<td>0.339</td>
</tr>
<tr>
<td>9p_{1/2}-7s</td>
<td>0.110</td>
<td>0.096</td>
<td>-</td>
<td>0.092</td>
</tr>
<tr>
<td>7p_{3/2}-7s</td>
<td>5.851</td>
<td>-</td>
<td>5.894</td>
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<td>5.927</td>
<td></td>
</tr>
<tr>
<td>8p_{3/2}-7s</td>
<td>0.934</td>
<td>0.908</td>
<td>0.924</td>
<td>0.918</td>
</tr>
<tr>
<td></td>
<td>0.909</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9p_{3/2}-7s</td>
<td>0.436</td>
<td>0.420</td>
<td>-</td>
<td>0.426</td>
</tr>
</tbody>
</table>

References:


On the calculations of the influence of a collisional correlation on the Dicke narrowing of a spectral line shape

H Cybulski¹, R Ciuryło¹

¹Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziądzka 5/7, 87-100 Toruń, Poland

Molecular line shapes are affected by several physical effects. In addition to well-known Doppler broadening and collisional broadening and shifting, many other effects like both the molecules’ center-of-mass velocity changes, Dicke narrowing, the speed dependence of collisional broadening and shifting or line mixing should be taken into account. In this work we focus on the Dicke narrowing effect for the collisionally broadened and shifted lines.

As it was indicated by Rautian and Sobelman [1] and discussed by others on classical and quantum ground [2-4] a correlation between the velocity-changing and dephasing collisions can result in a significant reduction of the Dicke narrowing effect. In some cases also an asymmetry of the line shape can appear [5,6].

Here, we employ the classical line-shape theory [1,7] to investigate this effect in more detail. We aim for an analysis of the influence of the velocity-changing and dephasing collisions’ correlation on the shape of spectral lines in cases of atom-molecule systems. Recently, it has been demonstrated that a shape of the interaction potential can affect significantly the calculated Dicke narrowed line profiles [8].

In our calculations classical (empirical) as well as high-level quantum-mechanically ab initio evaluated interaction potentials for some model systems are used.

References:

Studies of Stark broadening of Li I 460 nm and 497 nm spectral lines in laser ablation plasma

K Dzierżęga 1, M R Gavrilović 2, E Stambulchik 3, T Pięta 1, M Cvejić 2, S Jovicević 2, B Pokrzywka 4, W Zawadzki 1

1 Institute of Physics, Jagellonian University, ul. Łojasiewicza 11, 30-348 Kraków, Poland
2 Institute of Physics, University of Belgrade, P.O.Box 68, 11080 Belgrade, Serbia
3 Faculty of Physics, Weizmann Institute of Science, Rehovot 7610001, Israel
4 Institute of Physics, Pedagogical University, ul. Podchorąży 2, 30-084 Kraków, Poland

We present the results of experimental and theoretical studies of Stark broadening of Li I 460 nm and 497 nm spectral lines in laser-induced plasma (LIP). A Li LIP was induced by 1064 nm Nd:YAG laser ablation of Al₂O₃ : Li₂CO₃ : MgCO₃ (9 : 4 : 1) pellets in a vacuum chamber filled with argon at 200 mbar. For plasma diagnostics, the laser Thomson scattering (TS) technique was applied. In TS method, local values of $n_e$ and $T_e$ are directly derived from the electron feature of the TS spectrum without any assumption about the plasma chemical composition or its equilibrium state [1]. To that end, another, single mode, Nd:YAG laser at 532 nm was used. This laser beam was directed orthogonally to the plasma generating one. The emission from plasma and the laser-scattering light were observed perpendicularly to the plane of laser beams by imaging the investigated plasma plume onto the entrance slit of a Czerny-Turner spectrograph. The spectra of the scattered light and the plasma emission were recorded over wavelength range of 13.3 nm using a gated two-dimensional intensified charge-coupled device (ICCD) camera. Self absorption of studied Li I spectral lines was verified with the back-reflecting mirror method as described in Cvejić et al [2]. The sensitivity of the experimental system was corrected for, pixel by pixel of the ICCD, using a halogen-deuterium lamp.

![Figure 1. Sketch of the experimental setup (a) and experimental results for LIP 1000 ns after ablating laser pulse, b) plasma image with the origin at the target, c) the red shifted part of the electron feature of the TS spectrum after subtraction of plasma emission while illuminating plasma layer 0.6 mm away from pellet surface, and d) spectrum of the Li 460 nm spectral line from the same LIP layer as in (c).](image)

Spatially resolved measurements, performed for the time interval between 600 ns and 2.2 μs, show electron density and temperature to vary from $1.45 \times 10^{21}$ m$^{-3}$ to $3.53 \times 10^{22}$ m$^{-3}$ and from 1.96 eV to 1.06 eV, respectively, in the plasma core. The comparison between measured and calculated [3] line widths indicates very good agreement for the Li 460 nm line with forbidden component while they diverge for the isolated Li 497 nm line. This discrepancy increases with electron density and temperature, i.e. at earlier stages of plasma evolution.

References:

Solid rocket stability with reflective and non-reflective outflow

T S Elliot¹ and B H Flanigan²

¹ Department of Mechanical Engineering, Assistant Professor, University of Tennessee at Chattanooga, Chattanooga, TN 37403, USA
² Department of Mechanical Engineering, Graduate Research Assistant, University of Tennessee at Chattanooga, Chattanooga, TN 37403, USA

Hydrodynamic instabilities, or waves, that translate into pressure oscillations are analyzed through consideration of fluid-wall interactions in solid rocket motors. These pressure oscillations result in vibrations which can lead to changes in flight characteristics, design failure, or other undesirable effects. In recent years research efforts have been devoted to the modeling of pressure oscillations in order to understand their character [1] and design for mitigation. This study will utilize a two dimensional framework to understand and quantify the internal flow of a simulated solid rocket motor, illustrated in Figure 1 below, when considering either reflective or non-reflective outflow conditions. Reflective boundary conditions are typically used when the triggering of acoustic waves is desired whereas non-reflective conditions are used when solving viscous flows to allow free flow of vortices through the outflow boundary [2]. In this study both conditions are considered for their merits and correlations between them are discussed.

![Figure 1. Schematic of a simulated solid rocket motor with equally injecting headwall and sidewalls](image)

References:

Cavity and baffle design for acoustic attenuation of firearms

T S Elliott\textsuperscript{1} and B H Flanigan\textsuperscript{2}

\textsuperscript{1} Department of Mechanical Engineering, Assistant Professor, University of Tennessee at Chattanooga, Chattanooga, TN 37403, USA
\textsuperscript{2} Department of Mechanical Engineering, Graduate Research Assistant, University of Tennessee at Chattanooga, Chattanooga, TN 37403, USA

This study focuses on the development of a universal framework to perform spectral analysis of pressure signals and sound pressure levels over distance for arbitrary firearm suppression devices. A Large Eddy Simulation (LES) will be solved via the implicit-time formulation which will be compared with the output from the Flow Simulation solver built into SolidWorks. The work is motivated by the need for design optimization with regard to reduced sound pressure levels when suppression devices are used at training and competition sites. The concept of modeling and performing simulations to predicted the sound pressure levels is not a new development [1,2] yet many manufactures develop devices using very rudimentary calculations or in some cases intuition from past usage experience. The aim is to make using the Ffowcs Williams and Hawkings (FWH) equation [3] compatible with an existing flow solver where physical pressure oscillations are the primary output.

References:

Vibrational structure and cooperative electron-gamma–nuclear effects in molecular photoelectron spectra within Green’s functions and density functional methods

A Glushkov\(^1\), O Khetselius\(^1\), A Kuznetsova\(^1\), Yu Dubrovskaya and E Ponomarenko\(^1\)

\(^1\)Odessa State University – OSENU, Lvovskaya str. 15, Odessa, 65016, Ukraine

We develop an effective combined theoretical approach to vibrational structure in photoelectron spectra of molecules and present an effective computational code. The approach is based on the Green’s function method and density functional theory (DFT) formalism \([1]\). The density of states, which describe the vibrational structure in molecular photoelectron spectra, is calculated with the help of combined DFT-Green’s-functions approach. In addition to exact solution of one-bode problem different approaches to calculate reorganization and many-body effects are presented. In all cases no data about the molecular ion are needed and all transitions except those between linear and bent configurations are included. The density of states is well approximated by using only the first order coupling constants in the one-particle approximation. It is important that the computational procedure is significantly simplified with using the quasiparticle DFT formalism. Numerical data are listed for the CH, HF and other molecules. When the change of frequency due to ionization is small, the density of states can be well approximated using only one parameter \(g\):

\[
N_i(\varepsilon) = \sum_{n=1}^{\infty} e^{-\frac{\varepsilon_n}{m}} \delta(\varepsilon - \varepsilon_i + \Delta \varepsilon_i + n \cdot \hbar \omega), \quad S = g^2 \langle \hbar \omega \rangle^2.
\]

In case the frequencies change considerably, the intensity distribution of the most intensive lines can analogously be well approximated by an effective parameter \(S\). In table 1 the experimental \((S^{exp})\) and theoretical \((S^{th})\) values of the S parameter are presented for the molecules of CH, HF: \(S^0\) is the value without accounting correlation and reorganization corrections; \(S^{(b)}\) the values of the parameter with accounting correlation and reorganization corrections within our combined GF-DFT method.

Table 1. The experimental \((S^{exp})\) and theoretical \((S^{th})\) values of the S parameter are presented for different molecules (CH, HF): \(S^0\) is the value without accounting correlation and reorganization corrections; \(S^{(b)}\) – the combined GF-DFT method (b).

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Theory</th>
<th>(S^{th})</th>
<th>(S^{exp})</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>CH</td>
<td>(S^0)</td>
<td>0.22(1(\pi))</td>
<td>0.105(3(\sigma))</td>
</tr>
<tr>
<td></td>
<td>(S^{(b)})</td>
<td>0.2711</td>
<td>0.1134</td>
</tr>
<tr>
<td>HF</td>
<td>(S^0)</td>
<td>0.126(1(\pi))</td>
<td>1.90(3(\sigma))</td>
</tr>
<tr>
<td></td>
<td>(S^{(b)})</td>
<td>0.1920</td>
<td>2.0534</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.35</td>
<td>2.13</td>
</tr>
</tbody>
</table>

It is also presented consistent, quantum-mechanical approach to computing electron-nuclear \(\gamma\) transition spectra (set of vibration-rotational satellites in molecule) of nucleus in molecule and based on the using the DFT potential approximation for potential curves of the diatomic molecules. Estimates are made for vibration-rotation-nuclear transition probabilities in a case of the emission and absorption spectrum of nucleus \(^{127}\)I \((E^{(0)}_{\gamma}= 203\) keV\) linked with molecule H\(^{127}\)I and compared with other data \([2]\).

References:


Relativistic energy approach to heavy atoms in a strong field: Autoionization and multi-photon resonances

A Glushkov

1 Odessa State University – OSENU, Lvovskaya str. 15, Odessa, 65016, Ukraine

It is presented an advanced combined relativistic energy approach and relativistic operator perturbation theory (PT) and [1,2] and its application to studying interaction of the finite Fermi systems (heavy atoms, nuclei, molecules) with a strong external (DC electric and laser) field. The energy approach is based on the Gell-Mann and Low adiabatic formalism and method of the relativistic Green’s function for the Dirac equation with complex energy. The operator perturbation theory formalism includes a new quantization procedures of the Dirac (Schrödinger) equation states of the finite Fermi-systems in a strong field. The essence of the operator PT is the inclusion of the well-known method of "distorted waves approximation" in the frame of the formally exact PT. To overcome formal difficulties, the zeroth order Hamiltonian was defined by the set of the orthogonal eigen functions and eigen energies without specifying the explicit form of the corresponding zeroth order potential. In the case of the optimal zeroth order spectrum, the PT smallness parameter is of the order of G/E, where G and E are the field width and bound energy of the state level. It has been shown that G/E ≤ 1/n even in the vicinity of the "new continuum" boundary (n is the principal quantum number).

Results of the calculation for the multi-photon resonance and ionization profile in Na,Cs, Ba atoms are listed [2]. We have studied the cases of single-, multi-mode, coherent, stochastic laser pulse shape. New data on the DC, AC strong field Stark resonances, multi-photon and autoionization resonances, ionization profiles for a few heavy atoms (Eu, Tm, Gd, U) are presented. It has been firstly studied a giant broadening effect of the autoionization resonance width in a sufficiently weak electric (laser) field for uranium. It is declared that probably this effect is universal for optics and quantum chemistry of lanthanides and actinides and superheavy elements.

The direct interaction of super intense laser field (I~10^{25}-10^{35} W/cm^2) with nuclei is studied within the operator PT and the relativistic mean-field (plus Dirac-Woods-Saxon) model [2,3]. We present the results of AC Stark shifts of single proton states in the nuclei ^{16}O, ^{168}Er and compared these data with available data. New data are also listed for the ^{57}Fe and ^{171}Yb nuclei. Shifts of several keV are reached at intensities of roughly 10^34 W/cm^2 for ^{16}O, ^{57}Fe and 10^32 W/cm^2 for heavier nuclei. It is firstly presented a consistent relativistic theory of multiphoton-resonances in nuclei and first estimates of energies and widths for such resonances are presented for ^{57}Fe and ^{171}Yb nuclei.

References:

In gas laser ionization and spectroscopy of radioactive ion beams
and the need for spectral line characterization

C Granados, R Ferrer, L P Gaffney, M Huyse, Yu Kudryavtsev, E Mogilevskiy, S Raeder, S Sels, P Van den Bergh, P Van Duppen and A Zadvornaya

1KU Leuven, Instituut voor Kern- en Stralingsfysica, Celestijnenlaan 200D, B-3001 Leuven, Belgium

The in-gas laser ionization and spectroscopy technique (IGLIS) combines the chemical universality of a gas-cell for thermalizing nuclear-reaction products with the efficiency and high selectivity of a laser ion source to produce and study radioactive ion beams [1,4]. Radioactive nuclei produced in nuclear reactions, recoil from the target and thermalize and neutralize in a gas-cell via the interaction with the buffer gas, typically argon or helium at 100 to 500 mbar. Then, optical spectroscopy on the hyperfine atomic levels of the exotic nuclei is performed in order to obtain nuclear information such as magnetic dipole and electric quadrupole moments and differences in mean charge radii [2,3]. However, atom-atom interaction of the nuclear reaction products with the buffer gas broadens the atomic spectral lines masking important hyperfine structure and consequently important nuclear ground state properties cannot be extracted [3]. Typical values of the total FWHM of the spectral lines lies between 4 and 10 GHz. The spectral line broadening and shift due to collisions with the buffer gas was studied for both excited atomic and auto-ionizing states. Results on the collision broadening and shift will be present for $^{58}$Ni, $^{63}$Cu, $^{107}$Ag, $^{120}$Sn and $^{215}$Ac.

To overcome the inherent collisional shift and broadening present when performing spectroscopy in the gas-cell, the in-gas-jet ionization and spectroscopy technique was demonstrated in the case of stable copper [4] and short live actinium isotopes [5]. The low density and low temperature present in a supersonic gas expansion, reduces collisional shift and broadening effects by at least two orders of magnitude. In the case of neutron deficient actinium isotopes, a reduction from 3.8 GHz to 400 MHz was obtained in the gas-jet configuration. The ultimate width and shape of the spectral lines is determined by the Mach number of the supersonic jet.

In order to characterize the optimum gas-jet formation from a De Laval (convergent-divergent) nozzle the Planar Laser Induced Fluorescence (PLIF) technique was applied and successfully demonstrated for atomic species (copper). Application of the PLIF technique allows us to study temperature, density and velocity distributions in the jet, that will provide the best conditions for laser spectroscopy of radioactive beams. In addition, direct comparison between the fluorescence and ionization spectroscopy, the influence of the cluster formation in the gas-jet conditions and on the final shape of the atomic lines will be study.

Result on the characterization of the supersonic jet for stable copper and the on-line laser spectroscopy of actinium isotopes will be presented as well as the future plans for the IGLIS laboratory at the KU Leuven.

References

Plasma Kinetics Based Model for the Formation Mechanism of Catalyst Nanoparticles from the Thin Catalyst Film for the Carbon Nanostructures Growth

R Gupta¹, S C Sharma¹ and R Sharma¹

¹ Department of Applied Physics, Delhi Technological University (DTU), Shahbad Daulatpur, Bawana Road, Delhi-110042, India

The present model considers the thermal and energy balance of the catalyst film surface placed over the substrate surface during plasma processing i.e., plasma etching of thin film. The formation mechanism includes heat radiation, energy fluxes of different particles, kinetics of electrons, positively charged ions and neutrals originating from the plasma. It is found that catalyst nanoparticles with different diameters are formed when catalyst film having different thickness are placed over substrate surface [1]. The results also illustrate that plasma parameters (plasma density and plasma temperature) significantly affect the nanoparticle size. The diameter of the catalyst nanoparticle decreases when number density of etching gas increases [2]. In addition, it is also found that temperature of the substrate increases and attains the constant value after some time during this plasma treatment. The theoretical predictions are in concurrence with the experimental results.

References:

Theoretical investigation of the effect of hydrogen gas flow rate on the growth and field emission properties of the graphene sheet

N Gupta¹, S C Sharma¹ and R Sharma¹

¹ Department of Applied Physics, Delhi Technological University (DTU), Shahbad Daulatpur, Bawana Road, Delhi-110042, India

A theoretical model describing the plasma-assisted catalytic growth of graphene [1] that incorporates the charging rate of the graphene, kinetics of all the plasma species, formation of carbon clusters and large graphene islands [2] because of diffusion and accretion of ions on the catalyst nanoparticle has been developed. Using this model, it is shown that the variation in flow rate of the hydrogen gas can strongly affect the growth and field emission properties of the graphene sheet. Numerical calculations on the effect of hydrogen gas flow rate on the hydrocarbon ion density and its consequent effects on the height and thickness of the graphene sheet have been carried out for typical glow discharge parameters. It is found that upon an increase in the hydrogen gas flow rate, the thickness of the graphene sheet decreases. Using the results obtained, the field emission factor \(\beta \approx \frac{h}{t}\) [3] is estimated and it is found that \(\beta\) increases with the increase of hydrogen gas flow rate. Some of our results are consistent with the available experimental observations. The results of the present model can serve as a major tool in analyzing the field emission characteristics of the graphene sheet.

References:

Line shapes in the presence of nonlinear wave collapse in a plasma

I Hannachi¹,², J Rosato¹, R Stamm¹, Y Marandet¹

¹ Physique des Interactions Ioniques et Moléculaires, UMR 7345, AMU-CNRS, Marseille, France
² PRIMALAB, Faculty of Sciences, University of Batna, Batna, Algeria

In plasmas coupled to an external energy source like a beam of energetic electrons, one can observe the nonlinear coupling of Langmuir waves with ion sound and electromagnetic waves. This nonlinear interaction of waves changes the structural and radiative properties of plasmas [1]. Coherent wave packets are trapped in regions of high intensity, and are subjected to a wave collapse cycle. During this cycle the electric field of the wave can reach values several hundred times larger than the Holtsmark field.

We have studied the main features of wave packets in a fully ionized and unmagnetized plasma affected by nonlinear wave collapse, and propose here a simple model for evaluating the changes expected on a hydrogen line shape emitted under such conditions. According to analytical studies (using e.g. Zakharov equations or a nonlinear Schrödinger equation [2]) or simulations calculations [1], the electric field experienced by an emitter is a sequence of solitons, each one corresponding to a cycle of wave collapse in a localized region of the plasma. We model such an electric field with a stochastic renewal process using an exponential waiting time distribution and a half-normal probability density function for the electric field magnitude of the turbulent wave packet. We then calculate the dipole autocorrelation function and the shape of hydrogen lines by a numerical integration of the Schrödinger equation. The first results obtained with a simulation calculation of the hydrogen lines show that nonlinear wave collapse can provide an additional broadening to the Stark profile created by the background plasma. These calculations have been performed in a bulk hydrogen plasma with a density \(N_e=10^{18} \text{ m}^{-3}\) and a temperature \(T=2.8 \times 10^4 \text{ K}\).

![Electric field component acting on an emitter during a sequence of wave collapse](image)

*Figure 1.* Electric field component acting on an emitter during a sequence of wave collapse, as a function of time expressed in units of the inverse plasma frequency \(\omega_p^{-1}\) (\(\omega_p = \sqrt{N_e e^2 / m \epsilon_0}\), with \(e\) and \(m\) the electron charge and mass, and the permittivity of free space). The field is expressed in units of the Holtsmark field \(E_0\), which is the magnitude of a field created by a particle at the average interparticle distance in the bulk plasma. The fast oscillation is at the electronic plasma frequency, and the envelope of each soliton is Lorentzian.

References:

X-ray emission in interaction of highly charged xenon ions with surfaces

Ł Jabłoński1, D Banaś1, J Braziewicz1, J Czub1, P Jagodzinski2, A Kubala-Kukuś1, D Sobota1, I Stabrawa1, M Pajek1

1 Institute of Physics, Jan Kochanowski University, Kielce, Poland
2 Department of Mathematics and Physics, University of Technology, Kielce, Poland

The interaction of slow highly charged ions (HCI) with surfaces is dominated by a high Coulombic potential energy of the projectile, as compared to its kinetic energy [1]. These conditions provide unique opportunity for formation the so-called „hollow atoms” [2] in the process of neutralization of HCI at surfaces in which, first, the electrons are captured into high Rydberg state while inner shells remain empty. Such highly excited exotic „hollow atoms” quickly deexcite in a cascade of Auger and radiative transitions. Consequently, the emitted Auger electrons and X-rays carry information about the structure and relaxation processes for these exotic form of matter.

Here we report on the measurements of X-rays emitted in interaction of ~ 100 keV Xe\textsuperscript{q+} ions (q=25-35) with metallic Ta foil using a semiconductor drift detector (SDD). In these experiments the highly charged Xe\textsuperscript{q+} ions were produced in the electron beam ion trap (EBIT) trap of the EBIS-A facility [3-5], which can deliver a wide range of beams of slow HCI extracted from the EBIT, charge state analyzed in a dipole magnet, and focused on a sample mounted on a manipulator. The X-rays were measured with a 12-μm thick XFLASH detector having about 100 eV energy resolution for studied 1-2 keV photon energies. In these experiments the whole system was kept at UVH conditions, at 10\textsuperscript{-10} mbar level.

**Figure 1.** Measured spectrum of X-rays emitted in interaction of 119 keV Xe\textsuperscript{35+} ions with Ta foil.

The X-rays observed in interaction of slow Xe\textsuperscript{q+} ions with a metallic tantalum foil (see Fig.1) originate from radiative nl-3d transitions for ion charge states q=25-35 having vacancies in the M\textsubscript{4,5}–subshell (3d). In particular, two groups of x-ray transitions from 4l-3d and nl-3d (n \( \geq \) 5) were experimentally resolved and interpreted using calculated electron binding energies for nl-states. However, more detailed atomic structure MCDF calculations as well as a modeling the relaxation Auger and radiative processes are needed to fully describe the observed X-ray spectra. Such calculations are crucial to evidence, for instance, the internal dielectronic excitation process, which was observed in interaction of HCI with surfaces [6].

**References:**

Optical frequency comb spectroscopy of $\text{H}_2\text{O}$ and OH in a flame

L Rutkowski$^1$, A Khodabakhsh$^1$, A C Johansson$^1$, D M Valiev$^2$, L Lodi$^3$, Z Qu$^2$, R Ghorbani$^2$, O L Polyansky$^3$, J Tennyson$^3$, F M Schmidt$^2$ and A Foltynowicz$^1$

1 Department of Physics, Umeå University, 901 87 Umeå, Sweden
2 Department of Applied Physics and Electronics, Umeå University, 901 87 Umeå, Sweden
3 Department of Physics and Astronomy, University College London, London WC1E 6BT, UK

Absorption spectroscopy techniques based on continuous wave lasers are often used as a non-intrusive tool for combustion diagnostics, but the limited probed spectral range restricts the number of detected species and the choice of line pairs for thermometry. We employ near-infrared cavity-enhanced optical frequency comb spectroscopy for simultaneous detection of $\text{H}_2\text{O}$ and OH in a premixed methane/air flat flame. We compare $\text{H}_2\text{O}$ spectra to a line list that is more accurate than the HITEMP database and we retrieve concentration and flame temperature from the OH spectra.

The system is based on an Er:fiber femtosecond laser locked to an enhancement cavity with a finesse of ~150. The burner is placed in the center of the cavity and mounted on a vertical translation stage to allow changing the height above the burner (HAB). The cavity transmission is analyzed using a fast-scanning Fourier transform spectrometer equipped with an auto-balancing detector, which acquires one spectrum with 1 GHz resolution in 0.4 s [1]. Figure 1(a) shows a normalized flame spectrum compared with the transition frequencies and line strengths of $\text{H}_2\text{O}$ and OH. Figure 1(b) shows the improvement in accuracy of the new $\text{H}_2\text{O}$ line list compared to the HITEMP line list [2]. By taking ratios between spectra measured at different HABs, we isolate the OH lines from $\text{H}_2\text{O}$ [black, Fig. 1(c)]. Using one HAB as reference, we fit (red) the relative change of OH concentration and temperature between the two HABs involved in the ratio. The results obtained for different ratios are plotted in Fig.1(d) (markers), where they compare well with the theoretical behavior obtained from 1D Cantera calculations for stoichiometric ratio and a methane/air flow of 10 L/min (solid curves).

**Figure 1.** (a) Normalized flame spectrum at HAB of 2.5mm (black) together with a stick spectrum of transitions from the new $\text{H}_2\text{O}$ list (blue) and OH from HITRAN (orange, divided by 100) calculated at 1950 K. (b) A zoom of the spectrum compared to the new $\text{H}_2\text{O}$ line list (blue) and the HITEMP line list (red). (c) Ratio of two spectra taken at HABs of 5 and 2.5 mm (black) together with a fit (red, inverted) and the residual. (d) Flame temperature and OH concentration obtained from fits at different HABs (markers) compared to the 1D methane/air flame calculations (solid curves).

**References:**

Modelling X–Ray Line Shapes from Asphaltenes

H Alqhatani¹ J Shirokoff² J C Lewis¹

¹ Department of Physics and Physical Oceanography, Memorial University of Newfoundland, St. John’s, Canada A1B 3X7
² Faculty of Engineering and Applied Science, Memorial University of Newfoundland, St. John’s, Canada A1B 3X7

Structural studies of asphaltene in crude oil have been performed by X–ray diffraction (XRD). The XRD spectra were taken with a Rigaku Dmax 2200V/PC, and built–in Jade™ software was used for initial analysis [2]. XRD was performed with Cu–Kα radiation operating at 40 KV and 40 mA, with a scan rate of 0.001°2θ per second. The XRD data were first fitted with Pearson VII profiles and then with pseudo–Voigt profiles, and then modelled in Mathematica™ using a generalized Fermi function (GFF). These fits also included several different backgrounds (linear, exponential, and Lorentzian). The results are discussed in terms of accuracy with different combinations of background and line profile.

References:

Theoretical approaches for spectral line shapes of hollow ions
Ch Lin, H Reinholz, G Röpke

1 Universität Rostock, Institut für Physik, 18051 Rostock, Germany

Recent developments in laser technology draw close attention to hollow ion spectra induced by transitions of deep-lying bound electrons. As a diagnostic tool for dense plasmas, the hollow ion spectra have more advantages compared to conventional emission lines, since these spectra are less affected by coupling effects in plasmas [1]. Generally, phenomenological approaches are used to calculate spectral line shapes of hollow ions. In order to microscopically understand these inner-shell transitions in dense plasma, a systematically derived self-consistent quantum mechanical many-body theory is indispensable.

A quantum-statistical approach based on thermodynamic Green’s functions has been developed for spectral lines of hydrogen atoms and hydrogen-like ions in dense plasma. The shift and broadening of spectral lines are determined by the two-particle self-energy and vertex corrections [2]. Considering spectral line shapes of hollow ions, Kα radiation [3] is of particular interest. It depends strongly on the ion configuration (ionization state) and plasma environment (screening due to surrounding charged particles). Within a chemical picture, free and bound electrons are considered separately. The effects of bound electrons in a many-electron atom are taken into account by introducing an effective transition matrix. The influence of free electrons from the plasma on the emitter states is considered in a dynamically screened Born approximation.

On the other hand, spectral line shapes of an ion immersed in an interactive plasma environment can also be considered within the framework of open quantum systems [4]. In this quantum kinetic approach, the plasma surrounding is treated as a heat bath for the investigated emitter. The influence of the plasma environment on the shift and broadening of the spectral lines is described by its dynamic structure factor. For highly excited states (Rydberg states), this approach is applicable for calculating the transition rates of Rydberg states. By introducing a wave packet description for Rydberg atoms, the calculated results are in a good agreement with experimental data [4].

References:

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Amplification of THz radiation emission by a pre-bunched relativistic electron beam using ripple plasma wiggler

P Malik¹, S C Sharma¹ and R Sharma¹

¹ Department of Applied Physics, Delhi Technological University (DTU), Shahbad Daulatpur, Bawana Road, Delhi-110042, India

The fluid equations model has been carried out to study the effect of beam pre-bunching in a ripple plasma wiggler to generate and amplify the coherent terahertz (THz) radiation emissions. The radiation wavelength depends on the wiggler period. The enhancement in the growth rate and efficiency is being exploited with the resonance between the modulated frequency of electron beam and the frequency of the radiation wiggler field via Cerenkov interaction along the axial direction (when the frequency and wave number of modulated beam are comparable to that of unstable radiation wave). In addition, the frequency of the radiation wave increases at the expense of beam energy and modulation index $\Delta$. The growth rate of the unstable mode of wave increases with beam density and modulation index $\Delta$, and scales as one–third power of the beam density. It becomes larger as modulation index $\Delta$ approaches to unity.

References:

AlGaInN diode-laser technology for optical clocks and atom interferometry

S P Najda1, P Perlin1,2, T Suski2, L Marona2, S Stańczyk1,2, M Leszczyński1,2, P Wińiewski1,2, R Czernicki1,2, G Targowski1, C Carson3, D Stothard3, L J McKnight3

1 TopGaN Ltd., ul. Sokółowska 29/37, 01-142 Warsaw, Poland
2 Institute of High Pressure Physics PAS, ul. Sokółowska 29/37, 01-142 Warsaw, Poland
3 Fraunhofer Centre for Applied Photonics, Fraunhofer UK, Technology and Innovation Centre, 99 George Street, G1 1RD, Glasgow, U.K.

Optical clocks have demonstrated an improvement in temporal accuracy of several orders of magnitude over existing time standards based on caesium. Such systems hold great promise in many industrial sectors including financial time stamping, GPS-free navigation and network synchronisation. Atom interferometry has proven to be a reliable method of precision gravity sensing and finds application in geological studies, including earthquake warning systems and oil exploration. Such systems require a number of sophisticated lasers in a compact and reliable format for use outside of a laboratory environment, suitable for commercialisation and user transportation.

The AlGaInN material system allows for single transverse mode laser diodes to be fabricated with optical powers up to 100 mW and over a very wide range of wavelengths from U.V., 380 nm, to the visible, 530 nm. By tuning the indium content and thickness of the GaInN quantum well it is possible to directly target a wavelength of interest. Direct light generation at the required wavelength is crucial to reduce complexity of the overall system, to ensure compact systems suitable for transportations and to ensure a high wall-plug efficiency that is critical for space and mobile applications.

Hence, there is considerable interest in using AlGaInN laser technology for the next generation optical clocks and atom interferometry systems. This includes the \(5s^2S_{1/2} - 5p^2P_{1/2}\) cooling transition in strontium ion optical clocks at 422 nm, the \(5s^2^1S_0 - 5p^1P_1\) cooling transition in neutral strontium clocks at 461 nm and the \(5s^2S_{1/2} - 6p^2P_{3/2}\) transition in rubidium at 420 nm. These transitions are a few among an extensive list required. In addition to the requirements outlined above, narrow linewidths (<5 MHz) are required for the identified transitions and few kHz levels for other transitions. To meet these requirements we are pursuing both extended cavity laser (ECDL) geometries in the short term and distributed feedback architectures in the long term.

We have developed a range of AlGaInN diode-lasers [1] targeted to meet the wavelength and power requirements suitable for optical clocks and atom interferometry systems. A packaging system has been developed optimised for ECDL narrow-linewidth operation and includes anti-reflection coatings on the facets optimised for the design. Multiple ECDL designs have been developed including gratings in Littrow configuration and filter-based rugged geometry designs [2] optimal for narrow-linewidth operation. At the conference we will present details of the design of the structures and current performance related characteristics.

References:


Lateral grating DFB AlGaInN laser diodes for optical communications and atomic clocks

S P Najda¹, T Slight³, P Perlin¹², O Odedina⁴, T Suski², Ł. Marona², S Stańczyk¹², M. Leszczyński¹², P Wiśniewski¹², R Czernecki¹², G Targowski¹ and A E Kelly⁴

¹ TopGaN Ltd., ul. Sokołowska 29/37, 01-142 Warsaw, Poland
² Institute of High Pressure Physics PAS, ul. Sokołowska 29/37, 01-142 Warsaw, Poland
³ CST Global, Hamilton International Technology Park, 4 Stanley Blvd, Blantyre, Glasgow, Lanarkshire G72 0BN, United Kingdom
⁴ School of Engineering, University of Glasgow, Glasgow G12 8LT, United Kingdom

The AlGaInN material system allows for single transverse mode, ridge waveguide laser diodes to be fabricated with optical powers up to 100mW over a very wide range of wavelengths from u.v., 380nm, to the visible, 530nm, by tuning the indium content of the laser GaInN quantum well. AlGaInN blue-green laser diode technology allows the possibility of visible light communications that operate at very fast data rates (GHz) [1] and for next generation atomic optical clocks based on Sr (meeting the 88Sr⁺ cooling transition $[5s^2S_{1/2} - 5p^2P_{1/2}]$ by using 422nm & 461nm) and a blue cooling transition for Rubidium (Rb) $[4p^6S_{1/2} - 4p^6p^2P_{3/2}]$ at 420.2nm). Very narrow linewidths (<1MHz) are required for such applications, however in the present Fabry-Perot GaN LD’s a broad mode comb is observed in spectral output. Ideally, a GaN DFB laser with an integrated etched grating to select and stabilise the longitudinal mode would be considered, however there are significant technical challenges to overcome before a ‘conventional’ buried DFB GaN laser can be realised. Lateral gratings on AlGaInN ridge waveguide laser diodes are reported in [2] as an alternative to ‘conventional’ buried DFB’s and are more straightforward to fabricate while still achieving a good SMSR under pulsed operation. We report on efforts to improve lateral grating DFB performance to achieve even higher SMSRs and CW operation.

References:

Enhancement of THz radiation emission using space charge wave wiggler with relativistic effects of the electron beam

J Panwar¹, S C Sharma¹ and R Sharma¹

¹ Department of Applied Physics, Delhi Technological University, Shahbad Daulatpur, Bawana Road, Delhi-110 042, India

The emission of high power terahertz radiation (THz) is studied using space charge wave as a wiggler. The space charge wave is excited by using a pre-bunched relativistic electron beam (REB) in a plasma medium. The REB is pre-bunched due to the pondermotive force exerted by the two laser beams in the modulator. This energy modulated beam then travels through the drift space and gets density modulated. On interaction with the wiggler, the beam acquires an oscillatory velocity that couples with the modulated beam density to give rise to non-linear current density which acts as an antenna to produce terahertz radiation [1,2]. The growth rate of the excited space charge wave and the emitted radiation is evaluated and analyzed. The output radiation can be tuned by varying the wiggler parameters and the energy of the beam. The results of the present study can be extended to realize the practical applications of THz radiations.

References:

Self-Reversed Al Line Profiles in Laser-Induced Plasma

D M Surmick1, C G Parigger1

1 Center for Laser Applications, University of Tennessee Space Institute, Tullahoma, TN 37388

Laser-induced plasma is a complex and dynamical physical system, the physics of which can be diagnosed using broadened spectral emissions. Such physics include rapidly propagating shockwaves and the unique spectroscopic line shapes of atoms and molecules that arise from the expanding, hot, dense laser-induced plasma. Of current interest are Stark broadened lines, especially in regards to the spatial extent of the laser-induced plasma and for elevated electron densities where self-absorption effects become important. Distortions in the line shape due to self-absorption are particularly pronounced for ground state transitions. We investigate laser-induced plasma initiated following ablation of an aluminium alloy target in a gas atmosphere mixture of 90 percent hydrogen and 10 percent nitrogen using Nd:YAG 14 ns laser pulses with an average energy of 120 mJ/pulse. Self-absorption diagnostics are applied to the Al 3s23p→3s4s ground state transitions by retro-reflecting plasma emissions through the plasma breakdown volume. The plasma and its reflection are simultaneously imaged using a spectrometer-ICCD arrangement with an overall spatial and spectral resolution of 0.1 mm and 0.15 nm, respectively. Experimental, wavelength dependent correction factors are tabulated to determine the level of self-absorption and infer the electron density from Al line widths in the absence of line distortions due to self-absorption by measuring plasma emission ratios with and without its reflection [1]. Figure 1 shows measured vs. self-absorption corrected Al line profiles for a 60 ns time delay following ablation and at a distance of 0.5 mm from the target Al surface.

![Figure 1. Measured vs. self-absorption corrected Al line profiles. The blue lines indicate the unperturbed Al line centers at 394.4 and 396.15 nm.](image)

After application of the correction factors, the Al profiles appear narrower and deep absorptions near the line centers diminish. Such effects are expected under the influence of self-absorption. The corrected 394.4 and 396.15 nm profiles have line widths of 1.1±0.2 and 1.7±0.2 nm, respectively, as determined from Voigt profile fitting, which indicate electron densities in excess of \(10^{18}\) cm\(^{-3}\) [2, 3]. Corrected line profiles of this nature become invaluable when extracting the radial behavior of plasma density and temperature from spatially resolved, line-of-sight measurements along an axis of the plasma image plane. Both analyses show importance for early time and plasma shockwave diagnostics.

References:

Electron density and temperature variations in laser induced hydrogen plasma

G Gautam1, C G Parigger1

1 University of Tennessee Space Institute, 411 B.H. Goethert Parkway, Tullahoma, TN 37388, USA

Laser-induced optical breakdown is achieved by using Q-switched, Nd:YAG radiation focused into ultra-high-purity (UPH) hydrogen gas at a pressure of 1.08 ± 0.03 × 10⁵ Pa inside a cell. The plasma emission spectra are dispersed by a Czerny-Turner type spectrometer and detected with an intensified charge-coupled device (ICCD). The measured spectra are wavelength calibrated and detector sensitivity corrected. Spatially and temporally resolved line-of-sight spectra of Stark-broadened hydrogen Balmer alpha, H_α, and beta, H_β, lines are measured to diagnose the spatial and temporal variation of the electron density, N_e, and temperature, T_e.

Figure 1 shows the spatial variation of electron density and temperature for a time delay of 400 ns. The spatial distance indicated in Fig. 1 corresponds to the slit height. The laser radiation propagates parallel to the slit viz. from right to left. Full width at half maximu (FWHM) values were extracted from the Lorentzian fits to the experimental data for the evaluation of the electron density [1] by employing recently communicated empirical formulae [2]. The spatial variation of the electron excitation temperature is determined from the application of Boltzmann plots [3, 4] by utilizing integrated profiles of the H_α and H_β lines.

Spatial variations of N_e indicate a factor of 3 difference and an average value of 2.6 × 10¹⁷ cm⁻³ for a time delay of 400 ns. The temporal electron density variations are in the range of 8 × 10¹⁷ cm⁻³ to 0.5 × 10¹⁷ cm⁻³ for time delays of 0.15 μs to 1.4 μs. These electron densities agree with the line-of-sight values obtained from H_β lines [5, 6]. The average value of the electron excitation temperature is 52 × 10³ K. The temporal variations of temperature are in the range of 115 × 10³ K to 14 × 10³ K for time delays of 0.15 μs to 1.4 μs, consistent with previous hydrogen experiments [7].

References:

Multicomponent line profile restoring by means of ill-posed inverse task solution

G Revalde¹,², N Zorina², A Skudra²

¹ Ventspils University College, Inzenieru str. 101, Ventspils, Latvia
² Institute of Atomic Physics and Spectroscopy, University of Latvia, Skunu str. 4, Riga, Latvia
³ Institute of Technical Physics, Faculty of Materials Science and Applied Chemistry, Riga Technical university, P.Valdena 3, Riga, Latvia

In this work we present our calculation of ill posed inverse tasks by means of Tikhonov regularization [1]. The investigation of the criteria of usage of the Tikhonov regularization method for multicomponent overlapping line profiles restoring was done in three stages. The multicomponent "experimental" profiles were modeled by means of a nonlinear multiparameter $\chi^2$ [2] in the first stage. The values of the parameters were chosen so, that the "experimental" model profiles were maximally close to real spectral profiles, emitted from microsizes light sources [3]. After that the solution of the Fredholm integral equation of the first kind was performed to remove the instrumental function. The influence of the width of the instrumental function, number of the components of the profile and distance between components are discussed. At the end, the results were compared with modeled ones.

Figure 1. Comparison between "Real modeled" (modeled by means of non-linear multi-parameter modelling) profile and "Real solution" profile (obtained by means of Tikhonov regularization method)

On the Figure 1 we can see example of our calculation in case of two components, instrumental function was given as Gauss function (full width at half of maximum (FWHM) is 0.04 cm⁻¹).

References:

Spectroscopic diagnostics of the electron density in corona discharges

J Rosato¹, N Bonifaci², Z Li²,³, R Stamm¹

¹ PIIM, UMR 7345 Aix-Marseille Université / CNRS, Centre de St-Jérôme Case 232, F-13397 Marseille Cedex 20, France
² Laboratoire G2Elab CNRS & Grenoble University, 25 rue des Martyrs, 38042 Grenoble, France
³ Guizhou Institute of Technology, Caiguan road #1, 550003, Guiyang, China

Experiments have been carried out in gaseous He at the fixed temperature of 300 K and different pressures in the cell from 0.1 MPa up to 2 MPa. A corona discharge (ionization of gaseous He) has been performed at the vicinity of a tip electrode under high voltage. The discharge domain (ionization zone) has a volume less than an inter-electrode space (drift zone). The corona current has been measured for different pressures in a space-charge-limited regime. Spectroscopic observations of the light can be used to determine information of the local environment of the emitting atoms or molecules. The optical emission spectrum from impurities, like hydrogen, can also be used. In this work, we report on an investigation of the Ha and Hb spectral profiles and their dependence on the discharge current and pressure. It is shown that the electron density can be inferred from the Stark broadening of these lines.
Influence of Rydberg atom-atom collisional and (n - n’)-mixing process on optical properties of astrophysical and low-temperature laboratory plasmas

A A Mihajlov 1, V A Srečković1, Lj M Ignjatović1, M S Dimitrijević2,3,4 and Z Simić 2

1 Institute of physics, University of Belgrade, P.O. Box 57, 11001, Belgrade, Serbia
2 Astronomical Observatory, Volgina 7, 11060 Belgrade 74, Serbia
3 Observatoire de Paris, 92195 Meudon Cedex, France
4 IHIS Techno experts, Batajnički put 23, 11080 Zemun, Serbia

In this work, we will consider the influence of the (n-n’)-mixing processes during a symmetric atom Rydberg-atom collision processes on the intensity of chemi-ionization process. We will take into account H(1s) + H(n) and He(1s2) + He(n,l) collisional systems, where the principal quantum number n >> 1. The corresponding calculations of the chemi-ionization rate coefficients are performed for the temperature region characteristic for the solar and DB white dwarfs atmosphere.

It will be demonstrated that the inclusion of (n-n’)-mixing processes in the calculation, influences significantly on the values of chemi-ionization rate coefficients, particularly in the lower part of the block of the Rydberg states. As the previous results [1,2] showed that chemi-ionization and chemi-recombination processes change the stellar plasma atmosphere parameters, here we will consider the possible influences of the chemi-ionization processes in the presence of (n-n’)-mixing processes on the spectral line shapes in the solar and DB white dwarfs atmospheres as well as for laboratory obtained spectra.

References:

The inverse bremsstrahlung absorption coefficients and Gaunt factors in astrophysical plasmas

A A Mihajlov, V A Srečković, N M Sakan, M S Dimitrijević and Z Simić

1 Institute of physics, University of Belgrade, P.O. Box 57, 11001, Belgrade, Serbia
2 Astronomical Observatory, Volgina 7, 11060 Belgrade 74, Serbia
3 Observatoire de Paris, 92195 Meudon Cedex, France
4 IHIS Techno experts, Batajnički put 23, 11080 Zemun, Serbia

In this paper we will present the method of determination of the electron-ion inverse "Bremsstrahlung" characteristics in the stellar atmospheres where the plasma characteristics are changing in a wide diapason. It is shown that determination of these optical characteristics i.e. the absorption coefficients and Gaunt factors can be successfully performed in the whole region of electron densities and temperatures which is relevant for stellar atmospheres. The used method is based on cut-off Coulomb model potential which was used by now for the describing of some spectral characteristics of plasma [1,2]. The relevant quantum mechanical method of the calculation of the corresponding spectral absorption coefficient and Gaunt factor is described and discussed.

The results obtained for plasmas with the electron densities from $10^{14}$ cm$^{-3}$ to $10^{19}$ cm$^{-3}$ and temperatures from 3000 K to 50000 K within the wavelength region 100 nm $< \lambda < 3000$ nm are presented. These results can be of interest and use in the investigation of different laboratory plasmas.

References:

Investigations of atomic processes in the electron beam ion trap (EBIT) plasma by means of x-ray spectroscopy

D Sobota¹, D Banaś¹, Ł Jabłoński¹, P Jagodziński², A Kubala-Kukuś¹, M Puchala, I Stabrawa¹, M Pajek¹

¹Institute of Physics, Jan Kochanowski University, Kielce, Poland
²Departament of Physics, University of Technology, Kielce, Poland

In the electron beam ion trap (EBIT) the highly charged ions (HCI) are produced by a successive electron impact ionization of atom/ions radially and axially confined by magnetic and electric fields [1]. In the EBIT the electron impact ionization competes with the electron excitation and recombination processes leading to formation of the, so called, EBIT plasma characterized by a specific distribution of the ionic charge states. Consequently, the emission of X-rays from the EBIT as well as the charge state distribution of ions extracted from a trap carry information of atomic processes taking place in the EBIT plasma, namely the electron impact ionization, excitation and recombination.

In this paper we report on the measurements of X-rays, using a semiconductor drift detector (SDD), which were emitted from the EBIT filled with xenon gas bombarded by electron beam of energy 9 keV. These measurements were performed at the EBIS-A facility [2,3], which can deliver a wide range of beams of highly charged ions, including bare and few-electron species. The beams of Xe$q^+$ ions, with $q=25-35$, were extracted from the EBIT trap in a leaking mode and then charge state analyzed in a dipole magnet to measure their charge state distributions. Additionally, the X-ray spectra and charge state distributions of ions can be measured in a pulsed mode for a preset confinement time of ions in the trap, which gives access to study the dynamics of plasma equilibration in the EBIT.

![Figure 1. Measured X-ray spectrum from highly charged xenon ions in the EBIT.](image)

The measured X-ray spectra (see Fig.1) were found to be sensitive to the direct electron impact ionization and excitation (DE) as well as the radiative recombination (RR) processes. In particular, Fig. 1 shows the spectrum of X-ray transitions $n=3\rightarrow2$ and $n=4\rightarrow2$ following direct collisional excitation of corresponding states. For higher photon energies the X-ray lines originating from radiative recombination into the $n=2-5$ states are clearly separated. Detailed interpretation of observed X-ray spectra needs multi-configuration Dirac-Fock (MCDF) ionic structure calculations and solving the rate-equations describing a balance of discussed atomic processes in the EBIT plasma.

References:

Does non-cyclic Berry phase play any role in the formation of pressure-broadened spectral line shapes?

R Ciuryło1, J Szudy1 and W E Baylis2

1 Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziądzka 5, 87-100 Toruń, Poland
2 Department of Physics, University of Windsor, Windsor, Ontario N9B 3P4, Canada

Recently, the concept of Berry’s geometric phase [1] was included in the formalisms of adiabatic theories of pressure broadening to derive expressions for the intensity distribution both in the core [2] and far wings [3] of spectral lines radiated by atoms placed in an external electric field slowly rotating around a cone about a fixed axis. It was shown that the effect caused by Berry’s phase on pressure-broadened spectral lines may be important in cases when some parameters describing molecular system such as the external electric field traverse a closed path. Since the perturbers surrounding the radiating atom do not move along closed paths, the contributions to the Berry phase coming from the time dependence of the perturber coordinates $R(t)$ were assumed in Refs. [2] and [3] to be negligible. It was shown, however, by several researches that the geometric phase makes sense also for non-cyclic adiabatic evolution, corresponding to open paths in parameter space. Therefore, in the present work we discuss the problem of the influence of contributions to the Berry phase coming from the motion of perturbers along open paths on the shapes of pressure-broadened spectral lines. Following Zygelman [4,5] we examine possible implications of the Berry vector gauge potential for pressure broadening theory by the use of the Born-Huang adiabatic approximation. It is found that the effects due to non-cyclic Berry’s phase are negligible for strong allowed transitions. In general, they do not play any role for spectral features associated with $\Sigma - \Sigma$ transitions. However, the non-cyclic Berry phase effects are expected to have some importance for collision-induced spectra associated with dipole forbidden transitions.

References:

Modelling low temperature growth of carbon nanotubes in reactive plasma environment

A Tewari¹, S C Sharma¹ and R Sharma¹

¹ Department of Applied Physics, Delhi Technological University, Shahbad Daulatpur, Bawana Road, Delhi-110 042, India

Carbon nanotube growth in a reactive plasma medium assisted by catalyst is realized through a theoretical model. The model incorporates the effect of plasma sheath and plasma species kinetics on the growth kinetics of carbon nanotube on catalyst-substrate surface. The different processes such as adsorption, desorption, thermal dissociation and dehydrogenation, diffusion, and accretion among others are accounted in the present model. The enhanced growth rates of CNT are obtained at low substrate temperatures of 4000°C. The low –temperature CNT obtained through modeling can find applications in vertical transistors, field emission devices and field ionization applications among others.

References:

Multispectrum-fitting of phenomenological collisional line-shape models to a speed-dependent Blackmore profile for spectroscopic analysis and databases

P Wcisło¹, D Lisak¹, R Ciuryło¹, A S Pine²

1 Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziadzka 5, 87-100 Toruń, Poland
2 Alpine Technologies, 14401 Poplar Hill Road, Germantown, Maryland 20874 USA

A variety of phenomenological line-shape models [1-9] are compared with a speed-dependent Blackmore profile [10-12] describing an O₂ spectral line measured earlier with a very high signal-to-noise ratio, \( S/N > 10^5 \) [13,14]. In this reference Blackmore profile (SD₁₂B), the speed-dependence of the self-broadening and shifting is given by a hypergeometric function characterized by an isotropic long-range attractive \( r^{-5} \) interaction potential, and the velocity-changing collision operator is calculated from a corresponding short-range \( r^{-12} \) repulsion. Simultaneous fitting [15,16] of the phenomenological models to the Blackmore profile simulated at 15 pressures from 5 to 800 Torr provides model parameters, linear in pressure, with correlation reduced from single-spectrum fits. None of these fitting models are able to reproduce the reference spectra to within a \( S/N \) greater than \( 6 \times 10^4 \). The quality of fit [13], based on the peak intensity divided by the residuals, indicate which models are adequate for analysis of spectra measured with a given \( S/N \). The model dependence or systematic deviations of the fitting parameters is seen to be much larger than their least-squares statistical standard deviations. The model differences of the common parameters, such as line position, intensity and broadening, usually are inversely related to the quality of fit, but not always. These differences indicate the possible magnitude of systemic errors caused by oversimplified treatment of velocity-changing collisions. The application of these results to spectral analysis, improved databases [17], atmospheric remote sensing [18], trace gas metrology [19], and Doppler thermometry is discussed [20].

References:

Dispersion and relativistic corrections to the spectral line-shape models

Sz Wójtewicz¹, P Wcisło¹, P Amodio², L Gianfrani², D Lisak¹, R Ciuryło¹

¹ Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Grudziądzka 5, 87-100 Toruń, Poland
² Department of Mathematics and Physics, Second University of Naples, Viale Lincoln 5, 81100 Caserta, Italy

Recent developments in the ultra-high signal-to-noise-ratio spectroscopic measurements show that the commonly used theoretical line-shape profiles should be supplemented by neglected so far very subtle physical effects. Here we present the dispersion and relativistic corrections to the line-shape models on an example of simple Gaussian and Voigt profiles.

We discuss the dispersion corrections namely the frequency dependence of the Doppler shifting caused by dispersion [1,2] as well as by light frequency variation over the whole spectral line shape [2]. These effects can have non-negligible influence on the line-shape model and can affect it even at the level of $10^{-5}$ [2]. The dispersion correction may influence the determination of the line position at the level of kHz.

Moreover, we provided the relativistic formula describing the Voigt profile in the case of spontaneous emission [3]. Our formula has a proper behavior in two asymptotic cases: the classical Voigt profile and the relativistic Gaussian profile [4]. We presented an alternative expression, which simplify numerical evaluation for the most physically meaningful weak-relativistic regime. We estimated that at room temperature the relativistic correction can be at the level of $10^{-6}$.

The presented results are crucial in the Doppler-width thermometry [1] and precise molecular spectroscopy for fundamental studies [5].

References:

Anisotropic emission from an aluminium laser produced plasma

G A Wubetu¹,², T J Kelly¹, P van Kampen¹, H Fiedorowicz², A Bartnik², P Wachulak², W Skrzeczanowski² and J T Costello¹

¹ NCPST and School of Physical Science, Dublin City University, Glasnevin, Dublin 9, Republic of Ireland
³ Institute of Optoelectronic, Military University of Technology (MUT), Poland

In this work, anisotropic emission from laser produced plasma has been studied using time resolved imaging, as well as time and polarisation resolved spectroscopy in the optical spectral range. The results appear interpreted in the framework of recombination radiation from the plasma and a population imbalance of magnetic sub-shells.

Previous studies have shown that both the continuum [1,2] and line emission [3,4] can be partially polarized. When laser plasma is produced from a pure atomic target (in our case, aluminium) the broadband emission is made of electronic transitions where the initial state is in the continuum (either free – free transitions or free – bound transitions). It has been found that anisotropies in the broadband emission can lead to an increase in the signal to background ratio of the spectrum under study. This result is of interest to those studying Laser Induced Breakdown Spectroscopy (LIBS). In fact, an entire subset of LIBS is dedicated to studying the polarisation resolved spectra from multi-species targets (PRLIBS). The polarisation dependence of line emission has been studied in aluminium before [3,4]. However, this study focussed on narrow spectroscopic windows and very little has been reported to date on the mechanisms that lead to the anisotropy of the both the line and continuum emission.

In the first experiment we measured the time- and polarisation-resolved spatial anisotropy in plasma images. This was achieved by imaging the plasma through a Wollaston prism onto an ICCD detector. In the second experiment we measured the time resolved anisotropy of different spectral lines, namely: the Al I (394.4 nm and 396.1 nm), Al II (466.3 nm) and the Al III (569.6 nm and 572.3 nm). These were achieved by imaging the two orthogonally polarised images of the plasma plume onto the slit of a space resolving spectrometer. The results and mechanisms underlying the anisotropy will be discussed.

References:
LIST OF PARTICIPANTS
Piotr Ablewski (piotra@fizyka.umk.pl)
Mahmoud Abu-KHarma (mkharma@bau.edu.jo)
Spiros Alexiou (moka1@otenet.gr)
Nicole Allard (nicole.allard@obspm.fr)
Agnieszka Bartecka (bartecka@uni.opole.pl)
Andrzej Bartnik (andrzej.bartnik@wat.edu.pl)
Romain Baude (romain.baude@univ-amu.fr)
Katarzyna Bielska (kasia@fizyka.umk.pl)
Mateusz Borkowski (mateusz@fizyka.umk.pl)
Szczepan Brym (szbrym@matman.uwm.edu.pl)
Vasily Buyadzhi (vbuyad@mail.ru)
Annette Calisti (annette.calisti@univ-amu.fr)
Alain Campargue (alain.campargue@ujf-grenoble.fr)
Francesco Cappelli (francesco.cappelli@ino.it)
Roman Ciuryło (rciurylo@fizyka.umk.pl)
John Costello (john.costello@dcu.ie)
Hubert Cybulski (hubert@fizyka.umk.pl)
Agata Cygan (agata@fizyka.umk.pl)
Monika Czajkowska (monikac@fizyka.umk.pl)
Elisabeth Dalimier (elisabeth.dalimier@upmc.fr)
Thibault Delahaye (thibault.delahaye@lisa.u-pec.fr)
Alexander Devdariani (snbrn2@yandex.ru)
Jolanta Domysławska (jolka@fizyka.umk.pl)
Krzysztof Dzierżega (krzysztof.dzierzega@uj.edu.pl)
Volker Ebert (volker.ebert@ptb.de)
Trevor S. Elliott (trevor.s.elliott@gmail.com)
Wissam Fakhardji (wissam.fakhardji@ltu.se)
Aleksandra Foltynowicz (aleksandra.foltynowicz@umu.se)
Robert Gamache (robertGamache@uml.edu)
Zekry Ghatass (z_ghatass@yahoo.com)
Alexander Glushkov (dirac13@mail.ru)
Veronica Gonzalez-Fernandez (veronica.gonzalez.fernandez@uva.es)
Iouli Gordon (igordon@cfa.harvard.edu)
Motoshi Goto (goto@nifs.ac.jp)
Camilo Granados (camilo.granadosbuitrago@fys.kuleuven.be)
Neha Gupta (nehagpt2105@gmail.com)
Magnus Gustafsson (magnus.gustafsson@ltu.se)
Rafał Hakalla (hakalla@ur.edu.pl)
Ibtissem Hannachi (ibtissem.hannachi@yahoo.fr)
Robab Hashemi (robab.hashemi@uleth.ca)
Takeshi Higashiguchi (higashi@cc.utsunomiya-u.ac.jp)
Łukasz Jabłoński (lukasz@ujk.edu.pl)
Patryk Jasik (p.jasik@mif.pg.gda.pl)
Alexandra C. Johansson (alexandra.johansson@physics.umu.se)
Paul Julienne (psj@umd.edu)
Ewa Kaszewska (e.a.kaszewska@faj.org.pl)
Maria Kiseleva (m.kiseleva@science.ru.nl)
Jarosław Koperski (ufkopers@cyf-kr.edu.pl)
Alexander Kouzov (alex@ak1197.spb.edu)
Grzegorz Kowzan (gkowzan@fizyka.umk.pl)
Jacek Krełowski (jacek@umk.pl)
Karine Le Bris (klebris@stfx.ca)
John C. Lewis (john.lewis@mun.ca)
Gang Li (gang.li@ptb.de)
Chengliang Lin (chengliang.lin@uni-rostock.de)
Daniel Lisak (dlisak@fizyka.umk.pl)
Valery Lisitsa (vlisitsa@yandex.ru)
Andrew Ludlow (ludlow@boulder.nist.gov)
Pratibha Malik (prat_aru@rediffmail.com)
Marco Marangoni (marco.marangoni@polimi.it)
Javier Martin-Torres (javmar@ltu.se)
Piotr Masłowski (pima@fizyka.umk.pl)
Tigran Vartanyan (tigran@vartanyan.com)
Ajit Virdi (virdi_123@rediffmail.com)
Piotr Wcisło (piotr.wcislo@fizyka.umk.pl)
Marcin Witkowski (marcin@skyhost.pl)
Szymon Wójtewicz (szymon@fizyka.umk.pl)
Getasew Admasu Wubetu (getasew.wubetu2@mail.dcu.ie)
Sergey Yurchenko (s.yurchenko@ucl.ac.uk)
Hamit Yurtseven (hamit@metu.edu.tr)
Mikołaj Zaborowski (zaborowski@fizyka.umk.pl)
Michał Zawada (zawada@fizyka.umk.pl)
23rd ICSLS

List of Exhibitors
Menlo Systems GmbH:
Ben Sprenger (b.sprenger@menlosystems.com)

COMEF Sp. z o.o Sp. k.:
Bogusław Burak (comef@comef.com.pl)
Michał Wikarek (comef@comef.com.pl)

Lasotronix:
Patryk Karopwicz (pjk@lasotronix.pl)
Marzena Sitek (pjk@lasotronix.pl)

Toptica Photonics AG:
Jan Schaefer (jan.schaefer@toptica.com)

MOGLabs Europe:
Christoph Przeszlakowski (christoph.p@moglabs.com)
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