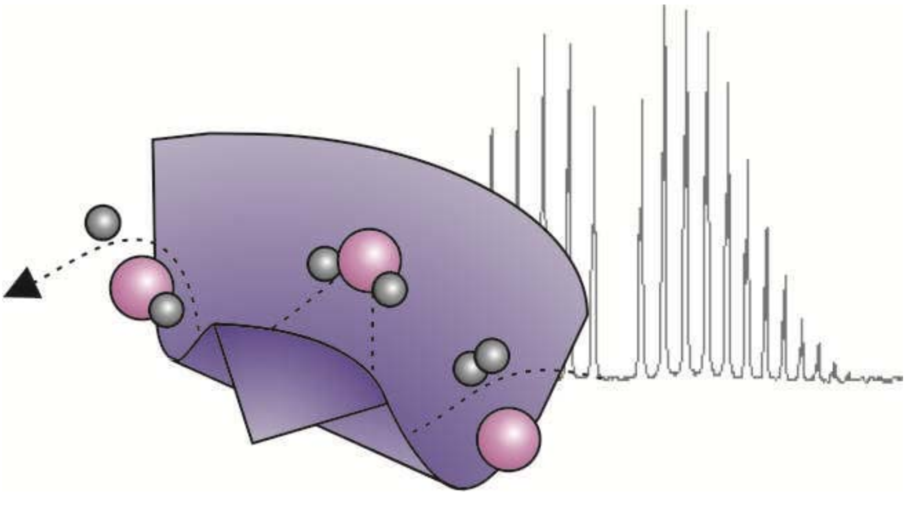
RSC Spectroscopy and Dynamics Group Meeting



St. Catherine's College, Oxford
5-7 January 2014

ROYAL SOCIETY
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We would like to thank the RSC and all of our sponsors for their generous support of this year's Spectroscopy and Dynamics Group meeting. Please support our sponsors by visiting their trade stands during the coffee breaks and poster session on Monday.

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Contents

1. PROGRAMME

Sunday 5 January

16:00 – 18:30	**Arrival and registration**, St. Catherine's College		
17:30 – 19:30	**Dinner**, University Club, Mansfield Rd		
	Session 1, PTCL lecture theatre, South Parks Rd		Chair: Claire Vallance
20:00 – 20:45	Invited tutorial talk	**Martina Havenith**	Ruhr-Universität, Bochum
20:45 – 21:30	Invited tutorial talk	**David Carty**	Durham University

Monday 6 January

07:30 – 08:30	**Breakfast**, dining hall		
	Session 2, Bernard Sunley lecture theatre		Chair: Thomas Preston
09:00 – 09:45	Invited talk	**Mark Johnson**	Yale University
09:45 – 10:05	Contributed talk	**Stephanie Harris**	University of Bristol
10:05 – 10:25	Contributed talk	**Daniel Horke**	CFEL, Hamburg
10:25 – 10:45	Contributed talk	**Alexander Weigel**	University of Oxford
10:45 – 11:15	**Tea/coffee**, Bernard Sunley foyer		
	Session 3, Bernard Sunley lecture theatre		Chair: Simon King
11:15 – 12:00	Invited talk	**Stuart Althorpe**	University of Cambridge
12:00 – 12:20	Contributed talk	**Gareth Richings**	University of Birmingham
12:20 – 12:40	Contributed talk	**Anna Andrejeva**	University of Nottingham
12:40 – 13:00	Contributed talk	**Maria Sanz**	Kings College London
13:00 – 14:00	**Lunch**, dining hall		
	Session 4, Bernard Sunley lecture theatre		Chair: Jon Tandy
14:00 – 14:20	Contributed talk	**Gediminas Galinis**	University of Leicester
14:20 – 14:40	Contributed talk	**Christopher West**	Durham University
14:40 – 15:00	Contributed talk	**Ingvar Kraatz**	University of Leeds
15:00 – 15:20	Contributed talk	**Matthew Robinson**	University of York
15:20 – 15:40	Contributed talk	**James Thompson**	Heriot-Watt University
15:40 – 16:00	**Tea/coffee**, Bernard Sunley foyer		
16:00 – 19:00	**Poster session and trade display**, Bernard Sunley foyer and meeting room		
18:00 – 19:00	**SDG Annual General Meeting**, Bernard Sunley lecture theatre		
19:00 – 20:00	**Dinner**, dining hall		
20:30 – 21:30	**SDGM Quiz**, St. Catherine's bar		

Tuesday 7 January

07:30 – 08:30	**Breakfast**, dining hall		
	Session 5, Bernard Sunley lecture theatre		Chair: Chris Rennick
09:00 – 09:45	Invited talk	**Nicholas Walker**	Newcastle University
09:45 – 10:05	Contributed talk	**Cheng Feng and Dan Spence**	University of Leicester
10:05 – 10:25	Contributed talk	**Jamie Young**	Warwick University
10:25 – 10:45	Contributed talk	**Maria Tesa-Serrate**	Heriot-Watt University
10:45 – 11:15	**Tea/coffee**, Bernard Sunley foyer		
	Session 6: Alan Carrington Memorial Session, Bernard Sunley lecture theatre		Chairs: Stuart Mackenzie and Daniel Zaleski
11:15 – 11:25	Invited talk	**Tim Softley**	University of Oxford
11:25 – 11:45	Invited talk	**Richard Tuckett**	University of Birmingham
11:45– 12:05	Contributed talk	**Nicolas Vanhaecke**	Fritz-Haber Intitut, Berlin
12:05 – 12:25	Contributed talk	**Helgi Hrodmarsson**	University of Iceland
12:25 – 12:45	Contributed talk	**Michal Ryszka**	Open University
12:45 – 13:45	**Lunch**, dining hall		
	Session 7, Bernard Sunley lecture theatre		Chair: Tom Sharples
13:45 – 14:30	Invited talk	**Mark Brouard**	University of Oxford
14:30 – 14:50	Contributed talk	**Rhiannon Monckton**	University of Manchester
14:50 – 15:10	Contributed talk	**Greg Dunning**	University of Bristol
15:10 – 15:30	Contributed talk	**Jemma Gibbard**	University of Oxford
15:30 – 16:00	**Tea/coffee**, Bernard Sunley foyer		
16:00	**Finish**		

2. TALK ABSTRACTS

I1 Solvation – new answers to an old problem

Martina Havenith

Ruhr-Universität Bochum

I2 Translational cooling of molecules

David Carty

Durham University

For almost fifteen years, the field of cold and ultracold molecules has been growing and changing rapidly. Such growth and change has been driven by the promise of exciting new physics and chemistry only possible by entering regimes of translational temperature (< 1 K or < 1 mK) that have been, and remain, largely unexplored. Most of the experimental effort has gone in to, and *still* goes into, devising ingenious methods for producing samples of translationally cold molecules. However, the field is beginning to reach a stage of maturation where molecular collisions and chemical reactions can be studied and researchers look likely, in this decade, to be able to make a quantum simulator using ultracold polar radicals. In this tutorial talk it will not be possible to give a comprehensive overview of the entire field, but it will be possible to talk about some of the more mature techniques that have been devised, such as buffer gas cooling and trapping, buffer gas beam formation and Stark and Zeeman deceleration, that can produce samples of molecules with temperatures between 10 mK and 1 K. Efforts being made to further cool molecules to bridge the gap between 10 mK and the µK regime will also be discussed.

I3 Cryogenic ion chemistry and spectroscopy: from ionic liquids to R6G

Mark Johnson

Yale University

I will discuss how the cooling, mass selection, and processing of cryogenic ions provides powerful opportunities for the detailed characterization of their structures as well as the rational synthesis of labile reaction intermediates. This is accomplished by first cooling the ions close to 10K and condensing onto them dozens of weakly bound, chemically inert small molecules or rare gas atoms. This assembly can then be used as a medium in which to quench reactive encounters by rapid evaporation of the adducts, as well as provide a universal means for acquiring highly resolved vibrational action spectra of the embedded species by photoinduced mass-loss. Moreover, the spectroscopic measurements can be obtained with readily available, broadly tunable pulsed infrared lasers because absorption of a single photon is sufficient to induce evaporation. The method is implemented with a hybrid photofragmentation mass spectrometer involving two stages of mass selection with two laser excitation regions interfaced to the cryogenic ion source. Specific recent examples include the structure of small building blocks of ionic liquids and the temperature dependence of the electronic spectrum of Rhodamine 6G.

C1 The Paternó-Büchi reaction – followed by transient absorption spectroscopy

Stephanie J. Harris[a], Daniel Murdock[a], Michael P. Grubb[a], Gregory M. Greetham[b],
Ian P. Clark[b], and Michael N. R. Ashfold[a]

[a] School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS.
[b] Central Laser Facility, Research Complex at Harwell, Science and Technology Facilities Council, Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0QX, UK.

The photo-initiated cycloaddition of 267 nm excited benzaldehyde-d_1 to cyclohexene, a well-known example of the Paternó-Büchi reaction, is studied using both ultrafast transient electronic and vibrational spectroscopy. Using this combination of techniques the progress of the reaction –starting with sub-ps intersystem crossing from the initially excited singlet state of benzaldehyde-d_1 to a triplet state from which it reacts with cyclohexene, forming a 1,4-biradical which subsequently decays to form the final oxetane product, can be followed. This study highlights the high-level of detail that the combination of these two techniques can provide on the mechanism and kinetics of organic photochemical reactions.

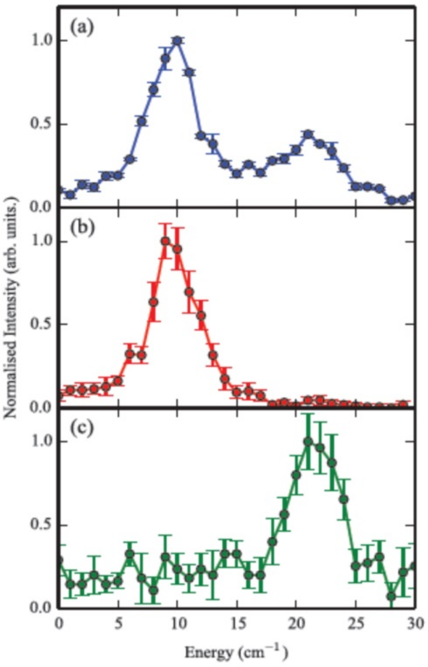
C2 Spatially separating *para* and *ortho* water – quantum state selected samples of gas-phase molecules

Daniel Horke[a], Y.-P. Chang[a], and J. Küpper[a,b,c]

a) Center for Free-Electron Laser Science, DESY, Notkestraße 85 22607 Hamburg, Germany
b) Department of Physics, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany
c) The Hamburg Center for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

We had previously demonstrated the ability to separate different species present in supersonically expanded molecular beams using the electrostatic deflector. This includes the separation of different conformers[1], cluster stoichiometries[2], and of individual quantum states of small linear rotor molecules.[3] These pure samples are ideally suited for studies of conformer-specific chemical reactivity[4] and they allow to significantly improve the experimentally achievable molecular alignment and orientation,[5] a prerequisite for novel imaging methodologies such as x-ray or electron diffraction from aligned gas-phase molecules.[6]

In this contribution we demonstrate how the electrostatic deflector was used to obtain quantum state selected samples of water molecules in the gas-phase. The equivalent proton spins in the water molecule lead to two distinct nuclear spin states – *para* and *ortho* – that occupy different rotational levels due to the different symmetries of the spin wavefunctions. We demonstrated the production of a cold (~ 8K) molecular beam of water, containing > 95% of population in the two absolute ground states, and subsequently spatially separated these using strong inhomogeneous electric fields. Furthermore, we demonstrated the selection of a specific *M* component, thereby providing fully *J*, *K* and *M* selected quantum state samples.



Rotational-state resolved REMPI spectra of water: (a) undeflected beam containing para and ortho water; (b) pure beam of ortho (M=1) water; and (c) pure beam of para (M=0) water.

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2. S. Trippel, *et. al.*, *Phys. Rev. A* **86**, 033202 (2012)

3. J. H. Nielsen *et. al.*, *Phys. Chem. Chem. Phys.* **13**, 18971 (2011)
4. Y.P. Chang *et. al.*, *Science* **342**, 98 (2013)
5. L. Holmegaard *et. al.*, *Phys. Rev. Lett.* **102**, 023001 (2009)
6. J. Küpper *et. al.*, arXiv:1307.4577, submitted (2013); A. Barty *et. al.*, *Annu. Rev. Phys. Chem.* **64**, 415 (2013); C. J. Hensley *et. al.*, *Phys. Rev. Lett.* **109**, 133202 (2012)

C3 Femtosecond spectroscopy on single nanoscopic particles

Alexander Weigel, Aleksander Sebesta, and Philipp Kukura

Physical and Theoretical Chemistry Laboratory, Department of Chemistry,
University of Oxford, South Parks Rd, Oxford OX1 3QZ, UK

Femtosecond spectroscopy is key to track even the fastest molecular motion and relaxation processes. Enormous activity has evolved in this field over the last two decades, but experiments have mainly focused on ensemble measurements. In an ensemble, vibrational and electronic coherences imprinted by the excitation pulse run rapidly out of phase, leading to an intrinsic loss of information. Femtosecond experiments on the singleparticle level avoid this drawback and can therefore give a much deeper insight into the molecular vibronic landscape. Most wellstudied chromophores absorb in the visible spectral region, where femtosecond light sources for singlemolecule experiments are currently unavailable. We have developed a highpower Titanium:Sapphire oscillator, and by focusing into a short YAG crystal we can directly generate white light with a repetition rate of 8 MHz. The output pulses span the full visible region from 450 nm to the near infrared and can be compressed to durations below 10 fs. A pulse shaper is used to generate pulse copies and pulse trains with specified interpulse delays and phases. The white light is then coupled into a homebuilt darkfield microscope, which allows tocollect fluorescence and scattering spectra of single particles without compromising the pulse structure of the excitation light. We present first experimental results on gold nanoparticles and quantum dots.

I4 Instantons and ring polymers

Stuart Althorpe

University of Cambridge

C4 Calculation of photoelectron spectra of aromatic molecules

Gareth RIchings *and Graham A. Worth*

School of Chemistry, University of Birmingham,
Edgbaston, Birmingham B15 2TT

In order to model the time-resolved photoelectron spectra of aromatic molecules, we use a first-order perturbation expansion to generate the total ion yield as a function of the time of the ionising pulse relative to the pump pulse[1]. This is achieved by combining the overlaps of wavepackets from a series of quantum dynamics calculations carried out using the MCTDH package, where the wavepacket in the pumped state is projected onto the ionic potential energy surface and allowed to propagate thereon. Summing the contributions, moderated with the laser pulse strength, from projections performed at a range of times after the pump pulse we get the total ion yield. Results for the toluene molecule are compared to calculations performed using discretised continua[2] to represent the free-electron wavefunction and also to experimental data[3].

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2. M. Seel and W. Domcke, *J. Chem. Phys.*, **95**, 7806 (1991).
3. J. A. Davies, A. M. Green and K. L. Reid, *Phys. Chem. Chem. Phys.*, **12**, 9872 (2010).

C5

Assignment of the vibrations of the S_1 state of chlorobenzene-h_5 and chlorobenzene-d_5

Anna Andrejeva

University of Nottingham

The labelling and assignment of the vibrational frequencies of the chlorobenzene molecule is investigated in its first electronically excited states (S_1). The assignments given utilise a recently proposed nomenclature[1], allowing the ring-localised vibrations to be compared straightforwardly across different monohalosubstituted benzenes. The assignments of the frequencies employ previous work but also the calculated wavenumbers for both fully hydrogenated monohalosubstituted chlorobenzene (-h_5) and the deuterated isotopologue (-d_5) employing time-independent density functional theory (TDDFT). Experimentally, one-colour resonance-enhanced multiphoton ionization (REMPI) spectroscopy was employed.

1. A. M. Gardner and T. G. Wright, J. Chem. Phys., **135**,114305 (2011)

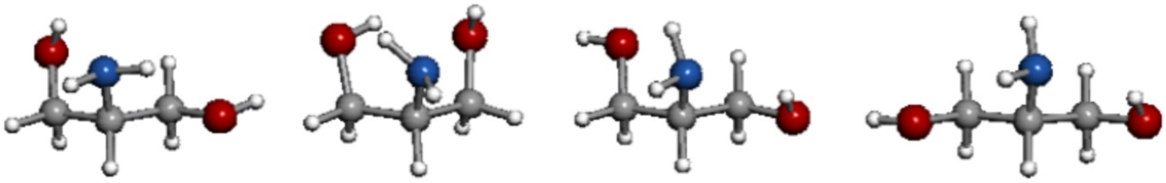
C6

The conformational landscape of bioactive serinol

D. Loru[a], M. E. Sanz[a], I. Peña[b], S. Mata[b], C. Cabezas[b], and J. L. Alonso[b]

[a]*Department of Chemistry, Kings College London, London SE1 1UL, UK*
[b]*Grupo de Espectroscopía Molecular (GEM), Laboratorios de Espectroscopía y Bioespectroscopía, Universidad de Valladolid, Valladolid 47005, Spain*

The rotational spectrum of the amino alcohol serinol CH_2OH-$CH(NH_2)$-CH_2OH, which constitutes the hydrophilic head of the lipid sphingosine, has been investigated using chirped-pulsed Fourier transform microwave spectroscopy in combination with laser ablation[1]. Four different forms of serinol have been observed and conclusively identified by the comparison between the experimental values of their rotational and ^{14}N quadrupole coupling constants and those predicted by *ab initio* calculations. In all observed conformers several hydrogen bonds are established between the two hydroxyl groups and the amino groups in a chain or circular arrangement. Interestingly, the most abundant conformer is stabilised by O-H···N and N-H··O hydrogen bonds forming a chain rather than a cycle. The higher-energy conformer detected presents a tunnelling motion of the hydrogen atoms of the functional groups similar to that observed in glycerol[2].



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2. V. V. Ilyushin, R.A. Motiyenko, F.J. Lovas, D.F. Plusquellic, *J. Mol. Spectrosc.* **2008**, *251*, 129.

C7 Incipient superfluid effects in molecule-helium clusters studied using non-adiabatic alignment

Gediminas Galinis[1], Luis G. Mendoza Luna[1], Mark Watkins[1], Russell Minns[2], Andrew M. Ellis[3], Richard Chapman[4], Cephise Cacho[4], Edmond Turcu[4], Emma Springate[4], Marius Lewerenz[5], Mirjana Mladenovic[5], Lev Kazak[6], Robert Irsig[6], Slavomir Skruszewicz[6], Sebastian Göde[6], Joseph Tiggesbäumker[6], Karl-Heinz Meiwes-Broer[6], Arnaud Rouzee[7], Klaus von Haeften[1].

[1] *Department of Physics and Astronomy, University of Leicester, UK*
[2] *Department of Chemistry, University of Southampton, UK*
[3] *Department of Chemistry, University of Leicester, UK*
[4] *Central Laser Facility, Rutherford Appleton Lab, UK*
[5]*Laboratorie Modelisation et Simulation, University of Paris-Est, France*
[6] *Institute for Physics, University of Rostock, Germany*
[7] *Max Born Institute, Germany*

Molecules embedded in helium nanodroplets demonstrate almost free gas-like rotation. This phenomenon is commonly refered to as *molecular superfluidity*. All our current knowledge on molecular superfluidity has been derived from rotational and ro-vibrational spectroscopic studies in the past 15 years. However, limitations exist in using frequency domain techniques. Consequently, we have used an alternative method to probe molecular superfluidity which employs a laser pump-probe method to non-adiabatically align helium-molecule complexes and to probe the state of alignment at any instance later. Periodic recurrences of alignment known as revivals provide information on rotational speeds and hence the interaction between the molecule and the surrounding helium. In this presentation the technique will be described and provisional results will be presented for the He-HCCH complex.

C8 Time-resolved photoelectron imaging of the chromophore of the green fluorescent protein

Christopher West

Durham University

The anionic form of *p*-hydroxybenzylidene-2,3-dimethylimidazolinone (HBDI) has been extensively employed as a model of the chromophore of the green fluorescent protein. In order to understand the intrinsic dynamics of HBDI-, we have performed time-resolved photoelectron spectroscopy. The S_1 state decays on a timescale of 1.4 ps via two dominant decay mechanisms: internal conversion and autodetachment. Internal conversion leads to large changes in the photoelectron spectra, which are assigned to rotation around the central allyl bridge. Autodetachment leads to photoelectrons with low kinetic energy. The relative yield between the two channels was determined and the lifetime for autodetachment was found to be approximately 30 ps.

C9 Femtosecond transient absorption spectroscopy of pyrrole and 2-ethylpyrrole in solution phase

Ingvar T. Kraatz, Benjamin J. Whitaker and Michael G.D. Nix

School of Chemistry, University of Leeds, LS2 9JT, United Kingdom

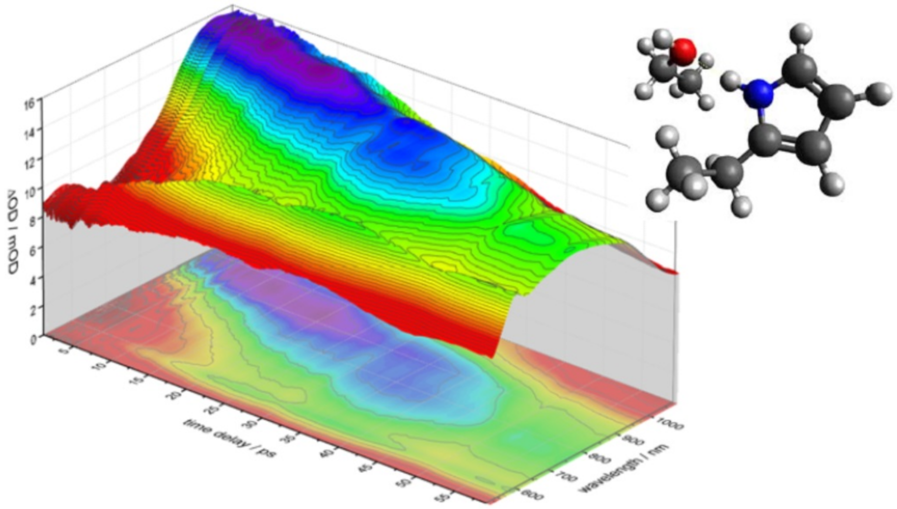
Extensive studies[1-3] of the excited state dynamics of heteroaromatic molecules revealed the importance of the repulsive $^1\pi\sigma^*$ coordinate in the photodissocation. Pyrrole, being the simplest prototype of this class of

molecules, has attracted much attention in gas phase, with studies focussing on the N-H bond fission[4-6]. Understanding differences and similarities in the photochemistry between gas and solution phases is crucial to translate conclusions drawn from isolated systems to molecular systems in a solvent environment. We conducted solution phase femtosecond transient absorption (fs-TA) studies of pyrrole and 2-ethylpyrrole (2-EP). Spectral signatures of the nascent radicals were assigned with help of time-dependent density functional theory (TD-DFT) excitation calculations.

Our fs-TA data suggest that the short time dissociation dynamics of pyrrole and 2-ethylpyrrole in ethanolic solution resemble the fast dissociation dynamics known from gas phase studies [REF]. The solution phase data further indicate radical product formation in both the ground state and first excited electronic states, as predicted by dynamics simulations but in contrast to gas phase ns data.

In the case of pyrrole, a fast (~1 ps) population flow is observed from the D_1 ($^2B_1$) state to the D_0 ($^2A_2$) state. This observation is in agreement with recent ab-inito multiconfigurational Ehrenfest calculations (AI-MCE)[7]. The fast population flow is governed by an additional concial intersection in the radical between the D_0 and D_1 state close to the D_1 minimum (Ref. [7]), which has not been considered in interpretations of gas phase data.

A significant difference is observed in the relaxation dynamics of the 2-ethylpyrrolyl radical in that the excited state (D_1) radical population appears to be stable. TD-DFT calculations indicate that the intersection between D_0 and D_1 states lies above the D_1 minimum. Furthermore, the 3s Rydberg character of the repulsive $^1\pi\sigma^*$ surface is responsible for a significant barrier along the N-H stretch coordinate and allows population to be trapped before dissociation. Our TA data also suggest a tunnelling process upon excitation close to the minimum of the repulsive state in the vertical Frank Condon region, which is absent with higher pump energy (above the S_1 barrier).



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C10 Development of a novel time-resolved electron diffraction apparatus

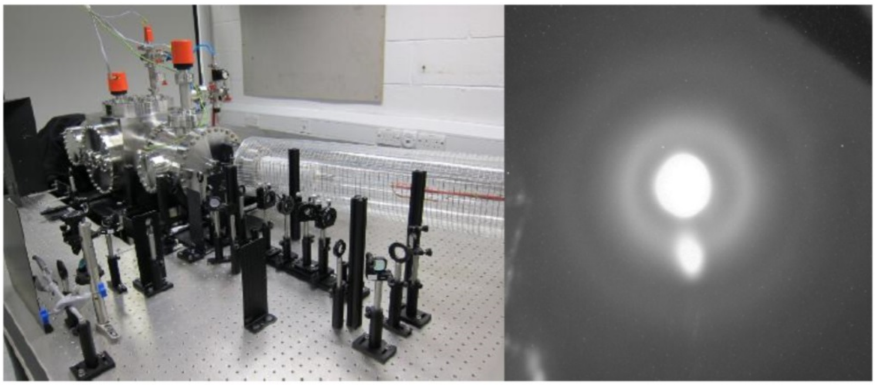
Matthew S. Robinson, Paul D. Lane, and Derek A. Wann

Department of Chemistry, University of York, Heslington, York, YO10 5DD

Electron diffraction has been a staple technique in determining the structure of molecules for nearly a century. However, until recently all electron diffraction experiments used a continuous electron beam, which limits us to being able to observe only static structures of molecules[1]. As molecules are constantly in a dynamic state, this time-averaged information is essentially a "blurred" image, like a photograph of a fast moving object taken with a long-exposure camera.

With the rise of femtochemical techniques, it is now possible to capture sharp, near-instantaneous diffraction images from molecular species using a pulsed electron beam[2]. Combining a laser pump and electron probe it is possible to watch how a molecule evolves over a period of time in its excited state.

The Wann group's newly assembled apparatus (below, left) is now producing diffraction patterns (below, right), and will be used to carry out time-resolved electron diffraction experiments for both crystalline and gas-phase samples. In this talk we will discuss the development of the apparatus, comparing its characteristics with those simulated using the SIMION and GPT programs[3]. We will present our initial diffraction results, as well as quantum chemical calculations that are guiding us in our choice of samples to study experimentally in the near future.



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3. D. A. Dahl, *International Journal of Mass Spectrometry*, 200, 200, 33.

C11 Following the relaxation dynamics of photoexcited aniline in the 273-266 nm region using time-resolved photoelectron imaging

James Thompson

Heriot Watt University

Time-resolved photoelectron imaging was used to investigate the relaxation dynamics of electronically excited aniline in the gas-phase following ultraviolet irradiation in the 273-266 nm region. We find that at all wavelengths studied, excitation is predominantly to the long-lived (>1ns) $S_1(\pi\pi*)$ state, which exhibits ultrafast intramolecular vibrational redistribution on a<1 ps timescale. At excitation wavelengths centred on resonant transitions in the aniline absorption spectrum that have previously been assigned to the higher lying $S_2(3s/\pi\sigma*)$ state, we also see clear evidence of this state playing a role in the dynamics. However, we see no indication of any non-adiabatic coupling between the $S_1(\pi\pi*)$ and $S_2(3s/\pi\sigma*)$ states over the range of excitation wavelengths studied.

I5 Broadband rotational spectroscopy of metal-containing molecules

Nicholas R. Walker

Newcastle University

Rotational spectroscopy has provided a wealth of information about the nature of Van der Waals, hydrogen and halogen bonding interactions. The technique provides unrivalled precision for molecular structure determination and can also be used to study tunnelling and internal rotation. Until recently, experiments have achieved high resolution but only at cost of the bandwidth of individual measurements. Electronics capable of digitising waveforms at gigahertz frequencies now allow experiments to be performed at high resolution, high bandwidth and with minimal or no cost to sensitivity. A design of broadband rotational spectrometer employing chirped-pulse excitation has recently been developed by Pate. A version of this instrument is used in conjunction with laser ablation and supersonic expansion to study metal-containing complexes at Newcastle University. Results will be presented to illustrate how new insights gained from broadband rotational spectra go beyond those achieved using earlier instruments. Opportunities and advantages for the study of metal-containing molecules will be explained. New challenges and strategies for disentangling complexity in rotational spectra will be discussed.

C12 Nanoparticle formation in helium nanodroplets: from quantized votices to giant magnetism

Dan Spence, Cheng Feng, Adrian Boatwright, Elspeth Latimer, Andrew M. Ellis, Shengfu Yang
Department of Chemistry, University of Leicester

Superfluid helium nanodroplets are emerging as a uniquely powerful and versatile tool for the synthesis of novel nanoparticles. In this presentation we report on two applications: (1) the formation of one dimensional nanostructure (nanowires) using the anisotropy provided by quantized vortices in superfluid helium; (2) the formation of pure Ni and Ni/Au core-shell nanoparticles using helium nanodroplets, which were then investigated a vibrational sampling magnetometer (VSM). We have found that for nanoparticles with a small core, e.g., 2.6 nm Ni core coated mono Au layer, the magnetism is hugely enhanced by 8 times compared with the bare Ni nanoparticles, approaching the theoretical limit. A possible explanation for this phenomenon will be provided.

C13 Geometry controlled dissociation of syringol

Jamie Young
Warwick University

C14 Gas-liquid collisions as a method for probing ionic liquid surfaces

M. A. Tesa-Serrate,[a] M. L. Costen,[a] J. M. Slattery[b] and K. G. McKendrick[a]

[a]*School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK*
[b]*Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK*

Ionic liquids (ILs) are low-temperature molten salts generally containing large organic cations. They are receiving increasing attention thanks to their interesting physicochemical properties, having been proposed as an environmentally friendly alternative to traditional solvents.[1] Many of their potential applications such as heterogeneous catalysis, gas chromatography and CO_2 capture involve the interaction between the ionic liquid and a gas. Knowledge of the interfacial structure and composition is essential to understand these processes; however there are very few truly surface-specific analytical techniques that can provide this type of information. An effective approach is to employ reactive collisions with gas-phase species which interact only with the outermost groups at the surface. In the present work, the interfacial reactivity of ionic liquids towards photolytically generated O(^{3}P) atoms has been characterised. The O(^{3}P) atoms react selectively with hydrocarbon chains in the liquid and produce OH radicals. OH products scattered back into the gas phase are then detected by laser-induced fluorescence (LIF). Following a previous proof-of-concept study,[2] a series of ILs containing the 1-alkyl-methylimidazolium cation have been investigated. The results demonstrate that the chemical composition of the interface is significantly different from the average of the bulk liquid, with the alkyl chains on the cation preferentially oriented towards the gas phase. This "surface aggregation" effect depends strongly on both the alkyl chain length and the steric bulk of the counter-anion.

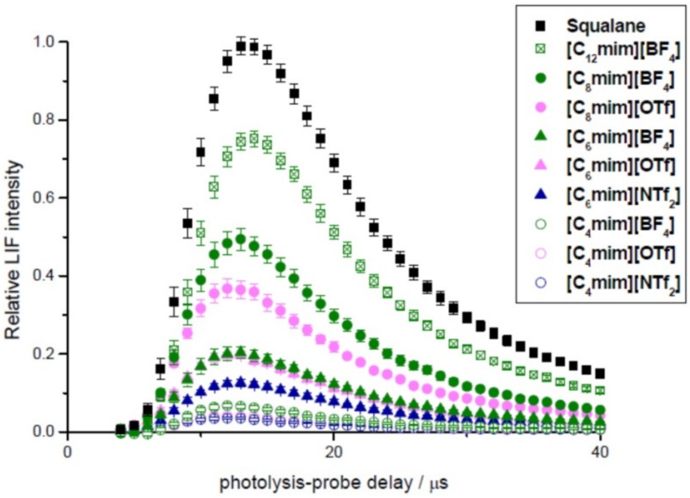

Figure 1. Appearance profiles of OH following reaction of O(^{3}P) with different ionic liquids containing the 1-alkyl-3-methylimidazolium cation ([C$_n$mim]$^+$) with *n* carbon atoms in its alkyl chain. The anions studied are tetrafluoroborate ([BF$_4$]$^-$), triflate ([OTf]$^-$) and bis(trifluoromethylsulfonyl)imide ([NTf$_2$]$^-$). Profiles are compared against an OH appearance profile from a pure hydrocarbon surface, squalane (2,6,10,15,19,23-hexamethyltetracosane).

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C15 Magnetic transition dipole moment unravelled from interferences with an electric transition dipole moment: the OH *A*–*X* system

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We determine the strength of the magnetic dipole allowed transitions in the $A^2\Sigma^+$, $v = 1 \leftarrow X^2\Pi$, $v = 0$ band of the OH radical. In a low external electric field, a small parity mixing slightly enables electric dipole allowed transitions, giving rise to a signal comparable to that of the much weaker magnetic dipole allowed transitions. This allows us to rule out the most prominent source of systematics of previous studies[1]. We measure the magnetic dipole transition moment relative to the electric dipole transition moment of the aforementioned band with an excellent accuracy, in very good agreement with ab initio calculations.

In addition, under specific conditions of applied electric and magnetic fields, and of laser excitation, the electric and magnetic transition dipole moments can interfere with each other. We use these interferences to measure the magnetic to electric dipole moment ratio in the A – X system of OH. The broadly applicable method does not rely on comparison of line intensities. Therefore, it allows one to measure the magnetic to electric dipole moment ratio even in systems in which the magnetic dipole allowed transitions are too weak to be detected.

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C16 New observations and perturbations in the (2+*n*) REMPI spectra of HI

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Raunvísindastofnun HáskólaÍslands, Dunhaga 3, 107 Reykjavík, Iceland.

Mass resolved resonance enhanced multiphoton ionization data for HI, for two-photon resonance excitations to Rydberg and ion-pair states in the 69 600 – 71 500 cm^{-1} region was recorded and analyzed. Several previously observed spectra due to resonance transitions were (re)assigned and the spectral data revealed several previously unobserved (2+n) REMPI spectra. Spectral perturbations, showing as deformations in line positions, line intensities, and line widths, were focused on to derive state interaction strengths, spectroscopic parameters for deperturbed states and parameters relevant to photodissociation processes. Perturbation effects, furthermore, have been helpful in spectra assignments and overall interaction and dynamical schemes to describe the observations are proposed.

C17 Excited state isomeric transitions and reactivity in hydrated nucleobases

Michal Ryszka

Open University

Multiphoton ionisation and electron impact experiments have provided new evidence for unimolecular and intermolecular reactive processes in excited nucleobases and their hydrated clusters. Progress towards producing beams of selected neutral cluster configurations for spectroscopy and collision experiments will be reported.

I6 Stereodynamics of the inelastic scattering of NO with the rare gases

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New velocity map ion-imaging results will be presented for the inelastic scattering of NO(X) by Ar, and other rare gases, in which the NO(X) molecule is fully quantum state-selected both before and after collision. State-to-state differential cross-sections (DCSs) and collision-induced angular momentum orientation and alignment of the fully Λ-doublet resolved inelastic scattering of NO($X^2\Pi_{1/2}$,v=0,j=1/2,f) with Ar have been measured at a collision energy of 530 cm^{-1}.

The dependence of the DCSs and angular momentum polarization on rotational and Λ-doublet state will be discussed in detail, with reference to simple classical and semi-classical models, as well as to exact quantum scattering calculations. A particular focus of the talk will be a discussion of the quantum mechanical origin of collision induced angular momentum orientation.

New experimental results will also be presented in which we have measured the DCSs and polarization on the inelastically scattered NO(X) products arising from collisions with oriented NO molecules. These results may be considered the first 'complete' experiment on the inelastic scattering of NO(X) by the rare gases.

C18 Electron-induced reduction reactions in amorphous solid water ices

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The low energy electron-stimulated reduction reactions of carbon monoxide in amorphous solid water (ASW) films were investigated for various film thicknesses and electron fluences. Layered water/CO films were grown on a Pt substrate by first depositing a thick ASW layer, followed by a single monolayer of CO, which was capped by a thick ASW layer. The films were irradiated with 100 eV electrons, and the concentration of reactants and products was monitored using temperature-programmed desorption and reflection absorption IR spectroscopy. The reduction intermediates and products HCO, H_2CO, H_3CO and CH_3OH were detected, as well as CO_2 from the oxidation channel. CO concentration profiles as a function of electron fluence were simulated using a simple Monte Carlo model that tracks H atoms through the ice lattice.

The results support an H atom migration mechanism, with H atoms diffusing through the film and taking part in the reduction of CO. It appears that H atoms diffuse deeper within the film than OH radicals, the latter of which are responsible for the oxidation pathway.

C19 The reactive scattering of Cl atoms with alkenes

Greg T. Dunning, Thomas J. Preston, Andrew J. Orr-Ewing

School of Chemistry, University of Bristol, Bristol, UK

The dynamics of Cl atom reactions with polyatomic organic molecules have previously been well studied, with fully state resolved differential cross sections acquired for the Cl+CH_4 reaction. In this study, state specific energy distributions were acquired for the HCl product following the reaction of Cl with propene, iso-butene and 2,3-dimethylbut-2-ene. Reactive scattering images were acquired using a dual beam set up, with the HCl state selectively ionised.

Hydrogen atom abstraction may occur through either a direct abstraction pathway, similar to the reactions with alkanes, or an addition-elimination pathway where a complex is formed by Cl addition to the double bond. Both these pathways are observed, with the direct abstraction producing vibrationally hot, rotationally cool HCl and the addition-elimination producing a rotationally hot, vibrationally cool product. In the case of the reaction of Cl with 2,3-dimethylbut-2-ene, a direct comparison to solution phase reaction studies may now be made.

C20 The interaction of H atom Rydberg atoms with a Cu(100) surface

Jemma Gibbard

University of Oxford

The interaction of Hydrogen atoms in a Rydberg state approaching a Cu(100) surface has been investigated. Cu(100) has a band gap along the surface normal and a series of image states at the surface vacuum interface. Resonance effects in the ionisation dynamics are therefore predicted at fields corresponding to the image state energies. An initial set of experimental measurements were promising but carried large error bars. Subsequently the velocity of the Hydrogen atom beam was scanned, changing detection probability in order to isolate any resonant effects, and interesting features in the surface ionisation profiles were seen. These features are further enhanced by cleaning the copper surface using an ion gun but these results display an unexplained velocity dependence.

3. POSTER ABSTRACTS

P1 Effect of Stark voltage on spectral line shapes in the millimeter wave spectrum of linalool

Stephanie Allpress, *Corey J. Evans*

Department of Chemistry, University of Leicester

The millimeter wave spectrum of linalool was recorded and assigned in the 48-63 GHz region. Calculations at the B3LYP/aug-cc-pVTZ level of theory identified the lowest lying conformer of (S)-(+)-linalool, whilst potential energy surface scans at the B3LYP/6-31G** level of theory calculated a torsional energy barrier that resulted in the splitting of the spectral lines. The millimeter wave spectrum of linalool was fitted using the XIAM program, which suggested further splitting of the spectral lines. Current investigations probe how different Stark voltages affect the line shapes of the spectral lines.

P2 See Abstract for contributed talk **C5**

P3 Synthetic Control of Retinal Photochemistry and Photophysics in Solution

Giovanni Bassolino and Philipp Kukura

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University of Oxford, South Parks Road, Oxford OX1 3QZ, UK

Understanding how molecular structure and environment control energy flow in molecules is a requirement for the efficient design of tailor-made photochemistry. In this work, we investigated the tunability of the photochemical and photophysical properties of the retinal chromophore in solution. Replacing the n-butylamine Schiff base linkage normally chosen to mimic the saturated linkage found in nature by aromatic amines results in the reproduction of the opsin shift and complete suppression of all isomerization channels. Synthetic modification of retinal by directed addition or removal of backbone substituents tunes the overall photoisomerization yield from 0 to 0.55, the excited state lifetime from 0.4 to 7 ps and activates previously inaccessible reaction channels yielding photoproducts such as 7cis and 13cis. There is a clear correlation between the presence of polarizable backbone substituents and photochemical reactivity. Structural changes that increase reaction speed were found to decrease quantum yields, and vice versa, showing an inverse correlation between excited state lifetime and efficiency in contrast to the trends observed when comparing retinal photochemistry in protein and solution environments. Based on the presented results, a simple model is suggested where backbone modifications and Schiff base substituents control barrier heights on the excited state potential energy surface and thereby determine speed, product distribution and overall yield of the photochemical process. This work provides scope for the artificial design of materials with high isomerization yields and specificity to an extent that were thought to exist only in an evolution-optimized, three-dimensional protein environment.

P4 Microwave spectrum and geometry of $C_2H_2\cdots CuI$

Dror Bittner

Newcastle University

Pure rotational spectra of $C_2H_2\cdots CuI$ have been measured using Balle-Flygare and chirped-pulse Fourier transform microwave spectrometers. The complexes were generated within a supersonically-expanding gas sample containing small percentages of C_2H_2, MeI and silver atoms introduced via laser ablation. The ground rotational spectra of two isotopologues, $C_2H_2\cdots{}^{63}CuI$ and $C_2H_2\cdots{}^{65}CuI$, have been fully characterised. Interpretation of the principle moments of inertia of the fitted spectra suggests a T shaped planar molecule of C_{2v} symmetry, with the metal atom close to the centre of mass forming a η^2 bond to C_2H_2. The r_0 bond distance of the metal to the midpoint of the C≡C bond, r(*⋯Cu), is determined to be 1.943(4) Å.

P5 Aluminium atoms 'orbiting' helium nanodroplets

A. Boatwright,[1] G. Sarma,[1] E. Cunningham,[1] S. Yang,[1] A. M. Ellis,[1] J. Jeffs,[2] L. Rimmer,[2]
N. A. Besley,[2] A. J. Stace[2]

[1] *Department of Chemistry, University of Leicester*
[2] *School of Chemistry, University of Nottingham*

Aluminium atoms generated by laser ablation within the path of a beam of helium droplets are shown to occupy both the ground electronic state ($3s^23p$; ^2P) and a series of metastable electronic excited states. Photoionization spectra originating from the metastable states allow transitions of Al to states above the ionization threshold to be recorded and we observe narrow absorption profiles with little or no shift when compared with the gas phase. We present evidence that these transitions arise from metastable Al atoms 'floating' on the helium droplet surface and explain this finding with the aid of ab initio calculations.

P6 From macroscopic to microscopic dissociative ionization dynamics: electron impact processes

James N. Bull[1], Jason W. L. Lee[2], and Claire Vallance[2]

1 Department of Chemistry, Durham University
2 Department of Chemistry, University of Oxford

The collision of free electrons with gas-phase molecules leading to ionization is one of the most fundamental processes in particle physics, and forms the basis of many small-molecule mass spectrometers. Despite electron impact first being suggested for mass spectrometry one century ago, comprehensive studies on the fundamental ionization dynamics for molecular systems are scarce due to the many-body nature of the process. This poster provides an account on the construction and application of two instruments over the last three years, targeted at measurement of absolute total ionization cross-sections (TICS), partial ionization cross-sections (PICS), as well as scattering and kinetic energy release distributions via velocity-map imaging (VMI). As listed, these properties become systematically more sensitive to the detailed dissociative ionization dynamics, and with the assistance of *ab initio* and trajectory calculations allow details of the ionization dynamics to be disentangled. As examples, TICS have been measured and modelled for a series of heterocyclic and aromatic species that can be considered as functional group analogues to the constituents of DNA and RNA sequences. These values are important input parameters in the modelling of genotoxic damage to living cells. PICS are summarised for a series of saturated and unsaturated perflourocarbons, which for over fifty years have been well-known to violate statistical theories of mass spectra due to interplays between non-statistical impulsive dissociation from excited states, and rapid intramolecular F-atom migratory rearrangements. These parameters are important in the modelling and tuning of plasma used as etchants in the semiconductor industry. Finally, a detailed analysis of the extraction of microscopic cross-sections from the electron-impact VMI of O_2 and CF_4 molecules will be presented.

P7 Spectroscopy and Kinetics of Criegee Intermediates

Rabi Chhantyal-Pun

University of Bristol

Criegee intermediates are intermediates involved in the ozonolysis of alkenes. Photochemistry and reactivity of Criegee intermediates are of significant interest in atmospheric chemistry. Recently simple Criegee intermediates have been detected in the laboratory setting via spectroscopic methods. Preliminary results on spectroscopy and kinetics of Criegee intermediates obtained via cavity ring down spectroscopy (CRDS) will be presented.

P8 Rotational Cooling of Cold, Trapped Diatomic and Polyatomic Ions

Nabanita Deb[1], Brianna Heazlewood[1], Chris Rennick[1] and Tim Softley[1]

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Chemistry Research Laboratory, 12 Mansfield Road, Oxford OX1 3TA

In recent years there has been much progress in the field of cold and ultracold molecular physics and a variety of experimental techniques for producing cold matter now exist. In particular, several groups have demonstrated the generation of trapped molecular ions at mK temperatures by sympathetic-cooling with laser-cooled atomic ions.[1,2] By implementing schemes to selectively prepare or to control the internal quantum state of the molecular ions, it will be possible to study chemical reactions under highly controlled conditions in an ion trap.

However, species produced in selected rovibrational states often have lifetimes of only a few seconds, as population is redistributed across several rovibrational states through interaction with the ambient blackbody radiation[3] (BBR). In this work, we propose ways to overcome the technical challenge of cooling the ion-trap through the use of lasers to pump the rovibrational population towards the rovibrational ground state.4 A variety of diatomic species are considered, including DCl^+, CsH, LiH and MgH^+.

This approach is extended to $C_2H_2^+$, where the interaction of a nonpolar polyatomic ion with BBR is investigated, with some interesting results. The exciting possibility of rovibrationally cooling this species is discussed in detail.

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P9 Transverse focusing effects in the Zeeman deceleration of hydrogen atoms

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3Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany
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Zeeman deceleration is an experimental technique in which inhomogeneous, time-dependent magnetic fields inside an array of solenoid coils are used to manipulate the velocity of a supersonic beam[1,2]. We have built and characterised a 12-stage Zeeman decelerator for hydrogen atoms in Oxford. Here, we give a detailed description of the experimental setup, and we present experimental results illustrating that the overall acceptance in a Zeeman decelerator can be signi_cantly increased by applying a low, anti-parallel magnetic field to one of the coils so as to form a temporally varying quadrupole _eld which improves particle confinement in the transverse direction[3]. The results show excellent agreement with three-dimensional numerical particle trajectory simulations, and they suggest the use of a modfied coil configuration to improve transverse focusing during the deceleration process.

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3. K. Dulitz, M. Motsch, N. Vanhaecke, T. P. Softley, submitted.

P10 Spectra and Dynamics of H_2S^+

Geoffrey Duxbury[1], Alex Alijah[2], and Christian Jungen[3]

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[2]*University of Reims, France*
[3]*Laboratoire Aimé Cotton, France*

Recently there has been a renewal of interest in the spectroscopy and dynamics of the formation and fragmentation of the hydrogen sulphide ion. In particular Han et al.[1] have obtained rotationally resolved spectra of higher vibrational states of the $\tilde{A}\,^2A_1 - \tilde{X}\,^2B_1$ system than were obtained previously[2], and Webb et al.[3,4] have carried out a comprehensive imaging study of the photo-fragmentation routes of highly excited H_2S^+.

Alex Alijah, Christian Jungen and I have extended our previous *l* basis approach to the calculation of the effects of orbital angular momentum in $H_2S^{+\;2}$ to include the stretch –bender extensions[5,6,7], with the options of using either the *K*- or *l* basis. This new code is being used to calculate the complicated orbital angular momentum and spin-orbit coupling effects responsible for the ro-vibronic pattern measured in some of the new experimental results, including the role played by predissociation.

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7 Duxbury, G. and Reid, J.P. *Mol. Phys*. 105, 1603 (2007)

P11 Solution phase photodissociation of XeF_2

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Gregory M. Greetham, Ian P. Clark, Mike Towrie
Central Laser Facility, Rutherford Appleton Laboratory, UK

XeF_2 has been shown to dissociate promptly in various organic solvents, following photolysis at 266 nm, to produce XeF and F. The dissociation is observed through an ultrafast pump-probe technique with near UV absorption via the B←X transition in the XeF product. The B $^2\Pi_{1/2}$ state of XeF is an ion pair state and so the B←X band origin varies with dielectric constant of the solvent.

In Ar and Ne matrices the XeF B←X absorption shifts to lower energy, which is a signature of a caged fluorine atom perturbing the B state potential surface. It is suggested that the remaining F atom created through the photolysis of XeF_2 causes a similar affect to the B state potential of the XeF in the liquid phase. The shifted spectrum that is observed from this perturbation has a 3 ps lifetime, indicating that the F atom either rapidly recombines to form XeF_2, or is removed from the solvent cage either through reaction with the solvent or diffusion into the bulk. Consequences for the use of XeF_2 as a photolytic precursor for F atom reactions in solution will be discussed.

P12 Ni/Au core-shell magnetic nanoparticles formed in helium nanodroplets

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Helium nanodroplets are emerging as a powerful and versatile tool for the synthesis of novel nanoparticles. In particular, the sequential pickup of molecules/atoms allows the addition of different materials to helium nanodroplets and thus the formation of core-shell nanoparticles. In this presentation we report our recent progress on the formation of pure Ni and Ni/Au core-shell nanoparticles using helium nanodroplets, which were then investigated using a vibrational sampling magnetometer (VSM). For nanoparticles with a small core, e.g., 2.6 nm Ni core coated with a gold monolayer, the magnetism is enhanced by 8 times compared with the bare Ni nanoparticles and approaches the theoretical limit. A possible explanation for this phenomenon will be provided.

P13 See Abstract for contributed talk **C20**

P14 Collision Induced Polarisation Over a Rainbow

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Inelastic scattering measurements have been made for the NO(X)—Kr system using a crossed molecular beam apparatus[1] coupled with velocity mapped ion imaging[2]. The initial state of the NO(X) was selected using hexapole focussing and the final state by (1+1') REMPI. This scheme allows for fully Λ-doublet resolved transitions to be observed [3], heightening the experiment's sensitivity to the attractive and repulsive forces that govern the collision dynamics.

The experimental apparatus also facilitates the determination of various polarisation moments (Figure 1) [4-5]. Measurements have recently been completed of both the alignment (plane of rotation) of the NO after collision with Kr and the orientation [6](sense) of rotation of NO(X) after collision with Kr. These measurements are extremely sensitive to the NO(X)—Kr PES [6] and provide insights into the interplay between the attractive and repulsive terms in the NO(X)-Kr potential and hence the observed dynamics.

We have also completed a theoretical study of the NO(X)—Kr alignment and have shown that although the collision system can be rationalised classically by the kinematic apse model[7], only by using a full quantum treatment can one reproduce all the features observed in the experimental data.

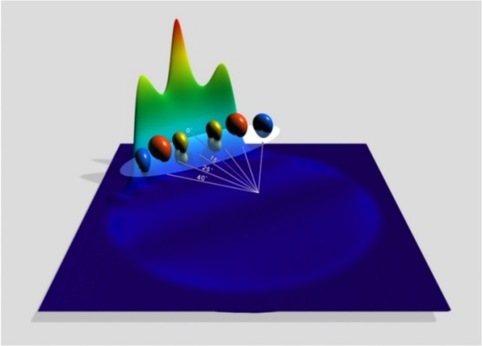

***Figure 1**: Quantum mechanically predicted angular momentum polarisation for the NO(X)—Kr collision with j'=3.5f. Only quantum mechanics reproduces the observed experimental polarisation. The background shows the theoretical angular distribution for the transition.*

P15 Density Functional Calculations of Anharmonic Frequencies in Ground and Excited States

Magnus Hanson-Heine

University of Nottingham

The work outlined in this poster covers three main topics:

1. Small molecule anharmonic corrections – this section analyses of the performance of different hybrid and gradient-corrected exchange-correlation functionals in calculating anharmonic vibrational frequencies for a wide range of small organic and inorganic molecules, including quantifying the effect of an increasing fraction of Hartree-Fock exchange.

2. Partial Hessian anharmonic corrections – A look at work developing faster methods for calculating anharmonic corrections for adsorbate molecules, molecules in solution, and highly localized vibrational modes, based on partial Hessian analysis.

3. Excited state frequencies – Finally, an assessment of the accuracy of frequencies computed using Kohn-Sham type DFT excited states, using the T1 states of 9-fluorenone and 2-naphthaldehyde as case studies.

P16 Ab-Initio Investigation of Group II Metal Hydride Complexes

Joe Harris

University of Nottingham

P17 Are arginine-halide clusters zwitterionic?

Andrew Harvey

University of York

We report the first MP2 computational study of the $Cl^{-}\cdot$ Arginine and $Br^{-}\cdot$ Arginine complexes, with the clusters being systematically classified into conformational families prior to optimization. The canonical tautomers in particular adopt numerous conformeric structures with close relative energies. Conformer energy differences are of similar magnitude to the canonical-zwitterionic tautomer differences, indicating that it is essential to obtain reliable conformer energies to determine whether the global minimum structure is zwitterionic or canonical for these prototype anionic systems. The zwitterionic and canonical minima are found to be very close in energy for $Br^{-}\cdot$Arginine, whereas the canonical form is significantly lower for $Cl^{-}\cdot$ Arginine. The calculations are used to interpret isotopically substituted IR spectra of the cryogenically cooled $Br^{-}\cdot$ Arginine cluster obtained by Johnson and coworkers.

P18 Reactions of cold ions and molecules

Brianna Heazlewood

University of Oxford

P19 See abstract for contributed talk **C2**

P20 See abstract for contributed talk **C16**

P21 Tuning Dynamics at Conical Intersections

R. Ingle, T.N.V. Karsili, B. Marchetti, M.N.R. Ashfold

University of Bristol

Conical intersection (CIs) are responsible for many of the ultrafast processes that are ubiquitous in photochemically driven biological and catalytic phenomena. It is therefore imperative that their versatilities and topologies are understood in great detail in order to tune processes that are facilitated by CIs. In this current project we outline experimental and theoretical projects that explore such avenues.

The photostability of DNA bases and base pairs can be understood by ultrafast internal conversion from the first excited state to the ground state, which is facilitated by a CI. We present theoretical results that show that the energies of a certain CIs can be tuned as well as the potential barrier en-route from S_1 to the CI by the changing the number of nitrogens substituted in the ring.

We also present experimental results that show how it is possible to control the radical electronic branching ratios and thus the photodissociation pathways in some functionalised heteroaromatics. By tuning the geometry of molecules around their CIs, it is possible to create photodissociation products either in their ground or excited state.

P22 Integrating cavity-enhanced spectroscopies with microfluidic systems

Dean James[1], James Foster[1], Cathy M. Rushworth[3], Aurélien Trichet[2], Jason Smith[2],
Hywel Morgan[3], and Claire Vallance[1]

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[2]Department of Materials, University of Oxford
[3]School of Electronics and Computer Science, University of Southampton

We are trialling the use of cavity enhanced spectroscopy to increase the detection sensitivity over conventional single-pass absorption measurements in microfluidics applications. This allows the probed sample volume to be reduced, with concomitant reductions in measurement time and reagent consumption.

P23 Mediating internal conversion by folding dynamics: a femtosecond time-resolved mass spectrometry study of a series of diamines

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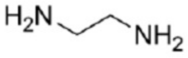
Department of Chemistry, University of Copenhagen, Universitetsparken 5,
DK-2100 København Ø, Denmark

The interaction between the two amino groups has been investigated in a series of 5 simple diamines (**1**-**5**).



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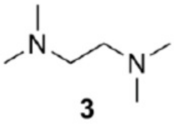

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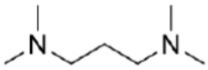

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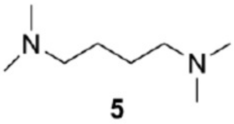

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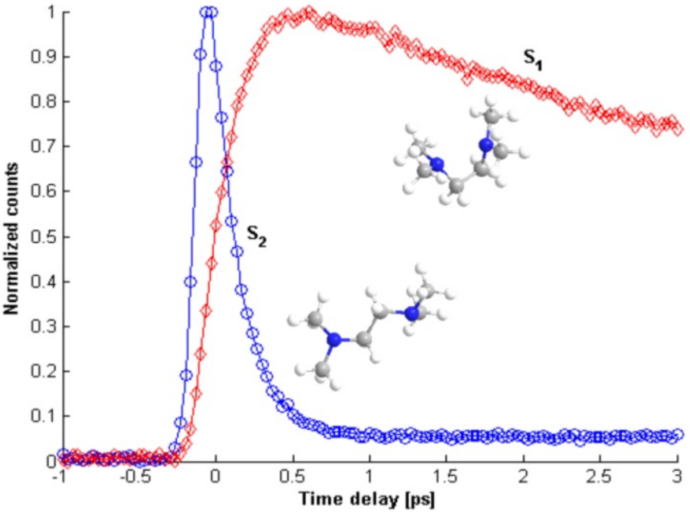
The purpose of the investigation was to determine the nature of the interaction, and how this interaction affects the excited-state dynamics. A pump-probe experiment with time-resolved mass spectrometry for detection was set up, to follow the excited-state dynamics of the diamines in the first few picoseconds after excitation to the S_2 Rydberg state.



The dynamics exhibited in the mass spectrometry transients is evidence of the transition from S_2 to S_1. Planarization of the amino groups and torsion in the alkyl chain is responsible for coupling the two states, mediating the internal conversion between them. Contributing to the notion that the torsional motion is in fact crucial is the observation that the process becomes slower when the ends get heavier, in going from the primary amino groups to the dimethylated tertiary amino groups. Calculations of the potential energy surfaces support this interpretation.

P24 Time-resolved photoelectron imaging study of the S_2 to S_1 internal conversion in simple amines

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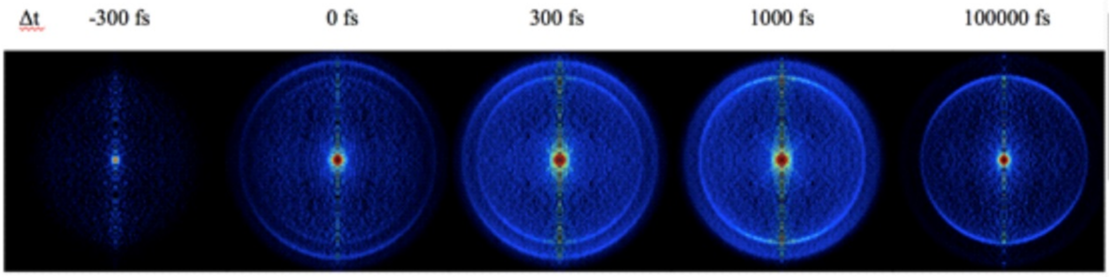
A series of small constitutionally isomeric aliphatic $C_5H_{13}N$ and alicyclic $C_5H_{11}N$ amines has been investigated with time-resolved photoelectron spectroscopy, using the VMI technique. The goal is to determine the effect of structural variations on the photophysics of amines following ultraviolet excitation. In particular the degree of N-substitution seems to be of importance, resulting in interesting differences in the dynamics[1].

Earlier studies have shown that for the tertiary amine N,N-dimethylisopropylamine (DMIPA), initial excitation to the 3p Rydberg state is followed by rapid internal conversion to the 3s state, which then decays with a longer time constant[2]. This is also seen in our data for both DMIPA and the unbranched N,N-dimethylpropylamine (DMPA).

An observation of interest is the differences in the evolution of the dynamics when going from tertiary to secondary and primary amines. One aspect of this is faster decay of the spectral features. If the decay reflects internal conversion from the initially excited state, this is opposite to expectations based on standard density-of-state arguments. This type of non-ergodic behavior has previously been observed in a series of cycloketones where the electronic states are coupled by a few specific vibrations[3]. The explanation may be similar for the amines, with coupling through the nitrogen inversion vibrational mode.

In addition, the spectra for the secondary and primary amines shows a broad spectral feature which could reflect a strong coupling of the lowest 3s state and a dissociative σ* state, as has been found for ammonia[4] and methylamine[5].



Abel inverted photoelectron VMI images for N,N-dimethylpropylamine at selected pump-probe delay times Δt.

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P25 See abstract for contributed talk **C9**

P26 Cold, Magnetically-Trapped Br Atoms

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We have produced a source of cold, magnetically trapped, bromine atoms. The Br atoms are produced by photodissociation of molecular bromine at 460 nm. The excess energy above the dissociation threshold produces Br fragments that recoil along the polarization axis of the laser. These Br fragments have velocity vectors that cancel that of the molecular bromine and are thus stationary in the lab frame. A pair of magnets forms a quadrupole-like potential which traps the low field-seeking Br atoms. The trapped atoms are then detected by 2+1 multiphoton-ionization (255 nm) delayed from the dissociation laser. We have detected these Br atoms at delays of 99 ms, i.e. up to the next laser shot, allowing for accumulation of density over successive laser shots. A molecular dynamics model has shown that this density can reach steady-state after a few seconds, reaching equilibrium of loading with loss by elastic collisions with background gas.

We have characterised the three largest contributions to trap loss: elastic collisions from the elastic collisions from the background Ar gas, Ar molecular beam, and Majorana spin flips. The long-time trap loss kinetics can be approximated by a pseudo-first order mechanism in which a collision transfers sufficient energy to eject an atom from the trap. We measure a decay rate of $1.31\pm0.29\ 10^{-9}\ \mathrm{cm}^3\ \mathrm{s}^{-1}$, which was used to fit for our trap depth of $U0/kB = (270\pm35)$ mK and hence the cross section of 201 ± 28 $\mathrm{Å}^2$ with a 95% confidence interval (Figure 4). Short-time losses are dominated by collisions of trapped atoms with fast Ar atoms in the molecular beam. Using the measured trap depth we determine that the molecular beam density peaks at 1.0×10^{12} atoms cm^{-3}. The rate of loss of Br atoms in the trap due to such collisions is measured to be $1.17\times10^{-14}\ \mathrm{cm}^3\ \mathrm{s}^{-1}$, corresponding to an elastic collisional cross section of 73,800 $\mathrm{Å}^2$. Finally, our Monte Carlo simulations show that the loss rate of Br atoms due to Majorana spin flips and have found that it will cause a loss of 5-20% of Br for one molecular beam load over a period of 5 seconds, therefore regarded as a negligible effect.

P27 Photostability of disulfide bridges

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Proteins are highly dependent on their tertiary and quaternary structure for proper molecular function. The conformation and stability of proteins are often strongly influenced by disulfide bridges [1] which are known to cleave photolytically [2]. From an evolutionary perspective the photochemical stability of nature's building blocks is of great importance and at a first glance disulfide bridges do not meet this requirement. Our femtosecond time resolved mass spectrometry experiments (TRMS) on dithiane (fig. a) showed a surprising intrinsic photochemical stability of the disulfide bond that is secured via the confinement of the cyclic structure. We showed that in spite of a repulsive excited state potential energy surface the molecule finds a safe return to the ground state through a conical intersection leading to the reformation of the disulfide bond [3]. These ultrafast dynamics are reflected in the oscillations observed in our TRMS experiments (fig. a).

We address whether the stability of dithiane is due to an intrinsic property of the S-S bond or arises from the carbon framework preventing the sulfur atoms from flying apart. Thus, we have investigated dithiane's open-chain counterpart diethyl disulfide (DEDS) (fig. b). The TRMS experiment show the linear disulfide undergoes ultrafast S-S dissociation on a sub-50 fs timescale without further ado (fig. c) [4]. Supported by the computed potential energy surfaces this shows that the photostability of dithiane must be ascribed to the cyclic structure exerting a restoring force that prevents the dissociation of the bond.

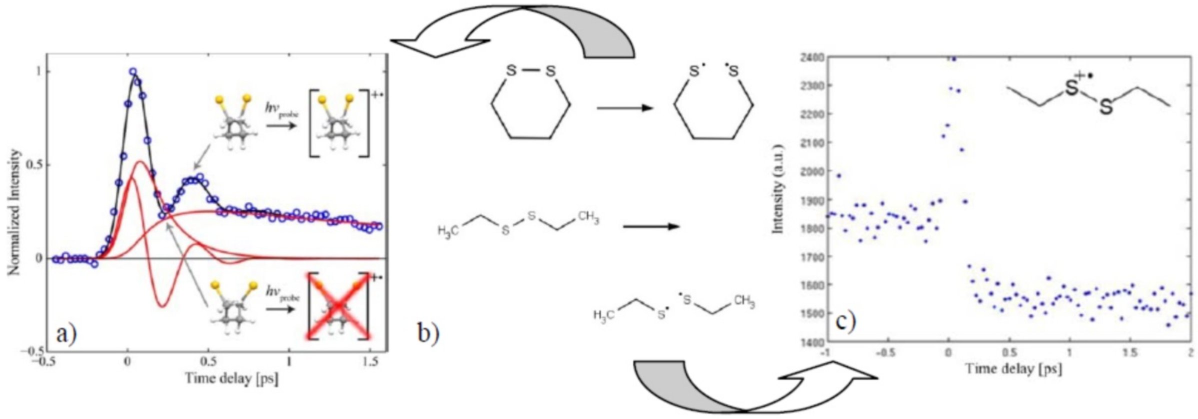

Fig. a. Fragment ion transient for dithiane using 284 nm pump and 400 nm probe pulse. b. Photolytical cleavage of dithiane (top) and DEDS (bottom). c. Fragment ion transient for diethyl disulfide using 266nm pump and 400nm probe pulse.

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P28 Quantized vortices and the formation of nanowires in superfluid helium droplets

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Department of Chemistry, University of Leicester

Helium nanodroplets have a variety of unique properties, some of which they share with bulk liquid helium. Until recently quantized vortices had only been seen in bulk helium and the evidence for their presence in superfluid helium nanodroplets was lacking. At Leicester we have now collected transmission electron microscopy (TEM) images of long chains of both spherical and rod shaped nanoparticles derived from the collision of large, doped helium droplets with a solid surface. Given that spherical nanoparticles have no intrinsic anisotropy, the particles must experience an aligning force that will guide the nanoparticles into chains and the only explanation is alignment along a quantized vortex. The presence of vortices has allowed us to grow 1-D nanowires for a variety of metals including, Au, Ni, and Cr, where these wires can have lengths of several hundred nm.

P29 The Pixel Imaging Mass Spectrometry (PImMS) sensor: the fundamentals and novel time-resolved imaging applications

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The Pixel Imaging Mass Spectrometry (PImMS) sensor has been developed in collaboration between the Departments of Chemistry and Physics in Oxford and the Rutherford Appleton Laboratory. The sensor is capable of simultaneously recording spatial and temporal data (to a precision of 12.5 ns) making it ideal for use in any time-resolved imaging experiments. This poster describes the operation of the sensor and details some of the novel applications to date.

P30 A Moving Trap Zeeman Decelerator

A. Mizouri, U. M. Krohn, V. Singh, L. A. McArd and D. Carty

Durham University

Our research is part of an experimental programme to build a quantum simulator using polar molecules. The aim of this programme, entitled "MicroKelvin Molecules in a Quantum Array" (MMQA), is to cool high densities of molecules to microKelvin temperatures and trap them in an optical lattice to create an ideal, tuneable and highly versatile tool for modeling strongly-interacting quantum systems and understanding the remarkable quantum phenomena they exhibit[1].

The general approach we are taking is to cool down large numbers of polar molecules using a modified design of a moving magnetic trap Zeeman decelerator[2]. This will be the first cooling stage down into the milliKelvin regime. The molecules will then be loaded into a microwave trap in their absolute ground state and be sympathetically cooled with ultracold atoms down into the microKelvin regime[3].

To detect the molecules, we intend to use a newly developed technique called cavity-enhanced laser-induced fluorescence (CELIF) that uses a cross-correlated combination of cavity ring-down and laser-induced fluorescence (LIF) detection to measure absolute densities of molecules with the sensitivity of LIF.

Here we present the achievements so far in our efforts to build a moving trap Zeeman decelerator, including our latest measurement of absolute densities (>10^5 cm^{-3}) of radicals in a molecular beam using CELIF.

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P31 See Abstract for contributed talk **C18**

P32 Ultracold collision of Li + CaH in a magnetic field

Masato Morita

Durham University

P33 Isomerization of the Azobenzene Radical Cation

Kristin Munkerup[1], Timothy Bohinski[2], Katharine M. Tibbets[2], Robert J. Levis[2], Theis I. Sølling[1]

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[2]*Temple University, Center for Advanced Photonics Research, Department of Chemistry,19122 Philadelphia, Pennsylvania, United States*

The photoisomerization of neutral azobenzene is well studied due to its applications as a photoswitch[1] and a molecular motor.[2] The radical cation dynamics of azobenzene is not well studied,[3] however understanding the behavior of various radical cation systems can help elucidate their role in chemical reactions[4-6] and lead to developing new forms of spectroscopy.[7] In this study, cis- and trans-azobenzene radical cations have been prepared using strong field tunnel ionization at infrared wavelengths (1200-1500 nm) and the dynamics investigated with femtosecond time-resolved mass spectrometry. The goal is to complement and extend the work by Ho et al.[3] who investigated trans-azobenzene radical cations with femtosecond pump-probe photoionization-photofragmentation spectroscopy in which the transients showed an oscillation in the parent and phenyl transient signals which was assigned to be the result of a torsional motion involving the phenyl groups on the radical cation ground state surface.

This study shows that radical cations of both trans- and cis-azobenzene dissociate into the same fragments indicating that the cis and trans forms have similar fragmentation pathways. Furthermore, both isomers have oscillations in the parent and phenyl fragment transients. These observations confirm the phenyl torsion to be the active motion that causes the observed oscillations, however the oscillations are out of phase and have different periods (Figure 1a and 1c) indicating different time evolution of the phenyl torsional motion.

Time-dependent DFT calculations on the B3LYP/6-31+G(d) level of theory have been used to perform a scan along the CNNC dihedral angle on the neutral ground state S_0 (red) and cationic ground state D_0 (blue) in Figure 1. The optimized geometry on the cation surface is when the CNNC dihedral angle is 90 degrees and as can be seen from Figure 1 the trans- and cis-azobenzene neutral geometries are far away from the optimal situation and therefore isomerize into the same isomer, the perpendicular azobenzene. This explains why the cis- and trans-azobenzene show the same fragmentation patterns and why they both have an oscillation in the transients.

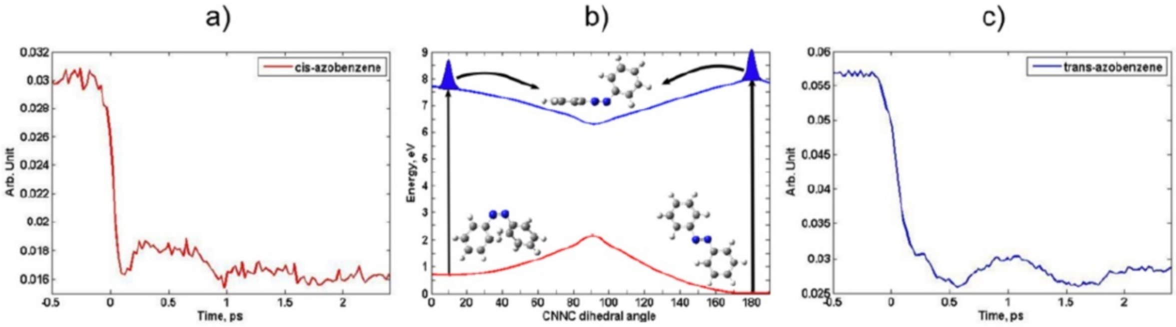

Figure 1. a) Parent transient signal of cis-azobenzene radical cation ionized with 1540nm pump and 800 nm probe probe. b) TDDFT results of a scan of the CNNC torsional angle on azobenzene. Red is the neutral S0 state blue is the D_0 cation ground state. Cis- and trans-azobenzene relax into the same geometry on the cation ground state surface. c) Parent transient signal of trans-azobenzene radical cation ionized with 1540 nm pump and 800 nm probe.

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P34 Time-Resolved Infrared Absorption Studies of the nσ* Mediated Ring-Opening Dynamics of Heterocyclic α-Carbonyl Compounds

Daniel Murdock, Joel Luke, Stephanie J. Harris, Michael P. Grubb, Ian P. Clark, Gregory M. Greetham,
Michael Towrie, and Michael N. R. Ashfold

Department of Chemistry, University of Bristol

Recent work has highlighted the important role played by optically "dark" n/πσ* electronic states in the photodissociation dynamics of electronically excited heteroaromatic molecules in both the gas and solution phases. The potential energy surfaces of states formed by σ*←n/π excitation are typically repulsive with respect to X–Y (X=O, N, S, etc.; Y=H, CH_3, etc.) bond extension and thus offer a route either to bond fission or to internal conversion via conical intersections located at extended X–Y bond lengths. The same paradigm should also apply to ring-opening reactions of heterocyclic molecules. This poster provides an overview of recent work performed on the UV-induced ring-opening reactions of three heterocyclic α–carbonyl compounds, furanone, thiophenone, and coumarin, in the solution phase, where ultra-fast transient vibrational absorption spectroscopy allows both the rates and quantum yields for such processes to be followed.

P35 CELIF: cavity-enhanced laser-induced fluorescence

Hendrik Nahler

Heriot-Watt University

P36 Stereodynamic effects in collisions of NO(X) + Ar

M. Brouard[1], H. Chadwick[1], C. J. Eyles[1], S. D. S. Gordon[1], B. Hornung[1], B. Nichols[1], F. J. Aoiz[2], S. Stolte[3]

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[2]*Departmento de Química Física, Universidad Complutense, Spain*
[3]*Atomic and Molecular Physics Institute, Jilin University, China*

Inelastic scattering measurements have been made for collisions of oriented NO(X) with Ar using a crossed molecular beam apparatus coupled with velocity mapped ion imaging, for a selection of spin-orbit conserving and spin-orbit changing transitions. The initial state of the NO(X) was selected using a hexapole field and the final state by (1+1') REMPI, allowing full Λ-doublet resolution of both the initial and final quantum state. The bond axis of the NO molecule was oriented prior to the collision using a static electric field generated by a four rod setup. Fast switching between the orientation field and velocity mapping conditions is needed to be able to image the scattered NO after the collision[1].

The state to state oriented differential cross-sections for scattering of NO with Ar have been measured, building on previous work on the steric asymmetry[2-3]. Complementary quantum mechanical calculations have also been performed and the agreement between the experimental and theoretical differential cross-sections is reasonable. The normalised difference between the two oriented DCSs varies with scattering angle, and can be qualitatively reproduced by model calculations that consider the interferences between four limiting scattering paths[4].

Preliminary measurements of the product rotational angular momentum alignment following collisions of NO(X) with argon have also been performed experimentally. The differences between the two orientations are not as pronounced as for the oriented differential cross sections. The results obtained can be explained classically by considering a simple kinematic apse[5] model, in which the projection of j onto the apse is conserved throughout the collision. Again, the polarisation parameters obtained from the experimental data are in good agreement with those obtained theoretically.

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P37 Photoion and photoelectron Spatial-map Imaging for plant sciences

Haoyu Niu, Cécilia Cauchy, and Claire Vallance

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The aim of my project is to develop spatial-map imaging to enable "chemically-resolved" imaging of plant samples with sub-cellular resolution. In our existing experimental setup, the sample is illuminated at a shallow angle by a UV laser, and spatial-map imaging optics are used to image the resulting photoions or photoelectrons onto a microchannel plate (MCP) detector coupled to a phosphor screen. Ions of a chosen mass are then acquired by gating the MCPs to the arrival time of interest and using a CCD camera to capture the image. In the future the instrument will be coupled to the PImMS ultrafast imaging sensor to allow images to be captured for every ion on each time-of-flight cycle. The images provide information on the identity of chemical compounds present at the surface of the sample and their spatial distribution across the surface. This could have a wide range of applications, including comparing healthy and diseased plant samples to determine the nature of the disease present.

To optimise the spatial mapping optics and determine the best achievable spatial resolution for the instrument, I have carried out ion trajectory simulations with the SIMION 8.0 software package. Optimising the sample preparation is key to achieving high quality imaging, and I have characterised a number of different sample preparation methods using an onion membrane as a test sample. Once these stages are completed, I will adapt the preparation techniques to be applicable to a wider range of plant samples.

My poster describes the simulations and optimization experiments we have carried out so far, and the sample preparation techniques we have tried.

P38 THz description of biologically relevant molecules

János Móczár and József Orbán

MTA TKI High Intensity Terahertz Research Group, Pecs, Ifjusag u. 6, 7624, Hungary

Terahertz spectroscopy is a powerful technique to provide information on low energy molecular state transitions and vibrations. The applied time domain terahertz spectroscopy (TDTS) method results in time resolved intensity data of the sample transmitted pulse that we convert to amplitude-frequency data set (transmittance spectrum).

We investigated biologically relevant molecules to study their spectral response for THz radiation. Characteristic absorbance peaks were determined for some amino acids and specific proteins of our interest. The structure and as a consequence the vibrations of proteins may vary on activation or due to ligand binding. The amount of collective modes increasing by size and complexity of molecules hinder characteristic spectroscopic responses to terahertz radiation therefore spectroscopic comparison of structural changes requires specific techniques.

This fundamental research will help to discover the relationship between the complex spectrum of amino acid chains and its building elements. Our aim is deeper understanding of biological function and role of proteins, especially enzymes and other proteins controlling cell dynamics.

P39 Picosecond Time-Resolved Photoelectron Spectroscopy of para-Fluorotoluene via the S_1 Vibrational Mode at 1990 cm^{-1}

Victoria Parkes

University of Nottingham

A pump-probe photoelectron velocity map imaging experiment was performed where the pump wavelength was resonant with the feature at 1990 cm^{-1} above the S_1 origin of *para*-fluorotoluene. The probe wavelength was chosen to provide a maximum photoelectron excess kinetic energy of ~3000 cm^{-1}. Both the pump and probe laser pulses were of 1 ps duration and the bandwidth of the laser was ~15 cm^{-1}, allowing a coherent superposition of eigenstates to be excited. The time delay between pump and probe was controlled and varied on the picosecond timescale such that a series of photoelectron spectra at different time delays were obtained from the inverted images. The intensities of the spectral peaks were plotted against time delay and fitted to a sum of cosines, in order that any quantum beating patterns associated with intramolecular vibrational redistribution might be quantified. In the present case, we observe quantum beating with an oscillation period of 5 ps overlaid on a rapid overall exponential decay. This is indicative of a coupled system whereby the bright state is strongly coupled to a so-called 'doorway' state. The observation of such an 'intermediate' IVR regime at such a high S_1 energy is remarkable, in that based on the density of states argument one might expect a simple exponential decay.

P40 Velocity map imaging of neutral copper clusters

Imogen Parry

Department of Chemistry, University of Oxford

P41 Imaging Vibrationally Excited HCl from Cl + Alkene Reactions

Thomas J. Preston, Greg. T. Dunning and Andrew J. Orr-Ewing

School of Chemistry, University of Bristol

Reaction between chlorine atoms and alkenes in single-collision environments can lead to HCl formation either through direct H abstraction or addition-elimination pathways. We measure the internal energy of the HCl product and the kinematics of the reaction products by combining resonance-enhanced multiphoton ionization of HCl and velocity-mapping the nascent ions. The Cl + propene reaction generates two distinct rotational temperatures of HCl in its ground vibrational state, 100 K and 4600 K. These two distributions herald two distinct pathways on the reactive surface. Reactions with propene, isobutene, and 2,3-dimethylbut-2-ene all produce vibrationally excited HCl, populating up to v=2. Direct dynamics calculations help reveal how different trajectories over these complicated potential energy surfaces influence the product state distributions.

P42 Photoelectron imaging of water cluster anions: design of a new spectrometer

Joshua P. Rogers, James N. Bull, and Jan R. R. Verlet

Durham University

P43 Using Velocity Map Imaging to study Bimolecular Roaming

Cassandra Rusher

Heriot Watt University

Dynamical studies of the photodissociation of a number of molecules, such as formaldehyde, have shown that there is competition with the classic transition state mechanism. These particular molecules undergo the formation of a frustrated radical state which leads to roaming of a fragment within the molecular space until it extracts the atom or fragment required to allow for full dissociation to occur.

This roaming pathway has recently been shown by Simon North and co-workers, to play a key role in the photodissociation mechanism of NO3. Calculations by Joel Bowman suggest that the roaming mechanism may also occur in the formation of NO3. An experimental set up has been developed to study the reaction of NO + O2 with the view to use velocity map imaging to study the dynamics of this reaction and to establish if roaming is occurring.

P44 Probing inelastic scattering of state-selected ND_3^+ with Ar using velocity-map imaging

Alan Sage, David Hadden, Andrew Orr-Ewing and Stuart Greaves

School of Chemistry, University of Bristol

ND_3^+ ions are created quantum state selectively via the well known C-X 2+1 REMPI transition and subsequently collided with Ar gas in a crossed-beam VMI machine. Preliminary ion images and differential cross sections are presented.

P45 Theoretical approach for photodissociation dynamics with *ab initio* multiconfigurational Ehrenfest method

Kenichiro Saita, Dmitrii Shalashilin

University of Leeds

Recently we report a result of the ab initio multiconfigurational Ehrenfest (AI-MCE) simulation of the photodissociation dynamics of pyrrole (*Phys. Chem. Chem. Phys*. **15**, 16227 (2013)). Pyrrole rapidly dissociates into a pyrrolyl radical and a H atom via a conical intersection and, on the other hand, the population exchange between the two states of pyrrolyl radical occurs on a longer scale than that of N–H bond fission. We are studying on the photodynamics of the pyrrole resembles as 2-ethylpyrrole, 2,4-dimethylpyrrole, etc.

P46 See Abstract for contributed talk **C6**

P47 UV spectroscopy of halide-ion-bound fluorobenzene derivatives in an ion trap

Ananya Sen

University of York

n this work we have investigated interactions between electron-deficient aromatic rings with electron-rich negative ions or groups. We have successfully electrosprayed such anionic complexes ($X^-.C_6F_nH_{6-n}$; X= F^-, Cl^-, Br^- and I^-; n = 3-6) into an ion-trap, mass-selected them and performed in detail UV photo detachment and UV spectroscopic studies on them. This involved modification of a Bruker-Esquire mass spectrometer to enable a pulsed UV laser beam (tunable OPO) to superimpose with the ion packet at the centre of the ion-trap. Preliminary experimental results show a difference in the UV spectrum of halides interacting with different halogen substituted benzene derivatives. Collision-induced dissociation has also been conducted to investigate the structure of the X-.C6FnH6-n complexes. DFT calculations are presented to aid the interpretation of the experimental results.

P48 Rotational Alignment of NO($A^2\Sigma^+$) from Collisions with Ne

Jeffrey D. Steill,[1] Jeffrey J. Kay,[1] Grant Paterson,[2] Thomas R. Sharples,[2] Thomas F. M. Luxford,[2] Jacek Klos,[3] Matthew L. Costen,[2] Kenneth G. McKendrick,[2] M. H. Alexander,[3] and David W. Chandler[1]

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We will describe a novel modification to the now well-established application of crossed molecular beams and velocity map ion imaging (CMB-VMI) to the study of rotationally inelastic collisions. In these experiments, laser excitation is employed to generate nitric oxide in its first electronically excited NO($A^2\Sigma^+$) state in order to carry out a detailed examination of the collision dynamics of an electronically excited molecule.

A molecular beam of NO(X) is crossed with a beam of collider gas within the source region of a velocity map imaging spectrometer. At the crossing region of the two beams, pulsed nanosecond laser radiation at ~226 nm is employed to prepare NO(A) in its (v = 0, N = 0, j = 0.5) level. After a time window of ~400 ns during which collisions of the prepared A state molecules are allowed to occur, the angular distributions of the velocities and angular momenta of rotational quantum states populated through these collisions are measured through (1 + 1′) REMPI via the NO(E) state and VMI detection.

As well as simply acting as a source of electronically excited NO, the initial state preparation step provides key advantages over traditional CMB-VMI experiments. A major problem in such experiments arises from the long temporal overlap of the two molecular beams (typically in the 100s of μs). This leads to a ‘fly-out’ of molecules produced with high lab frame speeds and build-up of molecules travelling slowly in the lab frame, resulting in distortions of the measured velocity distribution and significant problems in the interpretation of the resulting images. By creating a well-defined and brief time window over which collisions occur, the preparation of NO(A) in the crossing region of the two beams avoids this problem and hence simplifies the analysis of the images to obtain the true centre of mass frame scattering. In addition, NO(A) molecules are clearly not present in the beam prior to the state-preparation step, and hence the only substantial source of background ions are those which originate from (1 + 1) REMPI of NO(X) via the A state, effected by the state preparation laser. Since these ions are generated at the beginning of the collision time window, it is in principle possible to completely discriminate against them through a carefully designed set of ion optics and time-gating of the detector. Such an experiment would therefore be virtually background-free.

We report collaborative proof-of-principle experiments carried out by the authors at Heriot Watt University and Sandia National Laboratories, with theoretical calculations provided by the authors at the University of Maryland. Differential cross sections and scattering-angle dependent alignment of NO(A, v = 0, N' = 4, 5, 7, 9) produced through collisions with Ne have been measured and compared to both a simple classical ‘kinematic apse’ treatment and a full quantum scattering (QS) model of the dynamics on the most recent ab initio potential energy surface. The measured alignment parameters show substantial oscillations as a function of scattering angle which are well reproduced by the QS calculations but not by the classical model. This is in marked contrast to the behaviour of NO(X) + rare gas collision system, where previous measurements have demonstrated good agreement of the measured alignment with the predictions of a kinematic apse model.

P49 Relaxation dynamics of resorcinol

Michael Staniforth
University of Warwick

P50 Double Fluorescence and Ultrafast Intersystem Crossing – The peculiar Photophysics of Polycyclic Nitroaromatic Compounds

Anne B. Stephansen[2], Rafael López-Arteaga[1], Cesar A. Guarin-Duran[1], Theis I. Sølling[2], and Jorge Peón[1]

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Unusually fast intersystem crossing (ISC) and photoinduced release of the highly reactive NO· radical are the two primary S_1 deactivation channels for most nitroaromatic compounds.[1,2] Nitroaromatic compounds are in particular present in the air in urban areas, and since NO· has serious mutagenic and carcinogenic properties, these compounds are troubling environmental pollutants. This alone motivates investigation of the photophysics of nitroaromatic compounds. Furthermore, and more importantly for this investigation, the ISC happening on an ultrafast femtosecond timescale challenges the traditional description of spin-forbidden processes.

The efficient ISC is mediated by a strong coupling of the fluorescent $^1(\pi,\pi^*)$ state with an almost iso-energetic triplet receiver state with 3(n,π*) character, thus El-Sayed's propensity rules are obeyed. This contribution provides further evidence that the ISC mechanism must be an extreme manifestation of El-Sayed's rule by comparing the femtosecond time-resolved fluorescence measurements of 2-nitrofluorene with those of N,N-diethyl-7-nitro-9H-fluoren-2-amine.3 The presence of a donor substituent in a push-pull configuration turns out to induce drastic and remarkable changes in the photophysical properties. Whereas 2-nitrofluorene exhibits the "normal" nitroaromatic spectroscopic properties, the amino-substituted counterpart shows a marked shift in its S_1 energy redounding in loss of coupling with the triplet receiver state. This invokes fluorescence, and in polar solvents the diethylamino substituted compound even shows double peaked fluorescence. Both emissive states have significant charge transfer character, and their formation and equilibration happens on an ultrafast timescale. The present contribution aims at correlating structure and photophysical properties of nitroaromatic compounds as well as revealing the ultrafast nature of ISC.

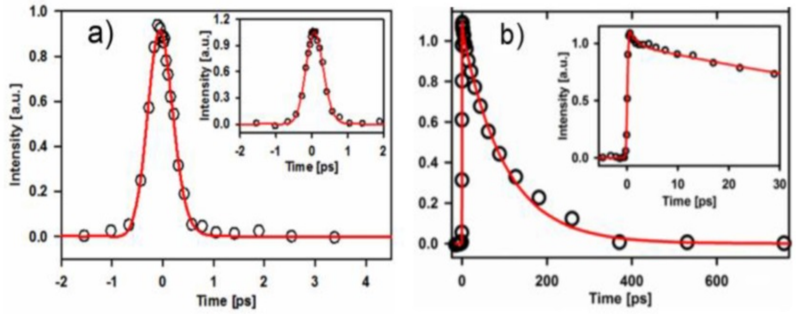

Figure 1: Examples of fluorescence up-conversion traces of (a) 2-nitrofluorene; and (b) N,N-diethylamino-7-nitro-9H-fluoren-2-a

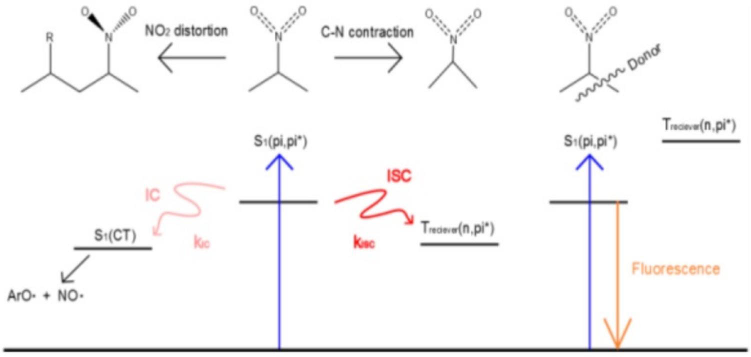

Figure 2: Schematic showing correlations of structure vs physical properties.

1. Morales-Cueto, R.; Esquivelzeta-Rabell, M.; Saucedo-Zugazagoitia, J.; Peon, J. *J. Phys. Chem. A* 2007, 111, 552.
2. Crespo-Hernandez, C. E. V., A. R. Sealey, B. *Mod. Chem. Appl*. 2013, 1, 1000106.
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P51 Spectroscopic study of the solvation of salts in water using helium nanodroplets

Jon Tandy, Andrew Shirley, Cheng Feng, Natércia Das Neves Rodrigues, Shengfu Yang, Andrew M. Ellis

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The solvation of NaCl in water inside helium nanodroplets has been examined for the first time using infrared depletion spectroscopy. Small water-salt clusters are formed by a double pick-up technique and then excited using an OPO. Infrared absorption transitions were then registered as depletion of signals in specific mass channels measured using a quadrupole mass spectrometer. Preliminary results measured in the O-H stretching region indicate the presence of several $NaCl(H_2O)_n$ clusters whose spectral bands match closely to theoretical predictions.

P52 Following the relaxation dynamics of photoexcited aniline in the 273-266 nm region using time-resolved photoelectron imaging

James Thompson

Heriot-Watt University

Time-resolved photoelectron imaging was used to investigate the relaxation dynamics of electronically excited aniline in the gas-phase following ultraviolet irradiation in the 273-266 nm region. We find that at all wavelengths studied, excitation is predominantly to the long-lived (>1ns) $S_1(\pi\pi*)$ state, which exhibits ultrafast intramolecular vibrational redistribution on a <1 ps timescale. At excitation wavelengths centred on resonant transitions in the aniline absorption spectrum that have previously been assigned to the higher lying $S_2(3s/\pi\sigma*)$ state, we also see clear evidence of this state playing a role in the dynamics. However, we see no indication of any non-adiabatic coupling between the $S_1(\pi\pi*)$ and $S_2(3s/\pi\sigma*)$ states over the range of excitation wavelengths studied.

P53 A new window into electron attachment dynamics: above-threshold ultrafast photoelectron spectroscopy of radical anions

J. R. R. Verlet, D. A. Horke, Q. Li, and L. Blancafort

Durham University

P54 Absolute density measurement of SD radicals in a molecular beam at the quantum-noise-limit

A. Mizouri, L.Z. Deng, J.S. Eardley, N. Warner, N.H. Nahler, D. Carty,* and E. Wrede

Durham University

P55 See Abstract for contributed talk **C3**

P56 Time-resolved photoelectron imaging of the chromophore of the green fluorescent protein

Christopher West

Durham University

The anionic form of p-hydroxybenzylidene-2,3-dimethylimidazolinone (HBDI) has been extensively employed as a model of the chromophore of the green fluorescent protein. In order to understand the intrinsic dynamics of HBDI-, we have performed time-resolved photoelectron spectroscopy. The S1 state decays on a timescale of 1.4 ps via two dominant decay mechanisms: internal conversion and autodetachment. Internal conversion leads to large changes in the photoelectron spectra, which are assigned to rotation around the central allyl bridge. Autodetachment leads to photoelectrons with low kinetic energy. The relative yield between the two channels was determined and the lifetime for autodetachment was found to be approximately 30 ps.

P57 The Art of Superpositions

Ben Whitaker, Mike Nix, Dave Lynch, Dominic Hopkinson, Lawrence Molloy and Andrew Wilson

University of Leeds

P58 Cavity Ring-Down Spectroscopy in the Near and Mid-Infrared for the Detection of Trace Gases

Luca Ciaffoni, Gus Hancock, Robert Peverall, Grant Ritchie, Kimberley Whittaker

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Applications for trace gas detection are numerous and diverse, ranging from the environmental and atmospheric to the industrial and medical. In many cases, absolute number densities are required and laser absorption spectroscopy is one technique that can provide such quantitative analysis. Often, high sensitivity and selectivity are also needed in order to monitor weakly absorbing species or those at low concentrations; such high sensitivities can be achieved by the use of cavity-based spectroscopic techniques or by the exploitation of the strong absorptions present in the mid-infrared (IR). Furthermore, a widely tunable laser source across a large wavelength range would be very beneficial as it would enable multi-species detection or the study of broadband absorbers.

In this contribution, we present our results of performing cavity ring-down spectroscopy (CRDS) in both the near and mid-IR to achieve such highly sensitive and broadband measurements.

In the near-IR, a novel, widely tunable telecom L-band (1563–1613 nm) digital supermode distributed Bragg reflector (DS-DBR) laser is utilised as the radiation source. This class of laser has never before been used in spectroscopy. We demonstrate its versatility and suitability as a spectroscopic laser source by exploiting its wide spectral coverage to monitor transitions at different, widely separated wavelengths and also to detect broadband absorbers.

In the mid-IR, we combine mid-IR radiation generated by mixing light from cw diode lasers using quasi phase matching (QPM) difference frequency generation (DFG) with CRDS to create a 3 µm DFG-CRD spectrometer. This is an attractive strategy for gas-sensing spectroscopic applications as it amalgamates the advantages of three separate concepts: the use of the mid-IR region of the spectrum (which allow high sensitivities and selectivity to be achieved by use of the strong transitions therein), the translation of the desirable characteristics of near-IR diode lasers to the mid-IR and the high sensitivities afforded by cavity-based techniques. We demonstrate the use of this DFG-CRD spectrometer by reporting the results of our spectroscopic studies of methane, acetone and deuterium.

Finally we report on the current state of our work to combine CRDS with widely tunable mid-IR generated by DFG using use the broadband DS-DBR laser as a signal source: such a widely tunable and sensitive spectrometer in the 3 µm region would be greatly advantageous in the detection of multiple species or broad-band absorbers for both medical and environmental applications.

P59 Electron Impact Total and Partial Ionization Cross Sections and Kinetic Energy Releases for Hydrocarbon Species Relevant to Fusion Edge Plasmas

Lorna Wilkinson, Weiwei Zhou, James Bull, Jason Lee and Claire Vallance

Department of Chemistry, University of Oxford, South Parks Road, Oxford, OX1 3TA, United Kingdom

As the energy crisis comes further into the public domain, the pressure is mounting to find a new energy source. The International Thermonuclear Experimental Reactor (ITER) is an international collaboration aimed at investigating nuclear fusion as a new commercial energy source. The tokomak at the heart of ITER is a cylindrical device within which the fusion plasma is confined by magnetic fields. The edge regions of the plasma are much cooler than in the centre, and neutral hydrocarbon species can form in this region from carbon atoms generated at the inner walls of the reactor. Collisions of these hydrocarbons with electrons in the plasma lead to ionization, fragmentation, and recombination processes, yielding a range of ions and neutrals that must be taken into account when modelling the plasma. Accurate modelling requires knowledge of the total and partial electron-impact ionization cross sections of the hydrocarbons, as well as the kinetic energy distributions for the various fragments.

The hydrocarbon species of interest are generally simple alkanes and alkenes. In the present work we describe experiments we will be carrying out over the next few months to determine total and partial ionization cross sections and kinetic energy releases for CH_4, C_2H_2, C_2H_4, C_3H_6 and C_3H_8.

P60 Velocity-map imaging anion photoelectron spectroscopy of gas-phase metal clusters.

Alex P. Woodham, Philipp Gruene, Marko Haertelt, Dan J. Harding, Andreas Osterwalder, André Fielicke

Technische Universität Berlin

Anion photo-electron spectroscopy has long been a powerful technique in the arsenal of gas-phase spectroscopists for accurate characterization of molecular species, and metal clusters are no exception to this [1]. Early experiments were limited to time-of-flight or magnetic bottle type detection schemes, which effectively limited the potential resolution and only information concerning the electronic structure of the cluster was reliably accessible. The development of electron velocity map imaging and with it the slow electron velocity imaging (SEVI) [2] technique instead allows for detection of photo-electrons produced close to threshold and an associated dramatic rise in resolution, allowing for the low-frequency vibrational modes of the cluster in both the initial (anionic) and final (neutral) state to be resolved. Further, the use of 2D positional imaging allows for information concerning the symmetries of the states involved to be gleaned from the variation of the observed intensity as a function of angle, i.e. the orbital angular momentum of the departing electron wave. Here we present the details of a new set-up designed and built in Berlin to perform these measurements, as well as initial results for the platinum trimer anion (Pt_3^-).

[1] a) T.M. Ramond *et al.,* J. Mol. Spec. **216** 1 (2002) 1-14. b) L.M. Wang and L.S. Wang*, Nanoscale* **4** 14 (2012) 4038-4053

[2] D. Neumark*, J. Phys. Chem*. A, **112** 51 (2008) 13287-13301

Possible 'surprise' posters

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5. MAP OF OXFORD

The railway station and bus station are about a 20-30 minute walk from St. Catherine's. There are taxi ranks at both stations.

Registration on Sunday January 5 is at St. Catherine's College from 4pm to 5:30pm. Dinner on the Sunday evening will be held at the University Club from 5:30pm to 7:30pm, and the evening tutorial lectures will be held in the PTCL lecture theatre from 8pm. All other talks will be held in the Bernard Sunley lecture theatre at St. Catherine's College.

Note that the St. Catherine's bar will not be open on the Sunday evening. Nearby pubs are indicated on the map in case you would like to continue discussions into the evening after the tutorial lectures.