

*Leiden Observatory workshop:
Photodissociation in astrochemistry*

3–5 February, 2015

Kasteel Oud Poelgeest, Leiden

Webpage: www.strw.leidenuniv.nl/cms/web/2015/20150203/info.php3?wsid=36
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Overview

This focussed workshop seeks to clarify the outstanding questions and priorities relevant to the forthcoming era of astrochemistry, and evaluate the present and future capabilities of spectroscopists and chemical physicists. We hope to encourage the investigation of photodissociation problems of immediate interest to astrochemistry. The format of the meeting is in the spirit of a true workshop, with plenty of time for discussions and interactions. The proposed topics for discussion are:

Problems in astrochemical photodissociation

- Which molecules are present in clouds, disks, and planet atmospheres exposed to intense UV radiation; how do they photodissociate: through lines or continuum; how do they (observably) influence their surroundings?
- What are the important ranges of temperature, density, extinction magnitudes, and UV wavelengths?
- What is the most useful kind of data? A completely assigned and modelled spectrum, raw experimental cross sections and linelists, superb accuracy over a small wavelength range (e.g., Ly alpha) or lower accuracy over a much larger range? Importance of self- and mutual shielding and tabulation of shielding functions; isotope selective processes?
- Photolysis in the gas phase vs ices; small versus large molecules (PAHs)
- Contributions to public databases:
 - Mainz UV/VIS database
 - Leiden photodissociation database of astrophysical molecules
 - PHIDRATES photoionisation and photodissociation rates
 - KIDA (KInetic Database for Astrochemistry)

Capabilities and challenges of laboratory experiments

- The generation of UV radiation: synchrotrons, lasers, plasmas, or electron excitation.
- The quantitative measurement of cross sections and dissociation: photoabsorption, fluorescence, or the detection of dissociation products and their excitation states; branching ratios to products.
- The synthesis and study of radical species and ions, as well as ices.

Theoretical methods

- Calculation of electronic structure and dipole moments
- Nuclear dynamics of excited states, modelling the branching ratio of ionisation, dissociation products, and fluorescence.
- More empirical theoretical models with increasing complexity: competition between dissociation and internal conversion for polyatomic molecules.

Arrival and departure

The workshop will be held in Kasteel Oud Poelgeest (www.kasteeloudpoelgeest.com), a beautifully renovated castle on the border of the city of Leiden. Leiden is easily reachable by train or car from the nearby international airport of Amsterdam, Schiphol.

The address of the venue (the postcode is particularly good for GPS location):

Kasteel Oud Poelgeest
Poelgeesterweg 1, 2341 NM Oegstgeest

The train connection between Amsterdam's Schiphol airport and Leiden Centraal Station is very good, with trains departing every 15 minutes and the journey requiring 20 minutes.

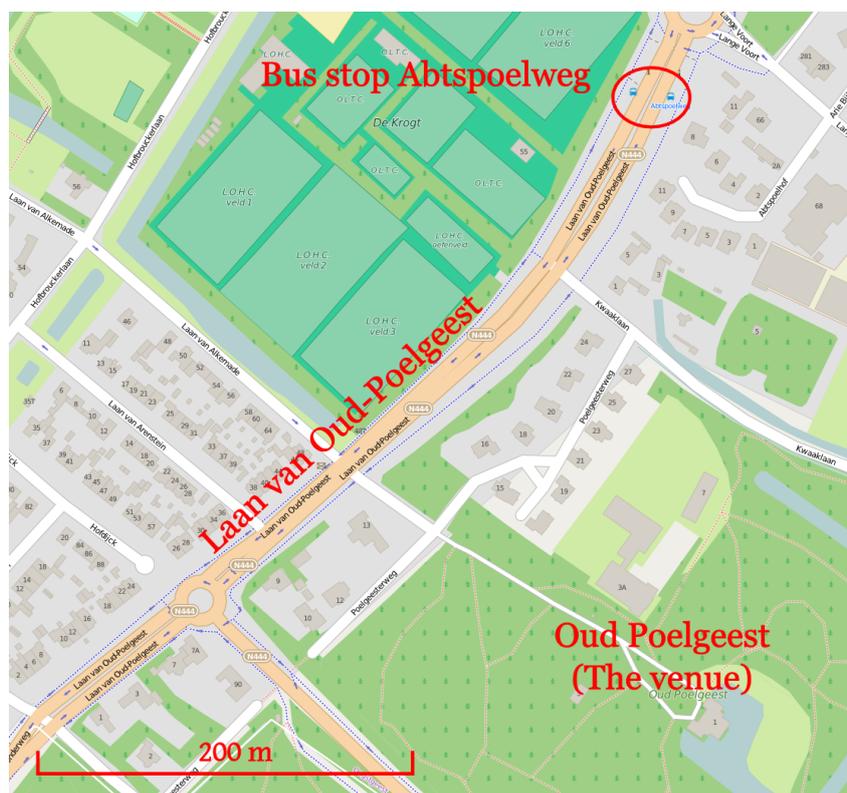
Travelling from Leiden Centraal to nearby Kasteel Oud Poelgeest is possible by bus. Good advice on public transport may be found here

9292.nl/en/journeyadvice/station-leiden-centraal/oegstgeest_kasteel-slot-kasteel-oud-poelgeest

The taxi fare between Schiphol airport and Poelgeest is around €65, and between Leiden and Poelgeest around €10.

In case you decide to visit Leiden Observatory (different from the Old Observatory) the address is:

Huygens & Oort Buildings (4th and 5th floors)
Niels Bohrweg 2
NL-2333 CA Leiden
www.strw.leidenuniv.nl



Meals and accommodation

Lunches, the conference dinner (February 3), and a buffet dinner at Poelgeest (February 4) are included in the registration fee for all attendees. Please inform us if any extras would like to attend the conference dinner. For those attendees who have requested the three nights accommodation package at Poelgeest this includes breakfasts on February 3, 4, and 5.

Registration and accommodation fees

The workshop fee is €120 (invitees exempt) and standard 3-night (nights of Feb. 2,3, and 4) accommodation package cost is €340. Payments for these or for any special arrangements can be made upon checkout from the workshop.

Acknowledgements

Thanks is due to the Dutch Science Organisation (NWO) and an Advanced ERC grant for providing financial support for the workshop and funds to assist delegates.

Program – Tuesday 3rd February

*Speakers are allotted 15+5, 25+5, or 30+10 minutes
speaking+question time*

- 9:30 *Arrival and coffee*
- 10:00 *Introduction to the workshop*
- 10:10 **Ewine van Dishoeck** (Leiden Observatory)
“Photodissociation processes in astrophysics”
- 10:40 **Mike Ashfold** (University of Bristol)
“The role of $\pi\sigma^$ states in molecular photodissociation processes”*
- 11:20 *Coffee break*
- 11:40 **Gerrit Groenenboom** (Radboud Universiteit, Nijmegen)
“Ab initio calculation of potentials, transition dipole moments, and fine structure branching ratios for photodissociation of diatomic molecules”
- 12:10 **Phillip Stancil** (University of Georgia)
“Computation of rovibrationally-resolved photo-destruction cross sections for interstellar, circumstellar, and stellar atmospheric environments”
- 12:40 *Discussion*
- 12:50 *Lunch*
- 14:10 **David Parker** (Radboud Universiteit, Nijmegen)
“VUV photodissociation of O_2 , CO_2 , COS , and methanol with velocity-map imaging detection”
- 14:40 **Marc van Hemert** (Leiden Institute of Chemistry)
“What can we learn from the VUV spectra of CH_3OH , CD_3OD , CH_3OD and CD_3OH that I recorded 40 years ago”
- 15:00 **Pablo Castellanos Nash** (Leiden Observatory)
“From PAHs to Fullerenes: Top-down interstellar chemistry”
- 15:20 **Paul Seakins** (University of Leeds)
“Laboratory studies of VUV methane photolysis and reactions of the resulting hydrocarbon radicals”
- 15:40 *Discussion*
- 15:50 *Coffee break*
- 16:10 **Evelyne Roueff** (LERMA, Observatoire de Paris)
“Photoprocesses under interstellar conditions. The combined answer of gas and dust to UV radiation”
- 16:40 **Markus Röllig** (University of Cologne)
“Photodissociation under varying dust absorption conditions”
- 17:00 **Wing Fai Thi** (MPI für extraterrestrische Physik)
“Photochemistry at protoplanetary disk surfaces: photodissociation, state-to-state chemistry, chemical-pumping to excited levels, and UV-pumping”
- 17:20 *Discussion*
- 18:45 *Board coach to conference dinner*

Program – Wednesday 4th February

*Speakers are allotted 15+5, 25+5, or 30+10 minutes
speaking+question time*

- 8:40 **Coffee**
- 9:00 **Carla Maria Coppola** (Università di Bari - INAF Arcetri)
*“Photodissociation of H₂ and HD in a non-thermal radiation
background: Application to the early Universe chemistry”*
- 9:30 **Olivia Venot** (KU Leuven)
“Photodissociation in hot exoplanet’s atmospheres”
- 10:00 **Antonio García Muñoz** (European Space Agency)
“Aeronomy of hot Jupiters”
- 10:20 **Discussion**
- 10:30 **Coffee break**
- 10:50 **Cheuk-Yiu Ng** (University of California, Davis)
*“State-to-state photodissociation of atmospheric molecules by
VUV-VUV laser velocity-map imaging method ”*
- 11:20 **Jordy Bouwman** (Radboud Universiteit, Nijmegen)
*“Dissociative ionization of nitrogen containing polycyclic aromatic
hydrocarbons”*
- 11:40 **Alan Heays** (Leiden Observatory)
*“Photodissociation and ionisation of molecules due to stellar and
cosmic-ray-induced radiation”*
- 12:00 **Discussion**
- 12:10 **Lunch**
- 14:00 **Jim Lyons** (Arizona State University)
*“Photodissociation in the solar nebula: Comparison of models and
meteorites”*
- 14:30 **Ruud Visser** (European Southern Observatory)
“Isotopic fractionation of nitrogen in protoplanetary disks”
- 14:50 **Catherine Walsh** (Leiden Observatory)
*“Photodissociation of N₂ and its impact on the nitrogen chemistry in
protoplanetary disks”*
- 15:10 **Inga Kamp** (University of Groningen)
“CO in the inner regions of protoplanetary disks”
- 15:30 **Discussion**
- 15:40 **Coffee break**

Program – Wednesday 4th February – continued

*Speakers are allotted 15+5, 25+5, or 30+10 minutes
speaking+question time*

- 16:00 **Xiaohu Li** (Leiden Observatory)
 “Photodissociation in dying stars”
- 16:20 **Nigel Mason** (The Open University, Milton Keynes)
 *“A database of VUV photoabsorption cross sections in the gas and
 solid phase using synchrotron radiation”*
- 16:40 **Valentine Wakelam** (Laboratoire d’Astrophysique de Bordeaux)
 “The KInetic Database for Astrochemistry”
- 17:00 *Discussion*
- 18:00 *Drinks*
- 18:30 *Buffet dinner*

Program – Thursday 5th February

*Speakers are allotted 15+5, 25+5, or 30+10 minutes
speaking+question time*

- 9:00 *Coffee*
- 9:20 **Guillermo Muñoz Caro** (Centro de Astrobiología, Madrid)
*“VUV-absorption cross sections of ices, photodissociation and
photodesorption”*
- 9:50 **Anita Dawes** (The Open University, Milton Keynes)
*“Vacuum ultraviolet photoabsorption spectroscopy of astrochemical ice
analogues”*
- 10:10 **Guilherme Almeida** (PUC-RJ, Rio de Janeiro)
*“Electron and photon impact on condensed organic molecules:
Astrochemical implications”*
- 10:30 *Discussion*
- 10:40 *Coffee break*
- 11:00 **Mingli Niu** (VU University, Amsterdam)
“Production of vibrationally hot H₂ (v=10–14) from H₂S photolysis”
- 11:20 **Rowin Meijerink** (Leiden Observatory)
“Modeling of the irradiated ISM in starburst galaxies and AGN”
- 11:40 **Wim Ubachs** (VU University, Amsterdam)
“Molecular hydrogen in the photosphere of white dwarf stars”
- 12:00 *Discussion*
- 12:10 *Lunch*
- 13:40 **Panayotis Lavvas** (CNRS, Reims)
“Nitrogen in Titan’s atmosphere”
- 14:00 **Sergio Pilling** (Universidade do Vale do Paraíba, Brazil)
*“Photodissociation induced by broadband soft X-rays in the surface of
the outer solar system moons”*
- 14:20 **Gaël Cessateur** (BIRA-IASB, Belgium)
“Photoabsorption in Jovian moons and cometary atmospheres”
- 14:40 *Discussion and final remarks*