IAU Symposium 350
Laboratory Astrophysics:
From Observations to Interpretation

Scientific Organizing Committee:
Farid Salama (Chair) ★ P. Barklem ★ H. Fraser ★ T. Henning ★
C. Joblin ★ S. Kwok ★ H. Lihmartz ★ L. Mashonkina ★ T. Millar ★
O. Shalabiea ★ G. Vidali ★ F. Wang ★ G. Del-Zanna

Local Organizing Committee:
H. Fraser (Chair) ★ D. Benoit ★ R. Coster ★ A. Dawes ★ S. Gärtner ★
D. Heard ★ S. Ioppolo ★ N. Mason ★ A. Meijer ★ P. Rimmer ★
E. Sciamma-O’Brien ★ F. Salama ★ C. Walsh ★ G. Del-Zanna

For more information and to contact us:
www.astrochemistry.org.uk/IAU_S350 ★ IAU350-labastro2019@open.ac.uk ★ @iaus350labastro
Abstract Book

Schedule†

Sunday 14th April .................................................. Pg. 2
Monday 15th April ................................................... Pg. 3
Tuesday 16th April .................................................. Pg. 4
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†Plenary talks (40’) are indicated with ‘P’, review talks (30’) with ‘R’, and invited talks (15’) with ‘I’. 
## Schedule

### Sunday 14th April

<table>
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<tr>
<th>Time</th>
<th>Event</th>
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<tbody>
<tr>
<td>14:00 - 17:00</td>
<td>REGISTRATION</td>
</tr>
<tr>
<td>18:00 - 19:00</td>
<td>WELCOME RECEPTION</td>
</tr>
<tr>
<td>19:30</td>
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BAR OPEN UNTIL 23:00

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### Monday 15th April

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<tr>
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<tbody>
<tr>
<td>09:00 – 10:00</td>
<td>REGISTRATION</td>
</tr>
<tr>
<td>09:00</td>
<td>WELCOME by F. Salama (Chair of SOC)</td>
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**SESSION 1**  
**CHAIR: F. Salama**

<table>
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<tr>
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<th>Speaker</th>
<th>Title</th>
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<tbody>
<tr>
<td>09:15</td>
<td>E. van Dishoeck (P)</td>
<td>Laboratory astrophysics: key to understanding the Universe</td>
</tr>
<tr>
<td>10:00</td>
<td>A. Boogert (I)</td>
<td>From Diffuse Clouds to Protostars: Outstanding Questions about the Evolution of Ices</td>
</tr>
<tr>
<td>10:15</td>
<td>O. Berné (I)</td>
<td>Observations and modeling of the photochemical evolution of carbonaceous macromolecules in star-forming regions</td>
</tr>
<tr>
<td>10:30</td>
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**SESSION 2**  
**CHAIR: C. Walsh**

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<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
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<tbody>
<tr>
<td>11:00</td>
<td>I. Sims</td>
<td>Experimental determination of reaction product branching ratios at low temperatures for astrochemistry</td>
</tr>
<tr>
<td>11:15</td>
<td>C. Jäger (R)</td>
<td>Laboratory experiments on cosmic dust and ices</td>
</tr>
<tr>
<td>11:45</td>
<td>A. Canosa (I)</td>
<td>Gas phase reaction kinetics of complex organic molecules at temperatures of the interstellar medium</td>
</tr>
<tr>
<td>12:00</td>
<td>S. Schlemmer (I)</td>
<td>The Spectroscopy of Molecular Ions related to H$_3^+$</td>
</tr>
<tr>
<td>12:15</td>
<td>D. Qasim</td>
<td>Synthesis of solid-state Complex Organic Molecules (COMs) through accretion of simple species at low temperatures</td>
</tr>
<tr>
<td>12:30</td>
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<td>LUNCH BREAK</td>
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**SESSION 3**  
**CHAIR: D. Heard**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
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<tbody>
<tr>
<td>14:00</td>
<td>N. Ysard (R)</td>
<td>Dust evolution: going beyond the empirical</td>
</tr>
<tr>
<td>14:30</td>
<td>C. Romero Rocha</td>
<td>Potential energy surfaces of elemental carbon clusters: from theory to applications in astrochemistry</td>
</tr>
<tr>
<td>14:45</td>
<td>C. Puzzarini (I)</td>
<td>Prebiotic molecules in interstellar space: rotational spectroscopy and quantum chemistry</td>
</tr>
<tr>
<td>15:00</td>
<td>Z. Awad</td>
<td>N-bearing Species in Massive Star Forming Regions</td>
</tr>
<tr>
<td>15:15</td>
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**SESSION 4**  
**CHAIR: A. Dawes**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
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<tbody>
<tr>
<td>15:45</td>
<td>M. Palumbo</td>
<td>Laboratory investigations aimed at building a database for the interpretation of JWST spectra</td>
</tr>
<tr>
<td>16:00</td>
<td>H. Cuppen</td>
<td>Simulations of energy dissipation and non-thermal desorption on amorphous solid water</td>
</tr>
<tr>
<td>16:15</td>
<td>C. Kemper (I)</td>
<td>The dust budget problem in galaxies near and far</td>
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END OF SCIENCE SESSIONS AT 16:30

<table>
<thead>
<tr>
<th>Time</th>
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<tbody>
<tr>
<td>17:15</td>
<td>COLLEGE TOURS</td>
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<td>17:30</td>
<td>POSTERS WITH REFRESHMENTS</td>
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END OF POSTER SESSION AT 19:00

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BAR OPEN UNTIL 23:00
## Tuesday 16th April

### SESSION 5  
**CHAIR: D. Benoit**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
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<tbody>
<tr>
<td>09:00</td>
<td>K. Altwegg (R)</td>
<td>Interpretation of in situ mass spectra at comet 67P</td>
</tr>
<tr>
<td>09:30</td>
<td>Y. Pendleton</td>
<td>A window on the composition of the early solar nebula: Pluto, 2014MU69, and Phoebe</td>
</tr>
<tr>
<td>09:45</td>
<td>A. Belloche</td>
<td>Molecular complexity in the interstellar medium</td>
</tr>
<tr>
<td>10:00</td>
<td>F. Pignatale</td>
<td>Fingerprints of the protosolar cloud collapse in the Solar System: refractory inclusion distribution and isotopic anomalies in meteorites</td>
</tr>
<tr>
<td>10:15</td>
<td>H. Sabbah</td>
<td>Characterization of Large Carbonaceous Molecules in Cosmic Dust Analogues and Meteorites</td>
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<td>10:30</td>
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### SESSION 6  
**CHAIR: H. Linnartz**

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<th>Time</th>
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<tbody>
<tr>
<td>11:00</td>
<td>V. Mennella</td>
<td>Catalytic formation of H$_2$ on Mg-rich amorphous silicates</td>
</tr>
<tr>
<td>11:15</td>
<td>K. Bowen</td>
<td>Laboratory Measurements of Deuterium Reacting with Isotopologues of H$_3^+$</td>
</tr>
<tr>
<td>11:30</td>
<td>N. Watanabe (I)</td>
<td>Detection of OH radicals on amorphous solid water</td>
</tr>
<tr>
<td>11:45</td>
<td>M. Nuevo</td>
<td>Formation of Complex Organic Molecules in Astrophysical Environments: Sugars and Derivatives</td>
</tr>
<tr>
<td>12:00</td>
<td>F. Dulieu</td>
<td>Hydrogenation and binding energies on dust grains as selective forces for the formation and observation of interstellar molecules</td>
</tr>
<tr>
<td>12:15</td>
<td>M. Stockett</td>
<td>Intrinsic absorption profile and radiative cooling rate of a PAH cation revealed by action spectroscopy in the cryogenic electrostatic storage ring DESIREE</td>
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<td>12:30</td>
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### SESSION 7  
**CHAIR: C. Joblin**

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<th>Time</th>
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<tbody>
<tr>
<td>14:00</td>
<td>S. Russell (I)</td>
<td>Carbonaceous chondrites as probes of protoplanetary disk conditions</td>
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<tr>
<td>14:15</td>
<td>V. Deguín</td>
<td>Amorphous Solid Water (ASW) particle production for collision experiments</td>
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<tr>
<td>14:30</td>
<td>P. Theulé (I)</td>
<td>Chemical dynamics in interstellar ice</td>
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<tr>
<td>14:45</td>
<td>M. Burchell</td>
<td>Survival of Shells of Icy Satellites Against Hypervelocity Impact</td>
</tr>
<tr>
<td>15:00</td>
<td>J. Thrower</td>
<td>Laboratory evidence for the formation of hydrogenated fullerene molecules</td>
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<tr>
<td>15:45</td>
<td>L. Wiesenfeld</td>
<td>Quenching of interstellar carbenes: interaction of C$_3$H$_2$ with He and H$_2$</td>
</tr>
<tr>
<td>16:00</td>
<td>F. Ciesla (R)</td>
<td>Chemical Evolution of Planetary Materials in a Dynamic Solar Nebula</td>
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**END OF SCIENCE SESSIONS AT 16:30**

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**END OF POSTER SESSION AT 19:00**

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**BAR OPEN UNTIL 23:00**

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### Wednesday 17th April

#### SESSION 8

<table>
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<tr>
<th>Time</th>
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<th>Title</th>
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<tbody>
<tr>
<td>09:00</td>
<td>Y. Aikawa (R)</td>
<td>Gas-dust chemistry of volatiles in the star and planetary system formation</td>
</tr>
<tr>
<td>09:30</td>
<td>J. Olofsson (I)</td>
<td>Dust production and characterization in young debris disks</td>
</tr>
<tr>
<td>09:45</td>
<td>B. Kerkeni</td>
<td>Understanding Propyl-cyanide and its isomers Formation: Ab initio Study of the Reaction Kinetics</td>
</tr>
<tr>
<td>10:00</td>
<td>S. Bromley</td>
<td>Using atomistically detailed simulations to understand the formation, structure and composition of astrophysical silicate dust grains</td>
</tr>
<tr>
<td>10:15</td>
<td>R. Teague (I)</td>
<td>Tracing The Physical Conditions of Planet Formation with Molecular Excitation</td>
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#### SESSION 9

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<tr>
<th>Time</th>
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<th>Title</th>
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<tbody>
<tr>
<td>11:00</td>
<td>A. Petrignani</td>
<td>High-resolution electronic spectroscopy study of neutral gas-phase PAH species</td>
</tr>
<tr>
<td>11:15</td>
<td>K. Lee</td>
<td>Interstellar aromatic chemistry: a combined laboratory, observational, and theoretical perspective</td>
</tr>
<tr>
<td>11:30</td>
<td>D. Dubois</td>
<td>Benzene Condensation on Titan’s Stratospheric Aerosols: An Integrated Laboratory, Modeling and Observational Approach</td>
</tr>
<tr>
<td>11:45</td>
<td>V. Vuitton (I)</td>
<td>Chemical composition of (exo-)planetary haze analogues by very high-resolution mass spectrometry</td>
</tr>
<tr>
<td>12:00</td>
<td>N. Sie</td>
<td>Temperature and Thickness effects on Photodesorption of CO Ices</td>
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**END OF SCIENCE SESSIONS AT 12:30**

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<td>13:30</td>
<td>CONFERENCE TRIPS</td>
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<td>Trips will finish between 16:30 and 17:30</td>
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### Thursday 18th April

**SESSION 10**

**CHAIR: E. Sciamma-O’Brien**

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<tr>
<th>Time</th>
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<th>Title</th>
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<tbody>
<tr>
<td>09:00</td>
<td>I. Kamp (R)</td>
<td>Protoplanetary disks, debris disks and solar system</td>
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<tr>
<td>09:30</td>
<td>N. Ligterink</td>
<td>The formation of prebiotic building blocks of peptides on interstellar dust grains</td>
</tr>
<tr>
<td>09:45</td>
<td>B. Sivaraman (I)</td>
<td>Complex molecules in astrochemical impact conditions</td>
</tr>
<tr>
<td>10:00</td>
<td>J. Pickering (R)</td>
<td>Recent advances in experimental laboratory astrophysics for stellar astrophysics applications and future data needs.</td>
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**SESSION 11**

**CHAIR: F. Wang**

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<th>Time</th>
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<tbody>
<tr>
<td>11:00</td>
<td>M. Montgomery (I)</td>
<td>The Wootton Center for Astrophysical Plasma Properties: First Results for Helium</td>
</tr>
<tr>
<td>11:15</td>
<td>I. Topala</td>
<td>Comparative study of 3.4 micron band features from carbon dust analogs obtained in pulsed plasmas at low and atmospheric pressure</td>
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<tr>
<td>11:30</td>
<td>T. Schmidt</td>
<td>Quantifying the aliphatic hydrocarbon content of interstellar dust using multiple laboratory spectroscopies</td>
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<tr>
<td>11:45</td>
<td>D. Gobrecht</td>
<td>From Molecules to Dust: Alumina cluster seeds</td>
</tr>
<tr>
<td>12:00</td>
<td>L. Zhang</td>
<td>Physical parameter estimation with MCMC from X-ray observations</td>
</tr>
<tr>
<td>12:15</td>
<td>M. Van de Sande</td>
<td>AGB outflows as tests of chemical kinetic and radiative transfer models</td>
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**SESSION 12**

**CHAIR: N. Mason**

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<tbody>
<tr>
<td>14:00</td>
<td>Poster Winner 1</td>
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<td>14:15</td>
<td>Poster Winner 2</td>
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<tr>
<td>14:30</td>
<td>K. Kotake (R)</td>
<td>Exploding and non-exploding core-collapse supernova models and the multi-messenger predictions</td>
</tr>
<tr>
<td>15:00</td>
<td>J. Mao</td>
<td>Density diagnostics of photoionized outflows in active galactic nuclei</td>
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<td>15:15</td>
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**PANEL DISCUSSION**

**MODERATOR: F. Salama (IAU S350)**

<table>
<thead>
<tr>
<th>Time</th>
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<tbody>
<tr>
<td>15:45</td>
<td>The Future of Laboratory Astrophysics (the role of IAU Commission B5)</td>
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<tr>
<td></td>
<td>J.-H. Fillion (PCMI), H. Fraser (IAU Comm B5), D. Hudgins (NASA SMD), H. Linhartz (NL), N. Mason (Europlanet), V. Mennella (INAF/ECLA), D. Savin (LAD), S. Schlemmer (Germany), O. Shalabiea (Africa/ME), F. Wang (China), N. Watanabe (Japan)</td>
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**END OF SCIENCE SESSIONS AT 17:15**

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**END OF POSTER SESSION AT 19:00**

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**BAR OPEN UNTIL 23:00**

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### Friday 19th April

**SESSION 13**  
*CHAIR: O. Shalabiea*

<table>
<thead>
<tr>
<th>Time</th>
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<th>Title</th>
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<tbody>
<tr>
<td>09:00</td>
<td>J. Tennyson (R)</td>
<td>The ExoMol project: molecular line lists for the opacity of exoplanets and other hot atmospheres</td>
</tr>
<tr>
<td>09:30</td>
<td>R. Bérard</td>
<td>Using cold plasma to investigate the mechanisms involved in cosmic dust formation: role of C/O ratio and metals</td>
</tr>
<tr>
<td>09:45</td>
<td>K. Lind (I)</td>
<td>Non-LTE spectroscopy for Galactic Archaeology</td>
</tr>
<tr>
<td>10:00</td>
<td>J. Lawler</td>
<td>Quantitative Atomic Spectroscopy, a Review of Progress in the Optical-UV Region and Future Opportunities using X-Ray FELs</td>
</tr>
<tr>
<td>10:15</td>
<td>A. Jerkstrand (I)</td>
<td>The origin of the elements: diagnosing the nucleosynthesis production in supernovae</td>
</tr>
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**SESSION 14**  
*CHAIR: G. Del Zanna*

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<thead>
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<th>Time</th>
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<tbody>
<tr>
<td>11:00</td>
<td>W. Liu (R)</td>
<td>Underground nuclear astrophysics experiment in Jinping China: JUNA</td>
</tr>
<tr>
<td>11:30</td>
<td>J. Grumer</td>
<td>Kilonovae and the lanthanides: an atomic theorists perspective</td>
</tr>
<tr>
<td>11:45</td>
<td>S. White</td>
<td>Generation of photoionised plasmas in the laboratory: analogues to astrophysical sources</td>
</tr>
<tr>
<td>12:00</td>
<td>M. Giarrusso</td>
<td>Laboratory plasmas for high-energy Astrophysics</td>
</tr>
<tr>
<td>12:15</td>
<td>H. Schatz (I)</td>
<td>Rare Isotope Physics in the Era of Multimessenger Astronomy</td>
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**SESSION 15**  
*CHAIR: H. Fraser*

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<tbody>
<tr>
<td>14:00</td>
<td>P. Young (R)</td>
<td>The Sun: our own backyard plasma laboratory</td>
</tr>
<tr>
<td>14:30</td>
<td>G. Del Zanna</td>
<td>Benchmarked Atomic Data for Astrophysics</td>
</tr>
<tr>
<td>14:45</td>
<td>U. Heiter (I)</td>
<td>Laboratory Astrophysics for the interpretation of stellar spectra</td>
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**END OF SCIENCE SESSIONS AT 15:00**

<table>
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<th>Time</th>
<th>Speaker</th>
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<tbody>
<tr>
<td>15:00</td>
<td>F. Salama (SOC)</td>
<td>SUMMARY</td>
</tr>
<tr>
<td>15:25</td>
<td>H. Fraser (LOC)</td>
<td>CLOSING REMARKS</td>
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CLOSE OF MEETING AT 15:30

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<table>
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<td>Student and PDRA poster presenters are indicated with an asterisk, *</td>
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Abstracts of Talks
Laboratory astrophysics: key to understanding the Universe (P)

van Dishoeck, E. F.¹
¹Leiden Observatory, Leiden University, Netherlands

Modern astrophysics is blessed with an increasing amount of high quality observational data on astronomical sources, ranging from our own solar system to the edge of the Universe and from the lowest temperature clouds to the highest energy cosmic rays. Spectra containing thousands of features of atoms, molecules, ice and dust are routinely obtained for stars, planets, comets, the ISM and star-forming regions, and now even for the most distant galaxies. Realistic models of exo-planetary atmospheres require information on billions of lines. Theories of jets from young stars benefit from plasma experiments to benchmark them. Stellar evolution theories and cosmology rely heavily on accurate rates for nuclear fusion reactions. The first stars could not have formed without the simplest chemical reactions taking place in primordial clouds. Particle physics is at the heart of finding candidates for the mysterious dark matter. There is no doubt that laboratory astrophysics, with 'laboratory' defined to include theoretical calculations, remains at the foundation of the interpretation of observations and truly 'makes astronomy tick'.

In this introductory talk, several recent developments in determining these fundamental data will be presented which have resulted in significant advances in our understanding of astrophysical environments. Often, a comparatively minor investment in basic studies can greatly enhance the scientific return from missions. Special attention will be given to recent results from infrared and millimeter facilities, including Herschel and ALMA, which reveal rich spectra of water and organic molecules in star- and planet forming zones. Their interpretation is greatly added by the application of ultra-high vacuum surface science techniques to astrophysical problems. Future needs of JWST will be discussed.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe, Solar System formation and the pre-solar nebula, Protoplanetary disks, debris disks, and the Solar System, Stars, stellar populations, and stellar explosions, Reaching beyond our galaxy: from extra galactic chemistry to dark matter

Research Area(s)
• Experimental laboratory astrophysics

Back to Schedule
The evolutionary sequence of diffuse to dense clouds and star formation governed by the physical processes of turbulence, compression, and gravitational collapse is accompanied by an impressive chemical evolution. Increasing densities shield the dust grains from the interstellar radiation field, leading to the formation of icy mantles on refractory dust grains. Telescope observations, analyzed using laboratory-measured ice spectra, have revealed that the icy mantles consist of layers dominated by H$_2$O and CO, respectively, that originate in different environments (Öberg et al. 2011, Boogert et al. 2015). Each layer is a complex mixture of simple molecules, with H$_2$O mixed with CO$_2$, CH$_4$, and NH$_3$ formed early in the cloud evolution, while CO can be pure or mixed with CH$_3$OH and OCN$^-$ and is formed later, at higher densities (Pontoppidan et al. 2004). The observations have raised important questions that directly relate to the interstellar ices as a reservoir for the formation of planetary system ices. New facilities coming online in the next years (e.g., the James Webb Space Telescope; JWST) are expected to provide important new constraints, and continued investment in laboratory ice experiments is warranted. The outstanding questions that I will likely address in this talk relate to the use of laboratory spectroscopy to detect frozen Complex Organic Molecules (Terwisscha van Scheltinga et al. 2018) and unravel sulfur ice chemistry (e.g., Dungee et al. 2018, Barr et al. 2018), the use of laboratory experiments to use ices as diagnostics of the thermal history (e.g., Poteet et al. 2013, He et al. 2018), and the use of laboratory experiments to determine new molecule formation pathways, for example for CH$_3$OH formation at lower cloud depths (e.g., Linnartz et al. 2015, Qasim et al. 2018).
Observations and modeling of the photochemical evolution of carbonaceous macromolecules in star-forming regions (I)

Berné, O.¹

¹Irap (CNRS and Univ. Toulouse), France

The goal of this contribution is to illustrate how spatially resolved spectroscopic observations of the infrared emission of UV irradiated regions, from star forming regions to the diffuse ISM, can be used to rationalize the chemical evolution of carbonaceous macromolecules in space, with the help of astrophysical models. For instance, observations with the Spitzer space telescope lead to the idea that fullerenes (including $C_{60}$) can form top-down from Polycyclic Aromatic Hydrocarbons in the interstellar medium. The possibility that this process can occur in space was tested using a photochemical model which includes the key molecular parameters derived from experimental and theoretical studies. This approach allows to test the likelihood that the proposed path is realistic, but, more importantly, it allows to isolate which are the key physical processes and parameters that are required to capture correctly the evolution of carbonaceous molecules in space. In this specific case, we found that relaxation through thermally excited electronic states (a physical mechanism that is largely unexplored, except by few teams) is one of the keys to model photochemistry of the considered species. Subsequent quantum chemical studies stimulated by the (limited) astrophysical model showed that a detailed mapping of the energetics of isomerization and de-hydrogenation is necessary to understand the competition between these processes in space.

Such approaches, involving experimentalists and theoreticians, are particularly promising in the context of the upcoming JWST mission, which will give access to the features of carbonaceous species (in emission and in absorption) and at an angular resolution which will enable to resolve new chemical frontiers in star (and even planet) forming regions.

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

Back to Schedule
Experimental determination of reaction product branching ratios at low temperatures for astrochemistry

Sims, I. R. 1, Hays, B. M. 2, Hearne, T. S. 3, Guillaume, T. 4, Abdelkader Khedaoui, O. 5, Gupta, D. 6, Cooke, I. R. 7, & the CRESUCHIRP team

1 Universite de Rennes 1, France, 2 Universite de Rennes 1, 3 Universite de Rennes 1, 4 Universite de Rennes 1, 5 Universite de Rennes 1, 6 Universite de Rennes 1, 7 Universite de Rennes 1

The CRESU (Reaction Kinetics in Uniform Supersonic Flow) technique, combined with laser photochemical methods, has been applied with great success to perform research in gas-phase chemical kinetics at low temperatures, of particular interest for astrochemistry and cold planetary atmospheres [1]. However, while many reactions have a number of potential product channels, measurements have concentrated to date almost exclusively on the overall rate constants. This is in part due to the difficulty of identifying a detection technique which is sufficiently sensitive and specific, yet able to measure quantitatively the concentrations of several species at the same time. Progress is being made in this area in several laboratories around the world, using for example synchrotron photoionisation mass spectrometry [2]. Here I will describe a new combination of the revolutionary chirped pulse broadband rotational spectroscopy technique invented by Brooks Pate and co-workers, with the CRESU technique, developed in a collaboration with the groups of Arthur Suits (U. Missouri) and Bob Field (MIT) which we have called Chirped Pulse in Uniform Flow (CPUF) [3]. Rotational cooling by frequent collisions with cold buffer gas in the CRESU flow at ca. 20 K drastically increases the sensitivity of the technique, making broadband rotational spectroscopy suitable for detecting a wide range of transient species, such as photodissociation or reaction products. In Rennes we are developing this technique to improve further its sensitivity and to apply it to reactions of astrochemical interest. I will describe our newly constructed Ka band (26.5-40 GHz) and E-band (60-90 GHz) spectrometers, and the latest results on product branching ratios at low temperatures.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe, Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
• Experimental laboratory astrophysics

Back to Schedule
Cosmic dust attests their existence by the interstellar extinction and polarization, IR emission and absorption spectra, and elemental depletion patterns. Dust grains are efficiently processed or even destroyed in shocks, molecular clouds, or protoplanetary disks. A considerable amount of dust has to be re-formed in the ISM. In various astrophysical environments, dust grains are covered by molecular ices and therefore, contribute or catalytically influence the chemical reactions in these layers. Laboratory experiments are desperately required to understand the evolution of grains and grain/ice mixtures in molecular clouds and early planetary disks. This talk considers recent progress in laboratory approaches on dust/ice experiments.

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics
Gas phase reaction kinetics of complex organic molecules at temperatures of the interstellar medium (I)

Canosa, A.\textsuperscript{1}

\textsuperscript{1}CNRS - Institut de Physique de Rennes (France), France

A great variety of complex organic molecules (COMs) have been identified in the interstellar medium (ISM) in the last 50 years. For quite a long time, COMs have been observed in lukewarm objects such as hot cores and hot corinos. Grain surface chemistry was claimed to be the source for the synthesis of such species during the warm-up of grains at $T > 30$ K and subsequent desorption. In contrast, only a few observations were available in the cold gas environments until recently. Investigations of the dense core B1-b and prestellar cores shed a new light on the mechanisms responsible for the presence of COMs in such objects ($T \sim 10$ K) for which the previous mentioned formation process on grains could not hold. Gas-phase reactions were reconsidered as a possible route to the formation of COMs in cold environments.

Within the framework of a collaborative project between the University of Rennes (France) and the University of Castilla-La Mancha (Ciudad Real, Spain), a new chemical reactor dedicated to low temperature studies has been developed in Spain. This apparatus is a new version of the CRÉSU (Reaction Kinetics in a Uniform Supersonic Flow) technique. It can be operated either with a continuous or pulsed flow at temperatures in the range 11.7 - 177.5 K. Coupled to the standard laser technique PLP-LIF (Pulsed Laser Photolysis - Laser Induced Fluorescence), this CRÉSU machine is designed to study radical-molecule reactions and the first investigations focussed on the kinetics of COMs toward OH radicals. The rate coefficients of the reactions have been obtained at various temperatures for molecules such as methanol, methyl formate, formaldehyde, ethanol or acetone. All of them were known to have a rate coefficient with a positive $T$-dependence at temperatures higher than 200 K. In the present talk, we will show that at lower temperatures, the reactivity significantly increases and becomes very fast at the temperature reigning in star forming regions.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

Back to Schedule
The Spectroscopy of Molecular Ions related to H$_3^+$ (I)

Schlemmer, S. 1, Asvany, O. 2

1 University of Cologne, Germany, 2 University of Cologne

H$_3^+$ is one of the key species in interstellar chemistry. The proton affinity of molecular hydrogen is small and therefore H$_3^+$ readily passes on its loosely bound proton to most other molecules in the interstellar medium. This leads to the formation of abundant molecular ions like HCO$^+$ or N$_2$H$^+$ which are used as diagnostic tools in many astronomical studies. Through the same process also other molecular ions are formed. In particular protonated forms of very abundant neutral species should be expected. However, the observational search for many of those ions is hampered since laboratory spectra of those ions are missing.

Recording such spectra in the laboratory is an experimental challenge since in many cases (i) the ions cannot be supplied in sufficient amounts to record traditional absorption spectra. In addition, deciphering such spectra is very difficult because the ions are commonly produced in discharges which (ii) produce many different species at the same time and (iii) many levels are populated under these hot conditions. In contrast, action spectroscopy in cold ion traps circumvents these difficulties. Here, the interaction of the ions with light is recorded by an alteration of the ion cloud composition by mass spectrometric means.

In our laboratory the method of light induced reactions (LIR) in ion traps has been developed continuously over the last 20 years in order to record spectra of only a few thousand mass selected, cold molecular ions. The spectral resolution of our IR measurements is high enough to predict THz spectra at sub-MHz accuracy which is sufficient to identify those ions in astronomical observations [1]. Double resonance techniques are employed to measure pure rotational spectra [2]. This data can be used to ultimately find those molecules in space [3].

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

Back to Schedule
Synthesis of solid-state Complex Organic Molecules (COMs) through accretion of simple species at low temperatures

Qasim, D. N.¹, Fedoseev, G.², Chuang, K.³, Taquet, V.⁴, Lamberts, T.⁵, He, J.⁶, Ioppolo, S.⁷, van Dishoeck, E.⁸, Linnartz, H.⁹

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Within the stellar formation cycle, the dense cloud stage is likely to be the earliest stage at which complex organic molecules (COMs) form on icy dust grains [1]. This is supported by solid-state experiments, which show that simple sugar-related species (e.g., glycolaldehyde) and sugar alcohols (e.g., ethylene glycol and glycerol) [2] can be formed at temperatures ≤ 15 K via radical-radical recombination reactions, i.e., without an ‘energetic’ input such as UV-irradiation of the ice. This recently experimentally explored field in astrochemistry is complimentary to decades of research that show that ‘energetic’ reactions can lead to the formation of COMs. In this contribution, I will give an overview of some of the latest work performed at the Sackler Laboratory for Astrophysics at Leiden Observatory on the formation of interstellar relevant COMs in the solid phase. Focus will be given to the formation and formation pathways of propanal and its derivative, 1-propanol, under interstellar analogue conditions resembling the CO freeze-out stage of star-formation. Propanal has recently been detected toward the low-mass protostar IRAS 16293-2422B, however its formation pathway is still unclear [3]. 1-propanol is of astrobiological relevance in that it is a primary alcohol, and it is hypothesized that such alcohols could have been the constituents of cell membranes during abiogenesis. The 1-propanol:propanal ratio from ALMA observations yields an upper limit of < 0.35-0.55, which is complemented by computationally-derived activation barriers. Thus, the formation of 1-propanol from propanal can be an astrochemically relevant pathway that will benefit from further validation by astrochemical modeling. Moreover, such molecules are and will be targets for ALMA and JWST observations, respectively. The detection of 1-propanol would build upon the idea that the components of primitive life on the early Earth are partially inherited from cold and lightless molecular cores.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

Research Area(s)
• Experimental laboratory astrophysics

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Dust evolution: going beyond the empirical (R)

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A key element when modelling dust in any astrophysical environment is a self-consistent treatment of the evolution of the dust material properties (size distribution, chemical composition and structure) as they react to and adjust to the local radiation field intensity and hardness and to the gas density and dynamics. The best way to achieve this goal is to ancore as many model parameters as possible to laboratory data. In this review, I will present a few examples to illustrate how outstanding questions in dust modelling have been/are being moved forward by recent advances in laboratory astrophysics and what laboratory data are still needed to further advance dust evolution models.

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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Potential energy surfaces of elemental carbon clusters: from theory to applications in astrochemistry

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The study of carbon clusters (Cₙ) has fascinated chemists and physicists over the years. First identified more than a century ago in astronomical bodies, Cₙ clusters are still a topic of increasing interest to both experimentalists and theorists alike [1]. Recently, we have focused onto the theoretical characterization of small Cₙs, notably C₃ and C₄ [2]. Special efforts were put into the computation and characterization of their global potential energy surfaces (PESs) by using of state-of-the-art ab initio calculations followed by analytic representation via the double many-body expansion (DMBE) method. Besides shedding light on some fundamental issues of such systems, their potentials contain important pieces of information that could therefore be employed as input for the construction of global truncated PESs of larger Cₙ species [3]. Yet, all these potentials carry inevitably precise information about the underlying species, and are therefore conceptually important tools for the study of their spectroscopy and chemical reaction dynamics. In our presentation, we will summarize all the above achievements as well as our recent attempts to obtain accurate reaction rate coefficients for the neutral-neutral C(n-x)+Cx → C(n-y)+Cy reactions. We hope that the inclusion of these data into astrochemical models of C-rich circumstellar envelopes and/or molecular clouds could lead to a refined understanding on the formation of more involved carbon chains molecules, PAHs, and their hydrogen deficient precursors.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

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• Theoretical calculations or simulations in laboratory astrophysics

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Prebiotic molecules in interstellar space: rotational spectroscopy and quantum chemistry (I)

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The starting point for the development of any astrochemical model is the knowledge of whether a molecule is present in the astronomical environment considered, with the astronomical observations of spectroscopic signatures providing the unequivocal proof of its presence. Among the goals of astrochemistry, the detection of potential prebiotic molecules (i.e., related to the formation of biomolecule building blocks) in astrophysical environments, and in particular in star forming regions, is fundamental in view of possibly understanding the origin of life. However, the detection of new molecules in space requires an exhaustive work to be carried out in the laboratory: on one side, it is necessary to understand whether the molecule under consideration might be present in the environment under study (thus requiring the investigation of possible formation pathways) and, on the other side, the spectroscopic signatures (mostly, rotational transition frequencies) need to be accurately determined over a large frequency range. Among the various chemical species, the compounds containing the CN moiety are considered prebiotic molecules as potential precursors of amino acids. The study of C-cyanomethanime [1] and ethanimine [2] will be presented as significant examples of the role played by rotational spectroscopy and quantum chemistry in this field. Another important prebiotic molecule is formamide, which has the ability to act as a precursor in the abiotic amino acid synthesis and perhaps also in that of nucleic acid bases. The investigation of its formation route will be addressed [3].

References

Scientific Theme(s)
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- Experimental laboratory astrophysics

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N-bearing Species in Massive Star Forming Regions

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Recent observations revealed that there is a difference in the spatial distribution of both nitrogen and oxygen bearing species towards massive star forming regions. These differences can be explained under different temperature regimes in hot cores [1]. In this study we attempt to model the chemistry of few nitrogen species; namely CH\(_3\)CH\(_2\)CN, CH\(_2\)CHCN, and NH\(_2\)CHO, using gas-grain chemical models [2,3]. A special attention is given to the role and efficiency of surface chemistry as it is suggested to be the key in manufacturing such species. We also investigate the influence of variations of the environmental physical conditions, among which are the density and the cosmic ray ionisation rate, on the fractional abundances.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

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Laboratory investigations aimed at building a database for the interpretation of JWST spectra

Palumbo, M.\(^1\), Baratta, G. A.\(^2\), Fedoseev, G.\(^3\), Fulvio, D.\(^4\), Scirè, C.\(^5\), Strazzulla, G.\(^6\), Urso, R. G.\(^7\)

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The James Webb Space Telescope (JWST) is expected to be launched in 2021. The Webb’s science instruments will provide us with high quality spectra acquired in the line of sight to young stellar objects whose interpretation requires a robust database of laboratory data. With this in mind, an experimental work is in progress in the Laboratory for Experimental Astrophysics in Catania (Italy) to study the profile (shape, width, and peak position) of the main infrared bands of molecular species expected to be present in icy grain mantles but not yet detected. Our study also takes into account the modifications induced on icy mantles by low-energy cosmic ray bombardment and by thermal processing. Here I will present some recent results which will contribute to identify and constrain the presence of deuterated species (such as HDO; \(^3\)), and nitrogen bearing species (such as HNCO and NO; \([1,2]\)) in icy grain mantles in star forming regions.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe, Solar System formation and the pre-solar nebula, Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Experimental laboratory astrophysics

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Simulations of energy dissipation and non-thermal desorption on amorphous solid water

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Dust particles covered by icy mantles play a crucial role in the formation of molecules in the Interstellar Medium (ISM). These icy mantles are mainly composed of water but many other chemical species are also contained in these ices. These compounds can diffuse and meet each other to react. It is through these surface reactions that new saturated species are formed. Photodissociation reactions are also thought to play a crucial role in the formation of radical species. Complex organic molecules are formed through an intricate network of photodissociation and surface reactions.

Both types of reactions release energy. Surface reactions are typically exothermic by a few eV, whereas photodissociation reactions are triggered by the absorption of a UV photon, resulting in the formation of highly excited products. The excited reaction products can apply this energy for desorption or diffusion, making products more mobile than predicted when considering only thermal hopping. The energy could further lead to annealing or deformation of the ice structure.

Here we would like to quantify the relative importance of these different energy dissipation routes. For this we performed thousands of Molecular Dynamics simulations for three different species (CO\textsubscript{2}, H\textsubscript{2}O and CH\textsubscript{4}) on top of a water ice surface [2]. We consider different types of excitation such as translational, rotational, and/or vibrational excitation. The applied substrate is an amorphous solid water surface (ASW) [3].

\textbf{References}
\begin{enumerate}
\item Fredon & Cuppen, H. M. 2018, Phys. Chem. Chem. Phys., 20, 5569
\end{enumerate}

\textbf{Scientific Theme(s)}
- Star formation and the cosmic matter cycle in the near universe

\textbf{Research Area(s)}
- Theoretical calculations or simulations in laboratory astrophysics

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The dust budget problem in galaxies near and far (I)

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In this talk I will discuss the origin of dust in our own and external galaxies. It has always been assumed that the source of interstellar dust is at least for a large part stellar. Using the Spitzer space telescopes to observe the Magellanic Clouds, we were in the unique position of doing a full census of dust producing stars and determine the dust production rate. On the other side of the equation we were able to determine the interstellar dust mass using maps obtained with Herschel. From these studies it is evident that the dust production doesn’t explain the interstellar dust mass. This is a problem also seen in the high red-shift universe, where it is know as the dust budget problem. In this talk I will explain why it is important to have an accurate determination of the interstellar dust mass in galaxies, and how systematic effects affect the dust mass determinations, ending with a justification to continue the work on determining dust opacities at far-infrared and submillimeter wavelengths in the laboratory.

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- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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Interpretation of in situ mass spectra at comet 67P (R)

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The Rosetta mission was following comet 67P for more than 2 years in close vicinity. ROSINA, the gas mass spectrometry suite on board Rosetta acquired during this time more than 2 million high resolution mass spectra. Total abundances as well as relative abundances of species were varying as a function of heliocentric distance, but also of sub-spacecraft latitude and longitude due to the irregular shape of the body. It is therefore not straight forward to e.g. deduce nucleus bulk abundances from measurements in the coma. In this talk I will present some examples on how laboratory work can help identifying the nucleus composition, but also the mechanism of cometary activity and the properties of cometary ices. Most laboratory work is being done on pure ices, mostly water ice whereas the comet is a mixture of ice and dust. Some potential pitfalls when interpreting cometary data by using pure ice lab data will be discussed.

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- Solar System formation and the pre-solar nebula

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A window on the composition of the early solar nebula: Pluto, 2014MU69, and Phoebe

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The initial chemical composition of any solar nebula will depend upon the degree to which 1) organic and ice components form on dust grains, 2) organic and molecular species form in the gas phase, 3) organics and ices are exchanged between the gas and solid state, and 4) the precursor and newly formed (more complex) materials survive and are modified in the developing planetary system. Infrared and radio observations of star-forming regions reveal that complex chemistry occurs on icy grains, sometimes before stars even form. Additional processing, through the protosolar disk and within the solar nebula further modifies most, but probably not all, of the initial materials. In fact, the modern Solar System still carries a fraction of its interstellar inheritance [1]. Here we focus on three examples of small bodies in our Solar System, each containing chemical and dynamical clues to its origin and evolution.

Phoebe, Pluto, and the small cold classical Kuiper Belt object (KBO) 2014MU69 each originated beyond Neptune. Saturn’s moon Phoebe is a captured KBO that carries high D/H in H2O [2], and complex organics, consistent with its formation in, and inheritance from, the outer solar nebula. Saturn’s largest ring is composed of primitive dust ejected from Phoebe’s interior by a relatively recent impact. Pluto’s internal and surface inventory of volatiles and complex organics [3], together with active geological processes including cryovolcanism, indicate a surprising level of activity on a body in the outermost region of the Solar System. Beyond Pluto, the New Horizons flyby of 2014MU69 will give the first view of an unaltered body composed entirely of material originally in the solar nebula at ~ 45 AU. These three objects provide a window on the composition of the early solar nebula and the degree to which the original material is retained in small Solar System bodies.

References

Scientific Theme(s)
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The search for complex organic molecules (COMs) in the interstellar medium (ISM) has revealed chemical species of ever greater complexity in various types of environment. This search relies heavily on the progress made in the laboratory to record and characterize their rotational spectra. Besides, our understanding of the chemical processes that lead to molecular complexity in the ISM builds on astrochemical numerical simulations that use chemical networks fed by laboratory and theoretical studies. On the observational side, the advent of the Atacama Large Millimeter/submillimeter Array (ALMA) and the expansion of the IRAM Plateau de Bure Interferometer now called NOEMA have recently opened a new door to explore the molecular complexity of the ISM. Thanks to the high angular resolution they can achieve, the spectral confusion of star-forming cores can be reduced, and their increased sensitivity allows astronomers to detect molecules of low abundance that could not be probed by previous generations of telescopes. The complexity of the molecules detected recently manifests itself not only in terms of number of their constituent atoms but also in their molecular structure. I will discuss results on molecular complexity in the ISM delivered by recent ALMA and NOEMA surveys.

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

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- Observations showing use of laboratory astrophysics in the interpretation/understanding of data
Fingerprints of the protosolar cloud collapse in the Solar System: refractory inclusion distribution and isotopic anomalies in meteorites

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Chondrites are made of a mixture of components that experienced different thermal histories and show differences in their isotopic compositions, especially in the most refractory phases, the Ca-Al-rich inclusions (CAIs) \cite{1}. The responsible processes are still debated. The age distribution of the CAIs indicates that their building blocks could have formed concurrently with the Sun, during the collapse of the parent cloud that formed our Solar System.

Here we investigate the dynamical and chemical evolution of different solids from the collapsing cloud to their transport in the forming protoplanetary disk with an outlook to the predicted isotopic anomalies resulting from heterogeneities in the parental cloud.

Our 1D disk model \cite{2} includes several processes such as gas and dust condensation/evaporation, dust growth/fragmentation, radiative and viscous heating, dead zone and a cloud infall in the form of a source term \cite{3}.

We find that the interplay between the thermal properties of the dust, the location in which the material is injected, the shape of the isotopic zoning in the clouds and the disk dynamic can produce aggregates whose petrographic and isotopic properties resemble those found in chondrites. Furthermore, we suggest formation timescales for different CAI types and assess the validity of isotopic chronometers like $^{26}$Al.

References
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Scientific Theme(s)
- Solar System formation and the pre-solar nebula

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

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Characterization of Large Carbonaceous Molecules in Cosmic Dust Analogues and Meteorites

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The Aromatic Research of Organics with Molecular Analyzer, AROMA [1], is an experimental set-up developed in the framework of the Nanocosmos ERC synergy project. Its main purpose is to analyze the carbonaceous molecular content of cosmic dust analogues and meteoritic samples. The experimental set-up consists of a laser desorption ionization (LDI) source and an ion trap connected to an orthogonal time of flight mass spectrometer. The ion source offers the possibility to study large carbonaceous molecules such as polycyclic aromatic hydrocarbons (PAHs) that are embedded in a variety of solid samples by performing LDI. The trap allows studying the structure of desired species by collision induced dissociation (CID). We demonstrate the potential of AROMA for the analysis of cosmic dust analogues and meteoritic samples. Hundreds of peaks are identified in the mass spectra with notable discrepancies across the different samples. We show that these differences can be used to trace the chemical history of each sample and are not a bias of our analysis. A double bound-equivalent (DBE) method is applied to sort the detected carbonaceous molecules into families of compounds. The DBE is representative of the unsaturation level of the molecules and thus corresponds to a direct measure of their aromaticity. It reveals in addition to PAHs, the presence of other populations such as aliphatic species, carbon clusters and fullerenes. A key molecule in the PAH family is m/z=202.08. We present how CID can help us disentangling the dominant isomeric structure at this position. The AROMA setup is now ready to tackle the question of the formation of carbonaceous nanograins in cosmic conditions. This question is the focus of experiments using the Stardust machine [2] and cold plasmas at low pressure [3]. Acknowledgments We acknowledge support from the European Research Council, Grant Agreement n. 610256 NANOCOSMOS, and support from La Region Occitanie, Grant No. 15066466.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

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Catalytic formation of H$_2$ on Mg-rich amorphous silicates

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In the interstellar medium (ISM), dust grains can be processed in a number of ways—heat, irradiation by cosmic and UV rays etc. Atomic H interaction of interstellar dust is another important processing mechanism, which eventually leads to the formation of molecular hydrogen. At a lower dust grain temperature ($< 20$ K), an efficient recombination of physisorbed H atoms on a variety of surface leading to H$_2$ formation has been well demonstrated both experimentally and theoretically. A series of experiments showed that H$_2$ formation could also occur on carbonaceous grain surface starting from simple nano-sized carbon particles to polycyclic aromatic hydrocarbons (PAHs) at higher grain temperature ($> 20$ K) [1,2] such as in photo-dissociation regions (PDRs). In these laboratory experiments, during H atom irradiation, surfaces with chemisorbed H atoms acts as a catalyst for H$_2$ formation through exchange reactions on aliphatic C-H bonds [1,2].

The present study has been extended to Mg-rich silicate grains with varying composition. Exposure to atomic H at 300 K on laser deposited amorphous silicates at room temperature leads to their hydrogenation. It has been analyzed by infrared spectroscopy through the formation of a broad 3.2 µm band depicting the O-H stretching mode. The mechanism of H$_2$ formation is an exchange reaction through O-H bonds on silicates. In addition, the O-H bands in Mg-rich silicates could contribute to the 3.2 µm absorption band of 67P/Churyumov-Gerasimenko comets observed through the VIRTIS (Visible, Infrared and Thermal Imaging Spectrometer) [3] on board the ESA’s Rosetta mission.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe, Solar System formation and the pre-solar nebula, Protoplanetary disks, debris disks, and the Solar System

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Laboratory Measurements of Deuterium Reacting with Isotopologues of H$_3^+$

Bowen, K. P.\textsuperscript{1}, Hillenbrand, P.\textsuperscript{2}, Liévin, J.\textsuperscript{3}, Urbain, X.\textsuperscript{4}, Savin, D. W.\textsuperscript{5}

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H$_2$D$^+$ and D$_2$H$^+$ are important chemical tracers of prestellar cores. At the densities of $\sim 10^6$ cm$^{-3}$ and temperatures of $\sim 20$ K typical for these environments, most molecules freeze onto dust grains. A notable exception is H$_3^+$ and its isotopologues, which become the dominant positive charge carriers in the gas, coupling the gas to any ambient magnetic fields, and thereby affecting the dynamics of the core collapse. H$_2$D$^+$ and D$_2$H$^+$ have a pure rotational spectrum that can be excited at prestellar core temperatures. This is to be contrasted with the symmetric H$_3^+$ and D$_3^+$, which have no pure rotational spectrum and are not observable in prestellar cores. Using H$_2$D$^+$ and D$_2$H$^+$ to probe prestellar cores and to infer the total abundance of H$_3^+$ isotopologues requires understanding the chemistry that forms and destroys these molecules. Of the eight key reactions that have been identified [1], five are thought to be well understood. The remaining three are the isotope exchange reactions of atomic D with H$_3^+$, H$_2$D$^+$, and D$_2$H$^+$. Semi-classical results differ from the classical Langevin calculations by an order of magnitude [2]. To resolve this discrepancy, we have carried out laboratory measurements for these three reactions. Absolute cross sections were measured using a novel dual-source, merged fast-beams apparatus [3] for relative collision energies between $\sim 10$ meV to $\sim 10$ eV. From these data we have generated thermal rate coefficients for astrochemical models. Here we will present our experimental results and discuss their astrophysical implications.

References


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Radicals are produced on/in ice dust mantles through both nonenergetic surface reactions and energetic processes like UV photolysis. At temperatures as low as 10 K, most of radicals cannot migrate on the surface once they are thermalized at the formation. However, when radicals start moving and encountering the other adsorbates during warming up, reactions of radicals play an important role in formation of complex organic molecules [1]. Therefore, information of diffusion and desorption of radicals from ice surface is essential for better understanding of chemical evolution. The number of experiments to approach the diffusion and desorption of radicals [2] is very limited because of those intrinsic technical difficulty. Especially, quantitative experiment on radical diffusion on ice has not yet been reported to my knowledge except for atomic radicals. I present the first experiment on detection of surface OH radicals produced by photolysis of pure compact amorphous ice, which enables us to derive the activation energy of surface diffusion. The detection of OH radical on the ice surface by conventional infrared measurements is very difficult because of overlapping with H$_2$O band. Instead, we have been successful in sensitively detecting the surface OH by the PSD-REMPI method [3].

References

Scientific Theme(s)
• Solar System formation and the pre-solar nebula

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The study of carbonaceous meteorites such as Murchison revealed the presence of a large variety and significant abundances of very complex organic molecules (COMs), which include amino acids, nucleobases, sugar derivatives, amphiphiles, and many other organic compounds of prebiotic and biological interest. Radiation of ices condensed on cold grains with energetic photons and/or particles was proposed as an efficient way to form such COMs in astrophysical environments. This hypothesis was confirmed by numerous laboratory experiments simulating photo-irradiation (ultraviolet, extreme ultraviolet, X rays) or particle bombardment (electrons, protons, heavy ions) of ices containing H$_2$O, CH$_3$OH, CO, CO$_2$, CH$_4$, H$_2$CO, NH$_3$, HCN, etc., condensed on cold (~5–80 K) substrates. These experiments resulted in the formation of amino acids, nucleobases, sugar derivatives, quinones, amphiphilic compounds, as well as a variety of other organic compounds that are similar to the COMs identified in carbonaceous meteorites. This work presents results for the formation of sugars, sugar alcohols, sugar acids, and their deoxy variants from the UV irradiation of ices containing H$_2$O and several combinations of carbon sources among CH$_3$OH, CO, and CO$_2$, and their comparison with meteoritic data. The formation mechanisms of these compounds and the astrobiological implications resulting from these experiments are also discussed in detail. This work summarizes the studies published recently about the formation of sugars, deoxysugars, and their derivatives [1–3], and shows new results obtained for different starting ice mixtures.

References

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- Solar System formation and the pre-solar nebula

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Hydrogenation and binding energies on dust grains as selective forces for the formation and observation of interstellar molecules

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Interstellar complex organic molecules (iCOMs) can be observed with great sensitivity in the gas phase thanks to their rotational signature. Recent advances in observation methods give hope that certain molecules could be associated with specific astrophysical conditions, if their main synthesis pathways can be determined. The evolution of atoms toward iCOMs can have a solid and cold phase, which we are studying. During the last few years, we have built a new experimental, to study the formation of molecules containing H,N,C and O. Our first conclusions suggest that it is indeed possible (and easy) to synthesize molecules such as NH\textsubscript{2}CHO (formamide).

On the other hand, the initially widespread idea that species can easily be hydrogenated and saturated seems to be misleading in many examples. Rather, it appears that the addition of atoms (H, N or O) can increase or decrease the molecular size. It is agreed that hydrogenation is the most common chemical reaction on the surface of grains. On the one hand hydrogenation induces some chemical transformation (mostly driven by competition between H addition and abstraction), on the other hand it releases energy to the deposited molecular film. These two aspects can lead to chemical selectivity on the surface of the grains, but also to selectivity when these species return in the gas phase via their chemical desorption [1]. During the presentation I will show some emblematic experiments that allow us to understand how to determine the chemical reaction pathways using formamide as example. Then I will explain how the action of hydrogenation can induce chemical desorption. Finally, I will show that the binding energies of pure species does not necessarily answer the question of the volatility of species [2], and that a detailed study of the hydrogenation and binding energies of iCOMs could provide leads to understanding the presence of some iCOMs in prestellar cores.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe, Solar System formation and the pre-solar nebula

Research Area(s)
- Experimental laboratory astrophysics

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Intrinsic absorption profile and radiative cooling rate of a PAH cation revealed by action spectroscopy in the cryogenic electrostatic storage ring DESIREE

Stockett, M. H.\textsuperscript{1}, Björkhage, M.\textsuperscript{2}, Cederquist, H.\textsuperscript{3}, Schmidt, H. T.\textsuperscript{4}, Zettergren, H.\textsuperscript{5}

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The multi-photon photodissociation (MPD) action spectrum of the coronene cation \((C_{24}H_{12}^+)\) has been measured as a function of storage time up to 60 s in the cryogenic electrostatic storage ring DESIREE. These measurements reveal not only the intrinsic absorption profile of isolated coronene cations, but also the rate at which hot-band absorptions are quenched by radiative cooling \[1\].

While it has become widely accepted that Polycyclic Aromatic Hydrocarbons (PAHs) are responsible to the infrared emission observed throughout the Interstellar Medium (ISM), other attributions of astronomical phenomena to PAHs remain unconfirmed or disputed. To interpret astronomical observations, laboratory spectroscopic and photophysical data is required. To this end, various experimental techniques (e.g. supersonic expansions, buffer gas cooling, and noble gas tagging) have been employed to cool gas-phase PAH ions to internal temperatures similar to those predominant in the ISM i.e. <100 K. In the present experiments, isolated PAH ions relax at their intrinsic radiative cooling rates in the cold (\(\sim 13 \text{ K}\)), collision-free environment of DESIREE.

Just after injection, the action spectrum is reddened by hot bands which fade with a time constant of 200 ms. This is consistent with radiative cooling via IR emission from vibrational transitions. The action spectrum recorded after relaxation is nearly identical to that reported by Joblin and coworkers \[2\], where coronene ions were cooled through collisions with He buffer gas in a cryogenic (35 K) ion trap. In both of these MPD measurements, the absorption profile is broadened with respect to that reported by Maier and coworkers using a He-tagging method \[3\], due to the lower internal temperature of the He-tagged ions. The position of the band maximum at 4570 Å is unaffected.

This contribution highlights the laboratory astrophysics potential represented by the new generation of cryogenic electrostatic storage devices.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics
Carbonaceous chondrites as probes of protoplanetary disk conditions (I)

Russell, S. S.¹, Bonato, E.², King, A. J.³, Bates, H.⁴, Schofield, P. F.⁵

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Carbonaceous chondrite meteorites can be used as tools to investigate the conditions and timescales of the evolution of the solar protoplanetary disk 4.6 Byr ago (e.g. [1]). These ancient rocks are composed of high temperature chondrules and calcium-aluminium-rich inclusions (CAIs) surrounded by a matrix that has often been affected by aqueous alteration. Chondrules are silicate rich rounded objects up to ~1mm across that formed by a flash heating event in a dense dust rich region of the solar system (e.g. [2]). CAIs are rounded or irregular object up to 1cm across that formed by condensation or melting/solidification within a more solar (reduced, hydrogen rich) environment. Matrix grains in the least altered meteorites are mainly composed of amorphous silicates with some crystalline olivine and pyroxene, with organic material and isotopically anomalous presolar grains. They are a good match for unprocessed protoplanetary dust [3]. Our work shows how even gentle heating in an asteroid alters this primordial dust, making it more crystalline and destroying and changing the organic component. We will present recently acquired data for matrix from meteorites that have experienced neither heating nor aqueous alteration. Characterising the mineralogy and geochemistry of this dust enables a better understanding of the origins and environmental conditions of the dust component of the solar protoplanetary disk.

References

Scientific Theme(s)
• Solar System formation and the pre-solar nebula

Research Area(s)
• Experimental laboratory astrophysics

Back to Schedule
Amorphous Solid Water (ASW) particle production for collision experiments

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Planet formation processes are experimentally investigated by low velocity collisions between protoplanetary analogues produced in the laboratory. Previous Collision studies have employed both silicates \cite{1} and crystalline ice particles \cite{2}. The latter yields sticking probabilities that are too low to account for the observed rates of planet formation leading to the so called ‘bouncing barrier’ \cite{3}. Nevertheless, proto-planetary disk particles may comprise both amorphous and crystalline ice material. Therefore, the study of amorphous ice particle collisions is vital to our understanding and has never been achieved because of the difficulty to produce, store and use such samples. Our work aims to design and use an experiment to produce $\mu$m HGW particles (Hyper-quenched Glassy Water), one of the three low density forms of amorphous water. We will do so by spraying water droplets in a cryoliquid which is liquid ethane. This technique has been developed by Cryobiologist to freeze samples in their living (ie not crystalline) state, but never with Astronomical purposes. Those particles will be used as protoplanetary analogues in microgravity for collision experiment.

References


Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Experimental laboratory astrophysics

Back to Schedule
Star formation regions are marked by the presence of interstellar complex organic molecules (iCOMs), the synthesis of some of them is thought to be strongly influenced by the surface of the interstellar grain ice mantle. The use of these iCOMs as chemical probes of star forming regions relies both on the knowledge of the complete network of solid-state network chemical reactions and on the knowledge of the dynamics at work in these reactions. The latter is based on a reaction-diffusion Langmuir-Hinshelwood mechanism.

I will present how it is possible to investigate the solid-state reaction network, from simple molecules to iCOMs and to constrain the dynamics of iCOMs formation in ice using a mechanistic bottom-up approach based on laboratory experiments on interstellar ice analogues. In particular I will show how reaction-diffusion can be separated and investigated independently [1,2] and I will show that the ice mantle modifies the simple Langmuir-Hinshelwood mechanisms [3].

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

Back to Schedule
Survival of Shells of Icy Satellites Against Hypervelocity Impact

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Icy worlds with interior subsurface oceans are of increasing interest for both planetary science and astrobiological reasons. The satellites of Jupiter and Saturn include several examples, such as Europa and Enceladus [1], and bodies such as Pluto may also have some form of interior ocean. There is no reason to suppose these are rare or unique to our Solar System. The lifetime of Solar System bodies is not however permanent - they are subject to evolutionary processes such as giant impacts which can catastrophically disrupt them. Impacts on ice have long been studied in the laboratory and via modelling (e.g. [2]). But the presence of an icy layer over an interior medium can change the outcome of an impact event (e.g. [3]). Recent experimental studies have looked at how this can change the energy density required for a catastrophic impact. Here we consider a more limited but related problem: How does a thick ice shell with no interior filling respond to impact events? This bridges the gap between solid ice bodies and ice shells with filled interiors and reveals how the shell itself behaves. Using a two stage light gas gun we have impacted decimetre scale ice shells in the laboratory at speeds in the range 2 to 5 km s\textsuperscript{-1}, to see how they respond. We have spanned the energy density which disrupts solid and water filled ice spheres of similar size and find that hollow ice shells behave differently. We report on what happens as energy density increases and one moves from cratering the ice shell, to penetration and finally disruption. The insights gained show how laboratory experiments can provide information on Solar System scale processes.

References

Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Experimental laboratory astrophysics

Back to Schedule
Laboratory evidence for the formation of hydrogenated fullerene molecules

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Large carbon containing molecules such as PAHs and fullerenes are thought to contain a significant fraction of the interstellar carbon budget. PAHs are widely detected throughout the ISM through IR emission. Similarly, C₆₀ and C₇₀ have been observed through IR emission to be present in stellar atmospheres [1] as well as in the diffuse ISM [2]. C₆₀⁺ has been determined as the carrier of the first two diffuse interstellar bands (DIBs) to be identified [3]. The interaction between such carbon bearing molecules and the most abundant element, H, is of particular importance in interstellar chemistry, having been proposed as a route to molecular hydrogen formation. Hydrogen induced unzipping of fullerenes has been proposed as route to forming PAHS, thus connecting these two classes of molecules. Several experimental and theoretical studies have revealed how, through superhydrogenation, PAHs can act as efficient catalysts for H₂ formation in regions such as PDRs where low temperature grain surface routes are not active. It remains unclear as to what extent such processes apply to fullerenes. I will discuss experimental evidence for the interaction of C₆₀ adsorbed on a graphite surface with H-atoms, showing that hydrogenated fullerene molecules can be formed. We consider both direct addition of H-atoms from the gas phase and a pick-up mechanism in which C₆₀ molecules are adsorbed on a pre-hydrogenated graphite surface. Scanning tunnelling microscopy and temperature programmed desorption have been used to study the hydrogenation process in situ and to probe the product mass distributions. Hydrogenated fullerenes are observed to desorb intact from a graphite surface allowing us to use mass spectrometry to determine the extent to which they can be hydrogenated. When adsorbed on a gold surface, H₂ is released from the hydrogenated fullerenes prior to fullerene desorption, allowing us to determine the barrier for H₂ release.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

Research Area(s)
• Experimental laboratory astrophysics

Back to Schedule
Quenching of interstellar carbenes: interaction of $\text{C}_3\text{H}_2$ with He and $\text{H}_2$

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In order to characterize the chemical composition, isotopic enrichments and possibly, history of the interstellar medium, it is necessary to get an accurate estimate of the molecular densities of the polar molecules observed. Since the intensity of the spectral lines depends on both photonic and molecular collisions, knowing the quenching/excitation rates is an essential ingredient, as soon as the spontaneous photon emission rates becomes comparable to the collisional quenching rate [3].

Many complex molecules are observed, and especially so, in pre-stellar and proto-stellar environments. Among those, hydrocarbons are particularly challenging, because of the absence of permanent electric dipole moment for the simplest ones, methane and $\text{C}_2\text{H}_n$, $n=2,4,6$. Among the closed-shell hydrocarbons, the carbenes $\text{c-C}_3\text{H}_2$ and $\text{l-C}_3\text{H}_2$ are the lightest ones to display a permanent electric dipole moment and hence, be detectable by rotational spectroscopy. The cyclic form, cyclopropenylidene, is ubiquitous in the Milky Way and external galaxies. Its abundance is high enough to warrant observations of $^2\text{H}$ and $^{13}\text{C}$ substituted species [2]. The linear form, propadienylidene, is less abundant but widely observed.

We present here a precise ab initio Potential Energy Surface for the interaction $\text{C}_3\text{H}_2$ with helium and molecular hydrogen, by means of an ab initio CCSD(T)-F12a formalism [1]. We conduct quantum dynamical scattering in order to get precise cross sections using a coupled-channel and coupled-states approach for solving the nuclear motion. We average sections to get rates for rotational quenching form 5 to 150K. We perform extensive tests on the potential energy surface and the quantum dynamics formalism, to validate the various methodological choices. We show that these new rates are vastly different, up to more than an order of magnitude, from the more approximate ones, present in the literature. We expect large differences in the astrophysical analyses of $\text{C}_3\text{H}_2$.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

Back to Schedule
Protoplanetary disks are known to be dynamic objects, through which mass and angular momentum are transported during the final stages of pre-main sequence growth. This dynamical evolution lasts millions of years, and is critical to understand as it will determine the properties of materials incorporated into planets.

In this talk, I will review how meteorites and cometary samples record a dynamic history of our own protoplanetary disk, the solar nebula, as these primitive planetesimals are found to be mixtures of dust grains and molecules which formed in a wide array of environments and physical conditions. I will then discuss our current ideas on how the chemical evolution of the nebula can be studied in the context of dynamical models. I will focus on the use of particle-tracking methods (e.g. [3]) in these studies, which allow us to directly record the conditions (temperature, density, radiation flux) that solids and gases would see over their lifetime in the solar nebula, and how such methods can be used to investigate the chemical evolution of species including the formation of organic molecules via irradiation of ices (e.g. [2]). Such dynamic evolution may also be important in the production of hydrocarbons and other species found in other protoplanetary disks (e.g. [1]). I will discuss the prospects for further studies using laboratory based experiments as a guide.

References

Scientific Theme(s)
- Solar System formation and the pre-solar nebula

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics
Gas-dust chemistry of volatiles in the star and planetary system formation (R)

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In this presentation, I will review two topics: (i) desorption and reactions of volatile species on ice surfaces and (ii) isotope fractionation.

ALMA enabled high spatial resolution observations of the central region of protostellar cores. While the circumstellar structures, e.g. the infalling gas and forming protoplanetary disk, are essential for star formation studies, chemical processes along the flow could transform the interstellar matter (ISM) to the disk material. Abundances of volatiles in the gas and solid phases keep changing via sublimation and reactions, as the gas and grains are heated by stellar irradiation and/or accretion shock. Since the brightness of the molecular emission lines varies spatially reflecting the temperature and abundance distributions, it is essential to consider both physical and chemical processes to interpret the observations. I will explain how the state-of-the-art theoretical models compare with observations and how the laboratory data and quantum chemical studies help the improvements of the model.

The isotope fractionations are found not only in the star-forming regions, but also in the primordial Solar system bodies such as comets. The molecular isotope ratios are thus considered to be possible tracers of chemical evolution from the ISM to the planetary matter. Major fractionation mechanisms are isotope exchange reactions and selective photo-dissociation via self-shielding. Quantum chemical studies and spectroscopic studies have been playing essential role in the quantitative evaluation of these mechanisms. Recently, nitrogen fractionation via self-shielding and ice formation is proposed; \textsuperscript{15}N\textsuperscript{14}N is selectively photo-dissociated, and \textsuperscript{15}N is frozen as NH\textsubscript{3} ice. The efficiency of the fractionation then depends also on gas-dust interactions such as photoevaporation yield.

Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

Back to Schedule
The dust that we observe in young debris disks is of secondary origin, the low-end of a collisional cascade that involves km-sized bodies and planetesimals. Observations at ever-increasing angular resolution and sensitivity are providing us very stringent diagnostics about the dust properties as well as the dynamical evolution of the small dust grains. In this review, I will try to compare side-by-side what we can learn from state-of-the-art observations and laboratory experiments, with a special emphasis on the phase function at near-infrared wavelengths (scattered and polarized light), the dynamics of small dust grains, as well as the fragmentation efficiency of pebbles and planetesimals.

**References**


**Scientific Theme(s)**  
- Protoplanetary disks, debris disks, and the Solar System

**Research Area(s)**  
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

*Back to Schedule*
A variety of molecules (180) have been detected in the interstellar medium (ISM) [1]. Many are organic with carbon backbone. Iso-propyl cyanide (i-C$_3$H$_7$CN) a branched alkyl molecule was recently observed [2] in the ISM. The molecule was detected in a giant gas cloud called Sagittarius B2, an active region of ongoing star formation in the centre of the Milky Way. Its abundance is 0.4 times higher than its straight-chain structure isomer, suggests that branched molecules may be generally abundant in the ISM. Propyl cyanide (C$_3$H$_7$CN) is the smallest alkyl cyanide that exists in several distinct isomers. i-propyl cyanide is the largest and most complex organic molecule found to date - and the only one to share the branched atomic backbone of amino acid: some of the building blocks of life.

However the routes leading to the formation of the different propyl cyanide isomers are not clear. There is a need to accurately determine the energetics, reaction barriers, and ultimately rate constants for such complex chemistry processes, in gas and on the icy mantle of dust grains. Our goal in this work is to understand the physical and chemical processes by which new complex organic molecules such as i-C$_3$H$_7$CN and n-C$_3$H$_7$CN form in the interstellar medium. We investigated the different reaction paths for their formation routes from ab initio, and kinetic calculations points of view. We considered the gas phase formation of the propyl-cyanide isomers from the bimolecular reaction of HCN with CH$_3$CHCH$_2$. The considered mechanism involves two-step reaction for each isomer.

We employed UCCSD(T)/aug-cc-pVTZ//UMP2(full)/aug-cc-pVTZ methodology to predict the structure of the formed species and the reaction energetics. Rate constants including quantum effects were calculated for the [200-2000K] temperature range.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

Back to Schedule
Using atomistically detailed simulations to understand the formation, structure and composition of astrophysical silicate dust grains

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\textsuperscript{1}University of Barcelona / ICREA, Spain, \textsuperscript{2}University of Barcelona, \textsuperscript{3}University of Barcelona

While dust takes up only one mass percent of the total matter in the interstellar medium, it plays a crucial role in its chemical evolution by catalyzing molecule formation and, through scattering the strong radiation from the interstellar medium (ISM), preventing molecular photodissociation in denser regions. Via a combination of lab characterization of pristine material, astronomical observations, the general properties of silicate dust particles have been reasonably well discerned. Fitting observed spectra with a combination of lab spectra of materials of different crystallinity, shape, size and composition has given valuable insight into the possible identity of silicate dust in a number of astronomical environments. Nanosilicates, although thought to be highly abundant \cite{Draine2001}, are more difficult to characterise by experiment and observation due to their extreme small size and correspondingly variable non-bulk-like properties. Employing state-of-the-art computational modelling we show that it is possible to directly and accurately calculate the structures and properties of nanosilicates \cite{Bromley2014,Goumans2012}. Specifically, we employ both classical atomistic and quantum mechanical electronic structure to highlight the power of this approach in three astronomically important contexts. Firstly, we show how atomistically detailed simulations can track the the nucleation of silicate nanograins from atomic/molecular precursors to grains of 50 nm diameter under any chosen conditions (e.g. circumstellar, ISM). From accurate evaluation of infrared spectra we then provide evidence for a population of ultra-stable ‘magic’ nanosilicates in the protoplanetary disks around Herbig Ae/Be stars, and also elucidate the subtle link between crystallinity/amorphicity in nanosilicates. Finally, we outline how these simulation methods could be used to assist in the interpretation of laboratory experiments dealing with dust analogues.

References
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Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

Back to Schedule
Understanding the physical conditions of planet formation are essential if we are to confront planet formation theories and subsequently understand the physical and chemical evolution of their atmospheres. The Atacama Large (sub-) Millimetre Array (ALMA) has driven substantial leaps in our understanding of the planet formation environment, the protoplanetary disk, and has enabled the detection of a multitude of molecular species over a range of transitions. Using traditional analyses of multiple transitions we are able to place exceptional, spatially resolved constraints on the local physical conditions in disks. I will present work using the simple diatomic species CS and CN which I have used to map the temperature and density structure of the nearest protoplanetary disk to us, TW Hya. In addition, I will present a new method which exploits the Doppler shift of emission lines in a rotating disk to super-sample the line profile which has enabled us to identify the previously unresolved splitting of hyperfine lines in the $N = 3 - 2$ level of CN. This revealed hyperfine anomalies in the CN emission around TW Hya which, with the aid of precise collisional rates, will potentially lead to a constraint on the local ortho-to-para ratio of H2 in a protoplanetary disk.

Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

Back to Schedule
High-resolution electronic spectroscopy study of neutral gas-phase PAH species

Petrignani, A.\textsuperscript{1}, Roeterdink, W.\textsuperscript{2}, Velásquez, H.\textsuperscript{3}, Buma, W.\textsuperscript{4}

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We present a study of neutral PAH species as possible carriers of the Diffuse Interstellar Bands (DIBs). We measured high-resolution gas-phase electronic UV/VIS spectra of cold neutral PAHs with 5 rings and more employing a (1+1') REMPI scheme on the jet-cooled molecules with mass selective detection. The spectra show strong vibronic coupling resulting in similar transition strengths for $S_1 \leftrightarrow S_0$ and $S_2 \leftrightarrow S_0$, whether allowed or forbidden, and transition going from the UV into the visible range. We also calculated the vibrationless electronic transitions using an all valence electrons theory and compared these to jet-cooled electronic spectra, validating its predictability to within 1% accuracy. We provide insight into possible carriers of the DIBs and further demonstrate that the electronic behaviour of PAHs is more strongly dependent on the isomeric structure than the size of the molecule.

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe, Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Experimental laboratory astrophysics

Back to Schedule
Interstellar aromatic chemistry: a combined laboratory, observational, and theoretical perspective

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The detection of benzonitrile (c-C\textsubscript{6}H\textsubscript{5}CN) in the cold, dark molecular cloud TMC-1 [1] has opened up a new field of interstellar organic chemistry. In light of this discovery, key, unanswered questions include what other small aromatic molecules exist in astrophysical environments, the connection of small aromatics and much larger polycyclic aromatic hydrocarbons (PAH) [2], and the chemical and physical role that aromaticity plays in the interstellar medium [3].

To address these questions, astronomical observations, laboratory measurements, and theoretical chemistry must be closely linked. In this talk, I will present the status of ongoing laboratory and quantum chemistry work on viable low temperature formation pathways and microwave spectroscopy of small aromatic molecules. This work is done in support of the GOTHAM, a large survey project of TMC-1 with the 100 m Green Bank Telescope.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

Research Area(s)
• Experimental laboratory astrophysics

Back to Schedule
Benzene Condensation on Titan’s Stratospheric Aerosols: An Integrated Laboratory, Modeling and Observational Approach

Dubois, D.¹, Iraci, L.², Barth, E.³, Vinatier, S.⁴, Salama, F.⁵, Sciamma-O’Brien, E.⁶

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Observations of Titan’s atmosphere made by the Cassini spacecraft revealed the presence of a high-altitude (>250 km) south polar cloud system with a benzene (C₆H₆) signature detected in the infrared [1]. The unusual condensation of C₆H₆ at these altitudes was made possible by a strong cooling in the stratosphere at southern latitudes, which followed a global circulation reversal after the northern spring equinox. In addition, aerosols present in the stratosphere may act as nuclei for the condensation and growth of these organic cloud particles. At present, however, laboratory data is insufficient for models to reproduce the formation and growth of such clouds, notably at Titan-like low temperatures. We present here results from the investigation of the condensation of benzene, combining laboratory, modeling and observational analyses synergistically. We have performed vapor pressure measurements of benzene at Titan-like temperatures using the Ames Atmospheric Chemistry Laboratory (ACL) [2] and studied favorable conditions for its condensation onto Titan aerosol analogs produced in the Titan Haze Simulation experiment on the NASA Ames COSmIC facility. The nucleation and condensation processes of benzene measured in the laboratory will serve as an input to the microphysical Titan model CARMA [3], which simulates the condensation, evaporation, sedimentation and coagulation of cloud particles. These comparisons will help us constrain the expected cloud formation altitude and particle size distributions. Moreover, using these outputs, we present a comparison with Composite Infrared Spectrometer (CIRS) observations in the 9-17 µm spectral region.

References

Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Experimental laboratory astrophysics

Back to Schedule
Aerosols are present in every substantial planetary atmosphere of the solar system and in that of exoplanets. Aerosols affect the chemistry, dynamics and flux of radiation in these atmospheres. They can provide organic material on the surface and modify its temperature and consequently have an impact on the habitability of the planet. On the other hand, they can hide spectral signatures and prevent characterization of atmospheric components. Nevertheless, the structure, composition and formation processes of the haze are still largely unknown. A most illustrative example is that of Titan. Although the Cassini-Huygens mission provided a wealth of data on Titan’s atmosphere and surface, in situ chemical analysis of the aerosols by the Huygens probe proved to be mostly unsuccessful and remote optical data allowed retrieving only sparse information about their molecular composition. Laboratory analogues (called tholins) can be synthesized by exposing representative gas mixtures to a plasma discharge or to UV radiation. Decades of study of these analogs (notably those of Titan or the Primitive Earth) made it possible to determine their physical and optical properties and demonstrated that their bulk composition was extremely complex from a chemical point of view. Only very high-resolution mass spectrometers can determine the atomic composition of each individual molecule making up the samples, while tandem mass spectrometry (MS-HRMS) and liquid chromatography (HPLC-HRMS) allow characterization of the molecular structure [1]. For example, ‘Titan’ tholins were found to contain 7 molecules corresponding to biological amino acids and nucleotide bases. Therefore, aerosols are a new source of prebiotic material and may increase the range of planets where life could begin [2]. In the context of the quest for biosignatures, development of very high-resolution mass spectrometers for spaceflight capable of in situ sampling of atmospheres and surfaces is mandatory [3].

References

Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Experimental laboratory astrophysics
Temperature and Thickness effects on Photodesorption of CO Ices

Sie, N.\textsuperscript{1}, Cho, Y.\textsuperscript{2}, Muñoz Caro, G.\textsuperscript{3}, Chen (Asper), Y.\textsuperscript{4}

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Abundant gaseous CO molecules have been observed in cold dense clouds, where the thermal desorption is inhibited. The secondary UV field \cite{Shen2004} can lead to photon-induced desorption, which is dominated by desorption induced by electronic transition (DIET). According to Muoz Caro et al. (2016) \cite{MunozCaro2016}, the photodesorption yield of solid CO ice is linearly dependent on deposition temperatures from 8 K to 20 K. However, the structure transition of CO ice from amorphous to crystalline is at around 20 K, showing that the linear dependence of photodesorption on deposition temperature is not related to structure. In this work, CO ices were deposited at 13-25 K with different thicknesses, and the trend of photodesorption yield derived from each irradiation period as a function of CO remaining thickness can be fitted by an analogy to Fermi-Dirac integrals, providing a method to study the energy transfer efficiency and energy penetration depth. Chen et al. (2017) \cite{Chen2017} demonstrated that the temperature dependent energy shifts in VUV absorption spectra of CO ices is due to the spontelectric filed in the range of 20-26 K. The relation between spontelectric field and the energy transfer efficiency will be discussed in this work.

References

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Scientific Theme(s)

- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)

- Experimental laboratory astrophysics

Back to Schedule
Circumstellar dust analogues can be studied experimentally to determine their collisional behavior and their optical properties. These results affect simulations of circumstellar disks in various, substantial ways: Collision results determine how dust aggregates grow and how their aerodynamic properties change with time. This determines how solids move throughout the disk, how they accumulate, and how planetesimals might be formed. The optical properties determine the observational signature of these effects and allow us to constrain the spatial distribution of dust in disks, the sizes of the aggregates, as well as the temperature and optical depth of the dust emission. In this talk, I will present how theoretical models and their predictions depend on laboratory results and what we learned about disks from high spatial resolution radio interferometry.

Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

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Protoplanetary disks, debris disks and solar system (R)

Kamp, I.¹

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VLT instruments and ALMA with their high spatial resolution have revolutionized in the past five years our view and understanding of how disks turn into planetary systems. This talk will briefly outline our current understanding of the physical processes occurring and chemical composition evolving as these disks turn into debris disks and eventually planetary systems like our own Solar System. I will especially focus on the synergy between disk structure/evolution modeling and astrochemical modeling to highlight the most recent advances, and open questions such as (1) how much of the chemical composition in disks is inherited from molecular clouds, (2) what is the origin of the gas in debris disks and what can we learn from it, (3) the relevance of snowlines for planet formation. For each of the three, I will outline briefly how the combination of theory/lab astrochemistry, astrophysical models and observations are required to advance our understanding.

Scientific Theme(s)
• Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
• Observations showing use of laboratory astrophysics in the interpretation/understanding of data

Back to Schedule
The formation of prebiotic building blocks of peptides on interstellar dust grains

Ligterink, N. F. 1, Coutens, A. 2, Calcutt, H. 3, Kofman, V. 4, Terwisscha van Scheltinga, J. 5, Linnartz, H. 6, van Dishoeck, E. F. 7, Jørgensen, J. 8, & PILS team

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The emergence of life on Earth may have been aided by organic molecules formed in and supplied from the interstellar medium. Molecules such as formamide (NH$_2$CHO), methyl isocyanate (CH$_3$NCO) and acetamide (CH$_3$C(O)NH$_2$) belong to a select group of interstellar ‘peptide-like’ molecules considered to be relevant precursors to the formation of peptide chains. On Earth, peptide chains form by linking amino acids and eventually result in proteins, the biomolecular engines of life.

Recent ALMA detections place NH$_2$CHO, CH$_3$NCO and CH$_3$C(O)NH$_2$ in the planet-forming region (inner 60 AU) around the sun-like protostar IRAS 16293-2422B. This hints that these building blocks were also available at the earliest formational stages of our Solar System [1,2,3]. How these species form and are related to each other is an open question, however.

In this talk the formation of peptide-like molecules on icy surfaces of interstellar dust grains is discussed. In the laboratory, CH$_4$:HNCO mixtures frozen at 20 K are UV irradiated and analyzed with infrared spectroscopy and temperature programmed desorption - mass spectrometry. The experiments show the simultaneous formation of a number of organic molecules, including NH$_2$CHO, CH$_3$NCO, CH$_3$C(O)NH$_2$, various larger peptide-like molecules, and also methylamine (CH$_3$NH$_2$), a presumed building block of amino acids such as glycine.

Constrained by experimental parameters, a reaction network is constructed which shows that these molecules are related through a series of radical addition reactions, primarily starting from atomic nitrogen (N), NH and NH$_2$. A comparison between laboratory and observational data shows that the presence of peptide-like molecules in the interstellar medium can be explained by chemical reactions taking place in the ice mantles around dust grains. Subsequent incorporation of these icy grains into larger bodies, such as comets, makes the delivery of peptide-like molecules to a young Earth likely.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe, Solar System formation and the pre-solar nebula

Research Area(s)
- Experimental laboratory astrophysics
Complex molecules in astrochemical impact conditions (I)

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¹Physical Research Laboratory, India

Recently several molecules were observed to be present on the icy satellites of our solar system that largely remained unexplored until the last quarter of the 20th century. Space based observations dominated the contribution towards our understanding on the surface chemical composition of the icy bodies in the Solar System. Among the icy objects of the Jovian and Saturnian planetary systems few satellites such as Ganymede, Europa, Callisto, Dione, Rhea and Titan that are embedded in their respective planetary magnetospheres are observed to undergo rich chemical processes. This is due to the availability of wide range of energetic ions that are present in those magnetospheres which processes the icy surfaces of satellites by irradiation and implantation.

The heterogeneous chemistry that is responsible for the molecular synthesis at such extreme conditions are so far simulated in the laboratories in order to understand every step of the reaction leading to synthesis of newer and complex molecules. The sources of energy to break and make bonds are so far from energetic sources such as eV to keV electron, keV ions and few eV photons. Such energetic processing of simple molecules is known to synthesis complex molecules such as amino acids, sugar and even di-peptide links. Yet, the particle irradiation has its own limitation.

Nevertheless, the surface features of the icy satellites remind us the impact process to have played a major role in the molecular synthesis. Such impacts and the impact associated shock processing of molecules in extreme conditions largely remains unexplored to-date [1, 2]. Therefore, a different approach [3] to process the molecules of astrochemical interest is required. In this talk, I will present the results of our new experiment where complex molecules subjected to astrochemical impact conditions yielding complex structures.

References


Scientific Theme(s)

- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)

- Experimental laboratory astrophysics

Back to Schedule
Recent advances in experimental laboratory astrophysics for stellar astrophysics applications and future data needs. (R)


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I present an overview of recent advances in experimental laboratory astrophysics to provide atomic data needed in stellar astrophysics applications. Accurate atomic data for line wavelengths, energy levels, line broadening such as hyperfine structure and isotope structure, and f-values, particularly for the line rich iron group elements, are needed, and examples of recent measurements will be given.

These atomic data are essential for determination of elemental abundances. With modern facilities, telescopes and spectrographs, access to underexplored regions (IR, vacuum UV, VUV), and improved stellar atmosphere models (3D, NLTE), and extremely large datasets, astronomers are tackling problems ranging from studying Galactic chemical evolution, to low mass stars and exoplanets. Such advances require improved accuracy and completeness of the atomic database for analyses of astrophysical spectra.

References

Scientific Theme(s)
- Stars, stellar populations, and stellar explosions

Research Area(s)
- Experimental laboratory astrophysics

Back to Schedule
The Wootton Center for Astrophysical Plasma Properties (WCAPP) is a new center focusing on the spectroscopic properties of stars and accretion disks using ‘at-parameter’ experiments. Currently, these experiments use the X-ray output of the Z machine at Sandia National Laboratories - the largest X-ray source in the world - to heat plasmas to the same conditions (temperature, density, and radiation environment) as those observed in astronomical objects. The experiments include measuring (1) density-dependent opacities of iron-peak elements at solar interior conditions, (2) spectral lines of low-Z elements at white dwarf photospheric conditions, (3) atomic population kinetics of neon in a radiation-dominated environment, and (4) resonant Auger destruction (RAD) of silicon at accretion disk conditions around supermassive black holes. In particular, we report on recent results of our experiments involving hydrogen and helium at white dwarf photospheric conditions. We show that the measured shift and broadening of helium lines, both of which can be used as mass indicators of white dwarfs, is very different from that predicted by theory.

Scientific Theme(s)
- Stars, stellar populations, and stellar explosions

Research Area(s)
- Experimental laboratory astrophysics

Back to Schedule
Comparative study of 3.4 micron band features from carbon dust analogs obtained in pulsed plasmas at low and atmospheric pressure

Topala, I.1, Gerber, I. C.2, Chiper, A.3, Pohoata, V.4, Mihaila, I.5

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Carbon dust analogs are obtained in the laboratory for more than three decades, as an approach to study some chemical and typological features of interplanetary and interstellar carbon dust. Various synthesis methods or post processing techniques are explored in order to match the astrophysical observations or to obtain information on dust processing in space [2]. Many experiments proved the potential to grow aliphatic, aromatic or mixed aliphatic/aromatic carbon structures, which exhibits IR absorption features similar to infrared absorption spectroscopy data from space [3]. It is important to mention here some of the experimental approaches: condensation, physical vapour deposition, plasma enhanced chemical vapour deposition, combustion and pyrolysis, pulsed laser deposition. Recently, our group reported a new experiment, based on high power impulse atmospheric pressure plasma for low temperature deposition of carbon dust analogs, in form of both non-aromatic thin films and ‘fluffy’ aggregates [1]. In this study, we report a comparative experimental study, focused on the 3.4 micron band features for carbon dust analogs obtained in (1) a pulsed laser deposition setup with Nd:YAG laser and graphite target, (2) a low pressure radio frequency discharge and (3) an atmospheric pressure dielectric barrier discharge, in helium - saturated hydrocarbons gas mixtures. The aliphatic -C-H stretching band, known at the 3.4 micron feature, as well the CH$_2$/CH$_3$ ratio, the H/C value and the physical appearance at mesoscale (i.e. thin films or ‘fluffy’ aggregates), show a variability that is influenced by synthesis method, the pulsing regime and the experimental parameters of a specific technique. Then, the spectroscopic features of dust analogs are compared with observational data from sources presenting a high column density of sp$^3$ hybridized carbon atoms (Sgr A*, IRAS 08572+3915, IRAS 19254-7245, NGC 1068 and NGC 5506)

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics
Quantifying the aliphatic hydrocarbon content of interstellar dust using multiple laboratory spectroscopies

Schmidt, T. W.¹, Gunay, B.², Burton, M. G.³, Rawal, A.⁴

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In the interstellar medium, the cosmic carbon abundance includes carbon in both the gas and solid phases. However, there is a discrepancy between the amount of carbon identified in the interstellar medium and that proposed by astrophysical models.[1] It has been estimated that a considerable amount of carbon may be found in the interstellar dust. The mid-IR spectrum of the interstellar medium contains both aromatic and aliphatic hydrocarbon absorption bands, which are generally attributed to carbonaceous dust. The aliphatic component of the carbonaceous dust is of particular interest because it produces a significant 3.4 µm absorption feature when viewed against a background radiation source. The optical depth of the 3.4 µm absorption feature is related to the number of aliphatic carbon C-H bonds along the line of sight. It is possible to estimate the column density of carbon locked up in the aliphatic hydrocarbon component of interstellar dust from quantitative analysis of the 3.4 µm interstellar absorption feature providing that the absorption coefficient of aliphatic hydrocarbons incorporated in the interstellar dust is known. We produced interstellar dust analogues by mimicking the interstellar/circumstellar conditions in the laboratory.[2,3] The resultant spectra of these dust analogues closely match those from astronomical observations. The measurements of the absorption coefficient of aliphatic hydrocarbons incorporated in the analogues were carried out by a procedure which combined FTIR and 13C NMR spectroscopies. The absorption coefficients obtained for both interstellar analogues were found to be in close agreement (4.76(8) × 10⁻¹⁸ cm group⁻¹ and 4.69(14) × 10⁻¹⁸ cm group⁻¹, less than half those obtained using small aliphatic molecules. The results thus obtained permit direct calibration of the astronomical observations, providing rigorous estimates of the amount of aliphatic carbon in the ISM.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

Research Area(s)
• Experimental laboratory astrophysics

Back to Schedule
Asymptotic Giant Branch (AGB) stars contribute a major part to the global dust budget in galaxies. Owing to their refractory nature alumina (Al$_2$O$_3$) is a promising first condensate emerging in the atmospheres of oxygen-rich AGB stars [1]. The emergence of a specific condensate is predicted by the condensation sequence [2] and depends on the thermal stability of the solid, the gas density and its composition. The evaluation of the condensates is based on macroscopic bulk properties. The growth and size distribution of dust grains is commonly described by Classical Nucleation Theory (CNT). We question the applicability of CNT in an expanding circumstellar envelope as CNT presumes thermodynamic equilibrium and requires seed nuclei on which material can condense. Nano-sized molecular clusters differ significantly from crystalline bulk analogues [3]. Quantum effects of the clusters lead to non-crystalline structures, whose characteristics (energy, geometry) differ substantially, compared to the bulk material. A kinetic quantum-chemical treatment involving various transition states describes dust nucleation most accurately. However, such a treatment is prohibitive for systems with more than 10 atoms. Therefore, we chose a hybrid bottom-up approach: Molecules and clusters up to 10 atoms are treated quantum-chemically, intermediate sized clusters (10-50 atoms) are calculated using hybrid density functionals and the growth of larger sized particles is described classically. The treatment of the intermediate size regime uses the free energies of the lowest energy configurations that are significantly lower than the corresponding CNT-derived bulk cuts. We present efficient chemical-kinetic pathways for the formation of the monomer and the dimer and we show the most stable configurations of (Al$_2$O$_3$)$_n$ clusters with $n$=1-10, including “fingerprint infrared spectra that are compared to laboratory experiments and observations.”

References

Scientific Theme(s)
• Stars, stellar populations, and stellar explosions

Research Area(s)
• Theoretical calculations or simulations in laboratory astrophysics

Back to Schedule
Physical parameter estimation with MCMC from X-ray observations

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\textsuperscript{1}National Astronomical Observatories, Chinese Academy of Sciences, China, \textsuperscript{2}National Astronomical Observatories, CAS, \textsuperscript{3}National Astronomical Observatories, CAS

X-ray spectra from astronomical objects are important tools to infer their structure and physical parameters, such as density, temperature and velocity. We introduce the Bayesian approach to fit the observed X-ray spectra \cite{Zhang2018} which is useful to gather information accurately from observation and hence to provide reliable approaches for the line diagnostic, modeling, and experimental comparison \cite{Wang2017}. Its main advantages include (i) all model-based parameters are set to be free instead of artificially fixing some of the parameters during the data-model fitting; (ii) the contributions from weak lines are considered; (iii) backgrounds are treated as a correction to the observation errors; and (iv) the confidence interval of each parameter is given.

References

[1] Zhang et al., 2018, HPLSE, Vol. 6, 137

Scientific Theme(s)
- Stars, stellar populations, and stellar explosions

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

Back to Schedule
AGB outflows as tests of chemical kinetic and radiative transfer models

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The outflows of asymptotic giant branch (AGB) stars are rich astrochemical laboratories. We use chemical kinetic models to study their large molecular diversity. These models are continuously improved upon, however, several questions still remain. We will discuss the limitations of current chemical models, reaction networks and molecular data.

One of these questions are the specific locations of the molecular shells of cyanopolyynes HC\textsubscript{2n+1}N and hydrocarbon radicals C\textsubscript{n}H within the outflow of the C-rich AGB star IRC+10216, the most studied AGB star. The HC\textsubscript{2n+1}N show a radial sequence, with longer C-chains further from the star, as expected from a bottom-up formation synthesis scenario. However, the C\textsubscript{n}H are cospatial \cite{1}. Unlike most models, the outflow is not smooth but has clumpy overdense shells. Our new model takes into account the effect of the clumps’ overdensity as well as their effect on the radiation field \cite{2}.

We find that the reaction network is not complete, with a recent addition \cite{3} influencing the results greatly, while other so far unknown pathways are still possible. Moreover, reaction rates forming longer C-chains have not been measured. Radiative transfer modelling is necessary to compare our results to observations and requires accurate molecular data for the excitation calculations, which is only available for HC\textsubscript{3}N. Our results show that the locations of the molecular shells are sensitive to the molecular data, which are currently approximated from other measurements, and hence form a source of large uncertainty. The puzzle of the chemistry of the outflow of IRC+10216, or indeed of all AGB stars, can only be solved through a collaborative effort of the entire laboratory astrophysics community.

References

Scientific Theme(s)
- Stars, stellar populations, and stellar explosions

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

Back to Schedule
Exploding and non-exploding core-collapse supernova models and the multi-messenger predictions (R)

Kotake, K.\textsuperscript{1}

\textsuperscript{1}Fukuoka University, Japan

How massive stars end their lives has been a time-honored riddle of astrophysics over the decades. Based on multi-dimensional radiation-hydrodynamics simulations, I report several new results of core-collapse supernova models, leading to a neutron-star and black-hole formation in the centre. I will also discuss how one could extract the information of the supernova engines by deciphering the multi-messenger observables including neutrino and gravitational-wave emission.

References

Scientific Theme(s)
- Stars, stellar populations, and stellar explosions, Reaching beyond our galaxy: from extra galactic chemistry to dark matter

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

Back to Schedule
Density diagnostics of photoionized outflows in active galactic nuclei

Mao, J.1, Kaastra, J. S.2, Mehdipour, M.3, Raassen, A. J.4, Gu, L.5, Miller, J. M.6

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Photoionized outflows in Active Galactic Nuclei are thought to influence their nuclear and local galactic environment. However, the distance of outflows with respect to the black hole is poorly constrained, which limits our understanding of the kinetic power by the outflows. Therefore, the impact of AGN outflows on their host galaxies is uncertain. Given the density of the outflows, their distance can be immediately obtained by the definition of the ionization parameter. Here we carry out a theoretical study of density diagnostics of AGN outflows using absorption lines from metastable levels in Be-like to F-like ions. With the new self-consistent photoionization model (PION) in the SPEX code, we are able to calculate ground and metastable level populations. This enable us to determine under what physical conditions these levels are significantly populated. We then identify characteristic transitions from these metastable levels in the X-ray band. Firm detections of absorption lines from such metastable levels are challenging for current grating instruments. The next generation of spectrometers will certainly identify the presence/absence of these density-sensitive absorption lines, thus tightly constraining the location and the kinetic power of AGN outflows.

References

Scientific Theme(s)
- Reaching beyond our galaxy: from extra galactic chemistry to dark matter

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

Back to Schedule
The Future of Laboratory Astrophysics

Salama, F.¹, Fillion, J. H.², Fraser, H.³, Hudgins, D.⁴, Linnartz, H.⁵, Mason, N.⁶, Mennella, V.⁷, Savin, D.⁸, Shalabiea, O.⁹, Wang, F.¹⁰, Watanabe, N.¹¹

¹IAUS 350, ²PCMI, ³IAU Comm B5, ⁴NASA SDM, ⁵NL, ⁶Europlanet, ⁷ECLA, ⁸LAD, ⁹Africa/ME, ¹⁰China, ¹¹Japan

Modern multidetector/multimessenger astronomy spends hundreds of millions of pounds on international large-scale facilities and missions to advance our observations of the universe. Ground-based and space-based observations, missions, and solar system exploration all rely on fundamental data to enable us to reap the largest possible scientific returns from this "astronomical" efforts. Laboratory Astrophysics underpins this data need, serving a huge international community, whilst researchers in this field are pushing boundaries across physics, chemistry, geology, and biology research in their own right. But often laboratory astrophysics falls through the cracks - of funding, appropriate referencing, adequate databasing (with validation and metadata) and benchmarking.

The context for this discussion will be to ask how can we utilise a global approach to encourage all space agencies and funding bodies to recognise the needs of astronomy and planetary science for fundamental laboratory data? How can we transfer best practice from one international region or country to another, and how can we work together as a global community to have a consistent, concerted approach world-wide to raise the profile, financing, and recognition of our field? And how can laboratory astrophysics be developed beyond the "usual" national "big-hitters", promoting the STEM agenda world-wide and contributing to the development agenda pursued by many nations and the IAU.

A panel of international experts and program managers will present the various successful approaches to Laboratory Astrophysics across the globe and confront the challenges they face, as well as addressing questions* from the audience. We will take an honest approach to the issues faced by our field, and look for a "next steps" approach. In particular, we will consider how IAU Commission B5, recently founded to promote Laboratory Astrophysics, can best support and enhance a strong synergy between all international partners that will benefit the growth and the strengthening of the Laboratory Astrophysics community.

*Question sheets will be available Sunday - Wednesday for participants to submit questions for the expert panel - comments on the day are welcome and the outcomes of the discussion will formulate the future direction, working groups, and activities of IAU Commission B5 (Laboratory Astrophysics) and help to inform the represented organisations to their strategies "back home".

Back to Schedule
The ExoMol project: molecular line lists for the opacity of exoplanets and other hot atmospheres (R)

Tennyson, J.¹

¹University College London, United Kingdom

The ExoMol project (Tennyson and Yurchenko 2012) aims to provide molecular line lists for exoplanets and other atmosphere with a particular emphasis on those atmospheres which are significantly hotter than the Earth’s. ExoMol now provides line lists for about 40 molecules including, in most cases, isotopologues; see the review by Tennyson and Yurchenko (2017). This includes key molecules such as water, methane and ammonia plus a range of diatomics (including electronic transitions) and hydrocarbons. New line lists include those for TiO and acetylene. The ExoMol database (www.exomol.com) underwent a major reformat an upgrade (see Tennyson et al. 2016) and now provides information on a variety of topics including, of course, line lists, cross sections (generated from the same line lists), lifetimes and Lande g-factors. A new flexible code ExoCross can rapidly generate cross sections even from huge line lists. ExoCross also allows facile conversion between ExoMol and HITRAN formats. The ExoMol data is now being extended to consider molecules likely to be present in the atmospheres of hot rocky super-Earths ("lava planets").

References

Scientific Theme(s)
- Solar System formation and the pre-solar nebula

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

Back to Schedule
Using cold plasma to investigate the mechanisms involved in cosmic dust formation: role of C/O ratio and metals

Bérard, R.¹, Makasheva, K.², Sabbah, H.³, Demyk, K.⁴, Joblin, C.⁵

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The processes related to nucleation, growth and processing of dust particles are of interest both in laboratory cold plasma and in astrochemistry. We are willing to develop a gas phase laboratory experiment to explore chemical pathways of dust formation involving elements largely present in the envelope of evolved stars, namely hydrogen, carbon, oxygen, silicon, as well as metals such as magnesium or iron. Dust formation has been observed in an asymmetric radio-frequency argon discharge with pulsed injection of hexamethyldisiloxane (HMDSO, C₆H₁₈OSi₂) and sputtering of a metal target [1]. We specifically investigate here the impact of key parameters on the mechanisms involved in dust formation. These include the C/O ratio, by injecting additional O², and the presence of metal atoms. Different levels of investigation are presented. Dust formation in the plasma gas phase is followed in-situ through optical emission spectroscopy. Dust particles are collected for ex-situ analyses. Using the laboratory astrophysics setups ESPOIRS [2] and AROMA [3], we investigate the chemical and molecular compositions by infrared spectroscopy and mass spectrometry, respectively. The different diagnostics provide information on the chemical pathways involved in dust formation. The amount of injected oxygen determines a threshold point after which no dust is formed anymore, implying inhibition of dust seeds by oxygen. When the metal atoms are sputtered inside the plasma gas phase, the chemical and molecular composition radically change. We show that new chemical bonds are formed as well as a variety of molecular carbonaceous species, including both aromatics and aliphatics. We demonstrate the relevance of our approach to tackle the formation of cosmic dust. Acknowledgement We acknowledge support from the European Research Council under the European Union’s Seventh Framework Programme ERC-2013-SyG, Grant Agreement n. 610256 NANOCOSMOS.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

Research Area(s)
• Experimental laboratory astrophysics

Back to Schedule
Non-LTE spectroscopy for Galactic Archaeology (I)

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Stellar abundances are used to understand the formation and evolution not only of stars and stellar populations, but large spectroscopic surveys now probe far in space and time through Galactic Archaeology. Extracting information from stellar spectra in terms of stellar properties requires detailed modelling of the surface layers and of how the stellar spectrum is produced from a myriad of atomic and plasma processes therein. The basic premises of quantitative stellar spectroscopy have largely remained unchanged for many decades, including the crucial approximations that stellar atmospheres are one-dimensional, hydrostatic and constant in time and that all atomic and molecular level populations are in perfect equilibrium with the local temperature (local thermodynamic equilibrium, LTE). The advent of 3D non-LTE abundance analysis finally promises to place stellar abundance analysis on a firm footing. However, the development critically depends on the availability of atomic data for the relevant species, in particular complete sets of radiative and collisional transition probabilities for neutral and singly ionised atoms. I will review recent progress made in conducting non-LTE spectroscopy with accurate model atoms for large stellar surveys and highlight outstanding issues.

Scientific Theme(s)
- Stars, stellar populations, and stellar explosions

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

Back to Schedule
Quantitative Atomic Spectroscopy, a Review of Progress in the Optical-UV Region and Future Opportunities using X-Ray FELs

Lawler, J. E.\textsuperscript{1}, Sneden, C.\textsuperscript{2}, Den Hartog, E. A.\textsuperscript{3}, Cowan, J. J.\textsuperscript{4}

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The development of broadly tunable organic dye lasers and a simple technique for making atomic and ionic beams of all elements has established a reliable absolute scale for atomic transition probabilities of lines in the optical to near UV regions. The laboratory astrophysics program at the University of Wisconsin (UW), which emphasized the rare earth neutron-capture elements and more recently the Fe-group elements, concentrates on neutral and singly-ionized species transitions that are observable in astronomical spectra of cool stars. The UW program is one of several productive efforts on atomic transition probabilities. These programs generally use time-resolved laser-induced-fluorescence (TR-LIF) to accurately measure total decay rates and data from high resolution Fourier transform spectrometers (FTSs) to determine emission branching fractions. Astrophysical applications of the UW laboratory results will also be described. In the not too distant future X-Ray Free Electron Lasers (FELs) with injection seeding will become available. Although the radiative lifetimes many or most important X-Ray transitions will be too short for TR-LIF measurements, level width measurements can provide the same information as a decay curve. Existing X-Ray FELs operate as Self Amplified Spontaneous Emission or SASE lasers. Their output has near perfect transverse coherence but lacks the necessary longitudinal coherence for gas phase experiments. The implementation of injection seeding at the Linear Coherent Light Source or LCLS facility in the USA and at other facilities in Europe and Asia will provide the needed frequency control for gas phase experiments with narrow resonances.

This work is primarily Experimental related to: Stars, stellar populations, and stellar explosions or Star formation and the cosmic matter cycle in the near universe

Scientific Theme(s)
- Stars, stellar populations, and stellar explosions

Research Area(s)
- Experimental laboratory astrophysics

Back to Schedule
Determining the origin of the elements is a fundamental quest in astronomy. Supernovae are believed to be important production sites for elements ranging from carbon to nickel, and beyond. I describe state-of-the-art methods to model and interpret spectra of supernovae, with the goal to determine their nucleosynthesis yields and ejecta structure, which in turn reveals their stellar origins and explosion physics. I emphasize the crucial role of various types of atomic physics in this quest, illustrating the important co-development of atomic data calculations and supernova spectral calculations. I give a brief description of how the kilonova/neutron star merger era now allows this kind of work to be extended into determining the origin of the the r-process elements.

**Scientific Theme(s)**
- Stars, stellar populations, and stellar explosions

**Research Area(s)**
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

*Back to Schedule*
Jinping Underground experiment for Nuclear Astrophysics (JUNA) [1] will take the advantage of the ultra-low background of China Jinping Laboratory (CJPL) (rock depth 2400 m) and high current accelerator based on an ECR source and a highly sensitive detector to directly study a number of crucial reactions occurring at their relevant stellar energies during the evolution of hydrostatic stars. In its first phase, JUNA aims at the direct measurements of \( ^{25}\text{Mg}(p,\gamma)^{26}\text{Al} \), \( ^{19}\text{F}(p,\alpha)^{16}\text{O} \) [2], \( ^{13}\text{C}(\alpha,n)^{16}\text{O} \) and \( ^{12}\text{C}(\alpha,\gamma)^{16}\text{O} \) reactions near Gamow energy.

The experimental setup, which includes an accelerator system (400 kV with ECR source) with high stability and high intensity (10 emA for proton (commissioned), 2.5 emA for \( ^4\text{He}^{2+} \) (under development)), a detector system, and a shielding material with low background, will be established during the above research. The high efficiency detector system is composed of gamma (HPGe and BGO, all commissioned), neutron \( ^3\text{He} \) and liquid scintillator, commissioned) and charged particle arrays. The high-power target is under development.

The main parts of accelerator system and detector arrays are ready and will be tested on ground and installed underground in 2019. Some test experiment on base level, such as \( ^{19}\text{F}(p,\alpha)^{16}\text{O} \), as well as detector background measurement in CJPL, were performed in ground and underground bases. One of four experiments will be started in 2019 and the first batch of four experimental results will be released in 2021. In this talk, the current progress of JUNA will be given.

References

Scientific Theme(s)
- Stars, stellar populations, and stellar explosions

Research Area(s)
- Experimental laboratory astrophysics
Kilonovae and the lanthanides: an atomic theorists perspective

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Unlike the first five gravitational wave (GW) detections, the discovery of the GW170817 signal on Aug 17 2017 [1] was also confirmed by an electromagnetic counterpart - a gamma-ray burst (GRB 170817A) just 1.7 seconds after the event. This triggered an intense broadband observation campaign of about 70 observatories, eventually leading to the discovery of a bright optical transient (AT 2017gfo in NGC 4993 at 40 Mpc) about 11 hours after the GW event. While the first ultraviolet observations during the following days showed a blue transient that faded within 48 hours, the optical and infrared spectral regions revealed a significant reddening over 10 days, pointing towards a kilonova fuelled by the radioactive decay of r-process elements formed in the ejecta [1, 2]. This unprecedented joint gravitational and electromagnetic observation marked a significant breakthrough in multi-messenger astronomy, opening up for a much deeper picture of events like these.

The seemingly high abundance of r-process elements in the ejecta introduces new demands on fundamental atomic data as input to the modelling, and in particular of largely uncharted territories in the periodic table such as the lanthanides (Z = 57 to 71). These elements are however not uncharted without reasons - their complex electronic structure together with the fundamental relativistic nature of heavy elements, make them arguably the most challenging atomic species in the periodic table (together with the actinides).

In this contribution I present new theoretical results for all neutral and singly ionised lanthanide species determined using the multiconfigurational Dirac-Hartree-Fock method as implemented in the GRASP2018 atomic structure code [3], I briefly discuss the impact on kilonova models as well as why an adequate description of the fundamental properties of these elements remains a challenge to state-of-the-art atomic theory.

References

Scientific Theme(s)
- Reaching beyond our galaxy: from extra galactic chemistry to dark matter

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

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Generation of photoionised plasmas in the laboratory: analogues to astrophysical sources


1Queen’s University Belfast, United Kingdom, 2Queen’s University Belfast, 3Queen’s University Belfast, 4Queen’s University Belfast, 5Queen’s University Belfast, 6Queen’s University Belfast, 7Imperial College London, 8Imperial College London, 9University of Kentucky, 10Chinese Academy of Sciences

Previously, we have successfully implemented, on the VULCAN laser at the Central Laser Facility, a theoretically-proposed technique [1] for creating a photoionised plasma in the laboratory using X-ray line radiation rather than the usual quasi-blackbody radiation source. Using X-rays generated from a tin foil to irradiate an argon gas target, we demonstrated that line radiation can efficiently be used to mimic the effect of a higher radiation temperature on the photoionisation of the target gas, with values in excess of 1 keV being achieved [2]. In addition, the experiment reached photoionisation parameters $\xi = 4\pi F/Ne$ (where $F$ is the radiation flux and $Ne$ the electron density) close to 50 erg cm$^{-2}$ s$^{-1}$, higher than those obtained in earlier work (e.g. [3]). We have compared argon emission-line spectra in the 4.15 - 4.25 Angstrom wavelength range from our VULCAN experiments with the predictions of various modelling codes, including the Cloudy code employed by astrophysicists. Based on our experiences during the earlier VULCAN campaign, plus work on tin foils undertaken on the SG-II laser at the National Laboratory on High Power Laser and Physics in Shanghai in late 2017, we have designed a new experiment to be undertaken on VULCAN later in 2019. This incorporates major improvements over our previous research, such as the use of double-sided irradiation (producing a more uniform X-ray flux distribution), a diode array system to measure the soft X-ray flux (so its contribution can be included in our modelling), and an improved Thomson scattering diagnostic. Our experiment should generate the closest laboratory analogue to the extreme photoionised plasmas found in accretion-powered astronomical sources.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

Back to Schedule
Laboratory plasmas for high-energy Astrophysics

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Electron Cyclotron Resonance (ECR) laboratory plasmas represent a useful test-bench for interdisciplinary studies in Plasma Physics, Astrophysics and Nuclear Physics. These high-density ($n_e \sim 10^{10} - 10^{13}$ cm$^{-3}$) and high-temperature ($T_e \sim 0.1 - 100$ keV) plasmas are created in magnetic traps, where a gas injected in a chamber is highly ionized by microwaves and confined by magnetic fields [1]. From the astrophysical point of view, many cosmic environments are expected to be reproduced in these devices. Then the analysis of the ECR plasma emission, ranging from the X-rays to the near infrared, gives the possibility to test the atomic processes and data used for the diagnostic of high-energy astrophysical plasmas [2]. We present our instrumental set-up for a magnetic trap and initial results/plans for 3D high-resolution ($R = 164000$) spectropolarimetry to observe the plasma emission in the visible range. We also present the results of an application devoted to measure the Landé g-factors, fundamental atomic parameters to recover the astrophysical magnetic fields [3]).

References

Scientific Theme(s)
- Stars, stellar populations, and stellar explosions

Research Area(s)
- Experimental laboratory astrophysics

Back to Schedule
The Joint Institute for Nuclear Astrophysics Center for the Evolution of the Elements is to connect research in experimental nuclear physics, observational astronomy, theory, and computational modeling to address major open questions related to the origin of the elements and the properties of dense matter in neutron stars. Rare isotopes play a key role in this endeavor. They govern the creation of the elements in extreme stages of stellar evolution, supernova explosions, and neutron star phenomena such as mergers, X-ray bursts, and hot crusts. While these isotopes only exist for fractions of seconds, their properties shape the resulting cosmic distribution of elements and the astronomical observables including spectra, neutrinos, and gravitational waves. The long-standing challenge in nuclear astrophysics of the production of the relevant isotopes in the laboratory is now overcome with a new generation of rare isotope accelerator facilities now coming online. One example is the FRIB facility under construction at Michigan State University. These new capabilities in nuclear physics coincide with advances in astronomy directly related to the cosmic sites where these isotopes are created, in particular in time domain and gravitational wave astronomy. I will discuss the importance of rare isotope physics in interpreting multi-messenger observations and how advances in nuclear physics and astronomy when combined promise to lead us towards a comprehensive theory of the origin of the elements and neutron stars.

Scientific Theme(s)
- Reaching beyond our galaxy: from extra galactic chemistry to dark matter

Research Area(s)
- Experimental laboratory astrophysics
The Sun: our own backyard plasma laboratory (R)

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The Sun’s atmosphere increases in temperature from 6000 degrees at the surface to over a million degrees at heights of a few thousand kilometres. This surprising temperature increase is still an active area of scientific study, but is generally thought to be driven by the dynamics of the Sun’s strong magnetic field.

The combination of a 2-to-3 order of magnitude temperature range combined with a low plasma density makes the solar atmosphere perhaps the best natural laboratory for the study of ionized atoms. Charge states from neutral to fully-ionized are found for most astrophysically important elements. Atomic transitions at ultraviolet and X-ray wavelength regions generally show no optical depth effects, and the lines are not subject to the interstellar absorption that affects astronomical sources.

In this talk I will summarize how solar spectroscopists and atomic physicists have worked together to improve atomic models and develop a new understanding of the solar atmosphere. A particular focus will be on the CHIANTI atomic database [1] that I helped develop as a graduate student in Cambridge in the 90’s. Areas where new atomic data are needed will be highlighted, and I will look forward to future solar observing facilities - both on the ground and in space - that will provide new challenges.

References

Scientific Theme(s)
• Stars, stellar populations, and stellar explosions

Research Area(s)
• Observations showing use of laboratory astrophysics in the interpretation/understanding of data

Back to Schedule
Benchmarked Atomic Data for Astrophysics

Del Zanna, G.¹

¹University of Cambridge, United Kingdom

I briefly review the recent calculations of atomic data for ions of astrophysical interest which have been carried out by the Atomic Astrophysics group in Cambridge. The calculations have been benchmarked against high-resolution laboratory and astrophysical spectra. A framework for assessing uncertainties in atomic data has also been developed. Long-standing discrepancies in predicted spectral line intensities have been resolved, and a significant number of levels in coronal ions have finally been identified, improving the modelling of the extreme-ultraviolet and soft X-ray spectral regions. Recent improvements based on collisional-radiative modelling are presented. They are relevant for the modelling of satellite lines in the X-rays and for solving the long-standing problems in the chromosphere-corona transition in stellar atmospheres.

Scientific Theme(s)
- Stars, stellar populations, and stellar explosions

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

Back to Schedule
High-precision spectroscopy of large stellar samples plays a crucial role for several topical issues in astrophysics. Examples include studying the chemical evolution of the Milky Way Galaxy, tracing the origin of chemical elements, and characterizing planetary host stars. Data are accumulating from instruments that obtain high-quality spectra of stars in the ultraviolet, optical and infrared wavelength regions on a routine basis. The interpretation of these spectra is often based on synthetic stellar spectra, either calculated on the fly or taken from a spectral library. One of the most important ingredients for these calculations is a set of high-quality transition data for numerous species, in particular neutral and singly ionized atoms. We rely heavily on the continuous activities of laboratory astrophysics groups that produce and improve the relevant experimental and theoretical atomic data. I will give examples for the accuracy and precision with which the chemical composition of stars in different Galactic populations can be determined, the impact of recent advances in laboratory astrophysics, as well as future needs.

Scientific Theme(s)
- Stars, stellar populations, and stellar explosions

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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Abstracts of Posters
Reduction of C=O functional group through H addition reactions at 10 K: The cases of glyoxal, propanal and methylformate

Krim, L.1, Leroux, K.2, Guillemin, J.3, Jonusas, M.4
1Sorbonne University, France, 2Sorbonne university, 3Ecole Nationale Supérieure de Chimie de Rennes, 4Sorbonne university

Poster number: 1

Many astrophysical models propose that the formation of Complex Organic Molecules (COMs) detected in the ISM are due to reactions involving atoms (mainly H atoms, but also N, C and O) reacting with different astrochemical relevant species on the icy interstellar grains at temperatures around 10 K. However many of the reaction mechanisms proposed in the astrophysical models have never been investigated experimentally and need to be studied and quantified in laboratory. In fact, all the laboratory studies carried out up to now have been focused on the H-addition reaction on simple species such as CO, NO and H2CO. From these a few laboratory studies involving only simple precursors, astrophysical models have generalized the H-addition processing to all astrochemical relevant unsaturated organic species in order to establish links between unsaturated (usually detected in dense molecular clouds) and saturated COMs (usually detected in hot cores and corinos). However, such a generalization is not true since we have recently shown that the hydrogenation reactions of substituted aldehydes such as propanal, propenal and propynal do not lead to the formation of the corresponding alcohols under ISM conditions. In the present work we propose a comparative experimental study of H2CO + H, HCOHCO + H, CH3CH2CHO + H and CH3OCHO + H solid state reactions at 10 K under interstellar conditions in order to characterize the main reaction pathways involved into the hydrogenation processing of CHO functional group. Our experimental results prove that while the simplest aldehyde, formaldehyde, is easily reduced into methanol, glyoxal, propanal and methylformate behave differently under H-bombardments but they cannot be a source of alcohols larger than methanol. Consequently the presence of aldehydes and saturated alcohols, very often not in the same interstellar regions, does not imply that alcohol species are necessarily produced on icy grains via aldehydes H-addition reactions.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

Research Area(s)
• Experimental laboratory astrophysics

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The presence of interstellar polycyclic aromatic hydrocarbons (PAHs) is inferred from the mid-infrared (IR) emission bands that are observed at 3.3, 6.2, 7.7, 8.6 and 11.2 µm. This IR radiation is emitted as the PAHs cascade down to the ground state after they have been excited by interstellar (vacuum) ultraviolet radiation. PAHs have been observed towards a large number of galactic and extragalactic sources and it has been derived that PAHs constitute up to 15% of the total cosmic carbon budget.

Energetic processing of interstellar polyaromatics may result in ionization and/or dissociation. It has been hypothesized that this chemical evolution is reflected in subtle changes in the observed mid-IR emission bands. Observational and laboratory data suggest that dissociation of large interstellar polyaromatics eventually results in fullerene formation. The underlying chemical processes involved in the dissociation of aromatics are not yet understood.

Our group characterizes the dissociation of polyaromatics by means of vacuum ultraviolet synchrotron radiation and mid-infrared free electron laser radiation. By combining these techniques with quantum chemical computations we obtain insight into the isomerization and dissociation at a molecular level of detail. [1,2,3] I will review our most recent results and will emphasize their importance in light of astronomical observations.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics
Infrared spectra of complex organic molecules in astronomically relevant ice matrices

Terwisscha van Scheltinga, J.1, Ligterink, N. F.2, Boogert, A. C.3, Dishoeck, E. F.4, Linnartz, H.5

1Leiden Observatory, Netherlands, 2University of Bern, 3University of Hawaii, 4Leiden Observatory, 5Leiden Observatory

Poster number: 3

The number of identified complex organic molecules, COMs, in inter- and circumstellar gas phase environments is steadily increasing. Recent laboratory studies show that many such species form on icy dust grains. At present only smaller molecular species have been directly identified in space in the solid state. Accurate spectroscopic laboratory data of frozen COMs, embedded in ice matrices containing ingredients related to their formation scheme, are still largely lacking. This work provides infrared reference spectra of acetaldehyde (CH3CHO), ethanol (CH3CH2OH) and dimethyl ether (CH3OCH3) recorded in different ice environments and for astronomically relevant temperatures, as needed to guide or interpret astronomical observations, specifically for upcoming James Webb Space Telescope observations. Fourier transform transmission spectroscopy (500-4000 cm⁻¹ / 20-2.5 μm, 1.0 cm⁻¹ resolution) is used to investigate solid acetaldehyde, ethanol and dimethyl ether, pure or mixed with water, CO, methanol or CO:methanol. These are deposited on a cryogenically cooled infrared transmissive window at 15 K. A heating ramp is applied, during which IR spectra are recorded, until all ice constituents are thermally desorbed. We present a large number of reference spectra that can be compared with astronomical data. Accurate band positions and band widths are provided for the studied ice mixtures and temperatures. Special efforts have been put in those bands of each molecule that are best suited for identification. For acetaldehyde the 7.427 and 5.803 μm bands are recommended, for ethanol the 11.36 and 7.240 μm bands are good candidates and for dimethyl ether bands at 9.141 and 8.011 μm can be used. All spectra are publicly available in the Leiden Database for Ice.

Scientific Theme(s)
• Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
• Experimental laboratory astrophysics

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An updated constraint on variations of the fine-structure constant using wavelengths of Fe II absorption line multiplets

Duc Thong, L.¹

¹Institute for Computational Science, Vietnam

Poster number: 4

A new stringent limit relating to the variation of the fine-structure constant ($\alpha = e^2/(4\pi\epsilon_0hc)$) has been extracted from Ritz wavelengths of 27 quasi stellar object (QSO) absorption spectra lines of Fe II. The calculation was combined with laboratory wavelengths and QSO spectra to obtain the result $\delta\alpha/\alpha = (0.027\pm0.832) \times 10^{-6}$. This result suggests how dedicated astrophysical estimations can improve these limits in the future and can also constrain space-time variations.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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Infrared spectra of protonated and hydrogenated corannulene (C$_{20}$H$_{10}$) and sumanene (C$_{21}$H$_{12}$) using matrix isolation in solid para-Hydrogen - Implications to the UIR bands

Sundararajan, P.$^{1}$, Tsuge, M.$^{2}$, Baba, M.$^{3}$, Sakurai, H.$^{4}$, Lee, Y.$^{5}$

$^{1}$National Chiao Tung University, Taiwan, $^{2}$Institute of Low Temperature Science, Hokkaido University, $^{3}$Division of Chemistry, Kyoto University, $^{4}$Department of Applied Chemistry, Osaka University, $^{5}$National Chiao Tung University

Poster number: 5

PAHs gained attention in the interstellar chemistry as they are attributed to be the potential emitters of the UIR emission bands. However, till date, no single PAH could be positively assigned to the UIR band. Since proton sources such as H$^+$ and H$_3^+$ are abundant in space, the proton transfer reactions to produce protonated species are likely to occur. Because the proton affinities of PAH are high, protonated PAH are postulated to be present in the ISM [2]. Corannulene (C$_{20}$H$_{10}$) and sumanene (C$_{21}$H$_{12}$) are fragments of C$_{60}$ and have a bowl-like structure. They were proposed to be intermediates in the formation of fullerenes in space [1].

Our recent technique of using electron bombardment on a p-H$_2$ matrix to produce protonated/hydrogenated species cleanly and efficiently can provide direct IR absorption spectra covering a wide spectral range with narrow lines [3]. The experiments were carried out with a closed-cycle helium refrigerator (3.3 K), which was coupled with a FTIR that covers the mid-IR region. H + C$_{20}$H$_{10}$ and their neutral counterparts were produced upon electron bombardment of the matrix during deposition of C$_{20}$H$_{10}$ mixed in p-H$_2$ over a period of 10 h. The matrix was then maintained in darkness. The protonated species became diminished after maintaining the matrix in darkness, whereas its neutral counterparts were produced. Infrared absorption features, grouped according to the behavior after maintaining the matrix in darkness and upon secondary photolysis were assigned to several conformers of protonated isomers of C$_{20}$H$_{10}$ by comparison with the predicted IR spectra. Two protonated species of C$_{20}$H$_{10}$ (hub and rim) [Sundararajan, et al. 2018, ACS Earth Space Chem.] and their respective neutral counterparts are unambiguously identified. Similarly, sumanene was also investigated using this technique to produce protonated and hydrogenated C$_{21}$H$_{12}$. The implications of the IR spectra of these molecules on the UIR bands will be discussed in this presentation.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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Non-statistical fragmentation of C\textsubscript{60} and the formation of endohedral defect fullerenes

Stockett, M. H.\textsuperscript{1}, Wolf, M.\textsuperscript{2}, Gatchell, M.\textsuperscript{3}, Schmidt, H. T.\textsuperscript{4}, Zettergren, H.\textsuperscript{5}, Cederquist, H.\textsuperscript{6}

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Poster number: 6

The observation of fullerenes in various astronomical environments, and the identification of C\textsuperscript{+}\textsubscript{60} as the carrier of several Diffuse Interstellar Bands, has led to a surge in interest in the formation and destruction pathways of fullerenes under different astrophysical conditions. Non-statistical fragmentation (\textit{i.e.} prompt single-atom knockout) of fullerenes and other large molecules following collisions with energetic H and He atoms in supernova shocks is considered a key destruction mechanism [1].

We have investigated this process through laboratory experiments and classical Molecular Dynamics (MD) simulations of C\textsuperscript{−}\textsubscript{60} + He collisions at center-of-mass energies of 20–80 eV. As the electron affinity of C\textsubscript{60} is much lower than any of its dissociation energies, collisions depositing enough energy to induce statistical unimolecular dissociation most likely lead to electron loss and thus do not contribute to the measured negative ion product mass spectrum, eliminating the major source of background.

Non-statistical fragmentation is observed directly by detecting C\textsuperscript{−}\textsubscript{59}. We observe for the first time the endohedral defect fullerene complex He@C\textsuperscript{−}\textsubscript{59}. Secondary decay products of these ions, C\textsuperscript{−}\textsubscript{58} and He@C\textsuperscript{−}\textsubscript{58}, are also observed. We measure the threshold center-of-mass energy for knocking out a single carbon atom from C\textsubscript{60} in collisions with He. Combining this with our MD simulations, we determine a semi-empirical value for the (projectile-independent) threshold displacement energy, the minimum energy needed to remove a single carbon atom from the C\textsubscript{60} cage [2]. Our value, 24.1±0.5 eV, is much higher than generally assumed previously for fullerenes (around 15 eV), and is similar to that determined for graphene and Polycyclic Aromatic Hydrocarbons [3].

References


Scientific Theme(s)

• Star formation and the cosmic matter cycle in the near universe

Research Area(s)

• Experimental laboratory astrophysics

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Photochemistry vs. Radiation Chemistry of Cosmic Ice Analogs

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Poster number: 7

While gas-phase reactions and surface reactions on bare carbonaceous or silicaceous dust grains contribute to cosmic chemistry, energetic processing via photochemistry and radiation chemistry of cosmic ices is thought to be the dominant mechanism for the cosmic synthesis of prebiotic molecules. Radiation chemistry is defined as the ‘study of the chemical changes produced by the absorption of radiation of sufficiently high energy to produce ionization’. Ionizing radiation in cosmic chemistry includes high-energy particles (e.g. cosmic rays consisting mostly of protons) and high-energy photons (e.g. extreme-UV (12.4 - 124 eV), X-rays, and gamma-rays). In contrast, photochemistry is defined as photon-induced electronic excitation not involving ionization. In addition to photochemistry, vacuum-UV (6.2 - 12.4 eV) light may initiate radiation chemistry because the threshold for producing low-energy electrons in condensed matter is lower than the gas phase ionization energy for a given molecule. For example, photoelectric emission threshold of amorphous ice (the main constituent of cosmic ices) is \(\sim 10.2 \text{ eV}\), which is smaller than the gas phase ionization energy of 12.6 eV for water. Because most previous astrochemical studies have used light sources that produce \(> 10 \text{ eV}\) photons, discerning the role of photochemistry vs. radiation chemistry in astrochemistry is challenging. By using a source whose photon energy does not exceed 8 eV, we have studied ammonia and methanol cosmic ice reactions attributable solely to photochemistry. We will compare and contrast these results to those obtained in the same ultrahigh vacuum chamber with 1 keV electrons which initiate radiation chemistry in cosmic ice analogs.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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N-Bearing Species in Massive Star Forming Regions

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Poster number: 8

Recent observations revealed that there is a difference in spatial distribution of both nitrogen and oxygen bearing species towards star forming regions. These differences can be explained under different temperature regimes in hot cores. In this study we attempt to model the chemistry of few nitrogen species, namely CH\textsubscript{3}CH\textsubscript{2}CN, CH\textsubscript{2}CHCN, and NH\textsubscript{2}CHO, using gas-grain chemical models. A special attention is given to the role and efficiency of surface chemistry as it is suggested to be the key in manufacturing such species. We also investigate the influence of variations of the environmental physical conditions, among which are the density and the cosmic ray ionization rate, on the fractional abundances.

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

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On the formation of Urea in the ISM

Meijer, A. J.\textsuperscript{1}, Slate, E. C.\textsuperscript{2}, Barker, R.\textsuperscript{3}, Euesden, R. T.\textsuperscript{4}, Revels, M. R.\textsuperscript{5}

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Poster number: 9

The interstellar medium contains vast dust clouds, which can be chemically incredibly diverse. The grain species in these clouds are covered by a variety of small ice species, including H\textsubscript{2}O, CO, H\textsubscript{2}CO, CO\textsubscript{2}, MeOH, CH\textsubscript{4}, and NH\textsubscript{3}. These ices can photodissociate to generate radicals, which can lead to further, more complex molecules. Two such, more complicated, molecules are methylformate and glycoaldehyde, which have been studied quite extensively in the literature.

Another complex organic molecule is urea. This molecule, potentially important for the abiotic origin of life, has not yet been detected in the interstellar medium, unlike glycoaldehyde or methylformate. However, it was one of the identified products in the famous Urey-Miller experiment in the 1950s \cite{1} and it has been detected in meteorites, such as the Murchison Meteorite.\cite{2} Moreover, it has been formed in ice-processing experiments, although its precise formation mechanism is unknown.\cite{3} In this paper, we consider a number of different formation routes for the formation of urea using a variety of computational methods. We show that there are a limited number of viable candidate pathways.

References
\cite{1} Miller, S. L. and Urey H. C., 1959, Science, 130, 245.


\cite{3} Foerstel, M., Maksyutenko, P. Jones, B. M. et al., 2015, Chem. Comm. 52, 741.

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

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Since the detection of CH$_3$OH in different objects of the interstellar medium (ISM), astrochemical models have been used to interpret the observed abundances, taking into account all potential formation and depletion processes both in the grain surfaces and in the gas-phase. The rate coefficients ($k$) for many gas-phase reactions are not known at the temperatures of the dense molecular clouds of the ISM (down to 10 K) due to the difficulties of the experimental methods. Usually $k$ values used in these models are estimates or extrapolations from temperature dependences reported at high temperatures. One of the potential depletion processes of methanol is the gas phase reaction with OH radicals: OH + CH$_3$OH $\rightarrow$ Products (Reaction 1).

The rate coefficient for Reaction 1 have previously been reported at $T > 20$ K [1-3]. Since $k$ has not been determined at temperatures closer than 10 K, Antiñolo et al. [1] proposed an extrapolated value of $k(10K) = 1.1 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ to be used in astrochemical models.

In this work, we have revisited the kinetics of Reaction 1 extending the temperature range down to 11.7 K and up to 177.5 K. For that purpose, the pulsed CRESU technique has been used. We report for the first time, $k(T=11.7K)$, the lowest temperature achievable until now using a pulsed CRESU apparatus. Additionally to the studies of the evolution of $k(T)$, we have studied the pressure dependence of $k$ in a large range of gas densities ($1.5 \times 10^{16} - 4.3 \times 10^{17}$ cm$^{-3}$) and our results are combined with those reported in previous works to extend that $p$-range [1-3].

Finally, the potential pressure dependence, the potential astrophysical implications of $k(11.7 K)$ and the formation of CH$_3$O radical from Reaction 1 will be discussed at the conference.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics
Nanoscale Structure of Amorphous Solid Water. What Determines the Porosity in ASW?

Gaertner, S.¹, Headen, T. F.², Youngs, T. G.³, Hill, C. R.⁴, Pascual, N.⁵, Auriacombe, O.⁶, Ioppolo, S.⁷, Loerting, T.⁸, Bowron, D. T.⁹, Fraser, H. J.¹⁰

¹ISIS Facility, STFC Rutherford Appleton Laboratory & School of Physical Sciences, The Open University, United Kingdom, ²ISIS Facility, STFC Rutherford Appleton Laboratory, ³ISIS Facility, STFC Rutherford Appleton Laboratory, ⁴School of Physical Sciences, The Open University, ⁵School of Physical Sciences, The Open University, ⁶School of Physical Sciences, The Open University & RAL Space, STFC Rutherford Appleton Laboratory, ⁷School of Physical Sciences, The Open University & School of Electronic Engineering and Computer Science, Queen Mary University of London, ⁸Institute of Physical Chemistry, University of Innsbruck, ⁹ISIS Facility, STFC Rutherford Appleton Laboratory, ¹⁰School of Physical Sciences, The Open University

Poster number: 11

Vapour deposited amorphous solid water (ASW) is supposed to be the most common solid material in space. Low temperature depositions of ASW are porous, suggesting that in space it may incorporate trace gases, influencing e.g. the formation of complex chemicals and the cooling of star-forming regions [1]. Porosity also alters the collisional properties of a material, potentially affecting crucial steps in planet formation [2]. In three decades of research on the structure of interstellar ice analogues, complementary methods often yielded seemingly contradictory results. The porosity and ice phase depend on growth conditions, such as substrate temperature and rate, composition and directionality of the gas flow. Also, ASW is known to change with temperature and potentially with time to reach an energetically preferable state by crystallising and losing porosity. These changes again depend on the environmental conditions the ice is experiencing. We studied the structure of vapour-deposited D₂O in the range of 18 to 180 K on intramolecular to 30 nm length scales, using neutron scattering as a non-invasive method (ISIS' NIMROD beamline, beamtime allocations RB1510246 & RB1610318). Building on earlier work [3], we can grow our ices in well-quantified and reproducible ways, taking out the aforementioned ambiguity regarding the deposition conditions. Structural changes evidence enhanced mobility from 100 to 150 K. Across the range 18 to 180 K, an Arrhenius type model describes the loss of surface area and porosity with a common set of kinetic parameters, but different high temperature equilibria. Therefore, surface area is not a measure for porosity, although the same mechanism (activation energy 428 K) drives both changes. Our findings indicate very loosely arranged molecules and imply that water will always change with time, even at low temperatures, changing our picture of ice astrophysics.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe, Solar System formation and the pre-solar nebula, Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Experimental laboratory astrophysics

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OH radical on interstellar ices: a quantum chemical study

Sameera, W.¹, Sameera, W.², Miyazaki, A.³, Watanabe, N.⁴

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Poster number: 12

The origin of radical species in the interstellar medium (ISM) and mechanistic details of their reactions remain a mystery. The radical species in the ISM play an important role in the formation of more complex molecules or radicals. These chemical processes occur on the icy mantles of interstellar grains at very low temperatures (typically 10 K). Radicals may adsorb on ice, diffuse, and subsequently react with other radical or molecular species on ice.[1] The rates of these processes are difficult to characterize from experimental studies alone. In this respect, modern quantum chemistry becomes critical.[2,3] We have used quantum mechanics/molecular mechanics (QM/MM) methods [3] to study OH radical binding on crystalline hexagonal water ice (Ih) and amorphous solid water (ASW). Depending on the number of dangling hydrogen (d-H) or dangling oxygen (d-O) at the binding sites, a range of binding energies was observed. In the absence of dangling atoms at the binding sites, the calculated binding energies are significantly weaker, allowing radicals to diffuse on the ice and react with other radical or molecular species on ice. Our study provides quantitative insights into OH radical desorption and diffusion on interstellar ices.

References

Scientific Theme(s)
• Solar System formation and the pre-solar nebula

Research Area(s)
• Theoretical calculations or simulations in laboratory astrophysics

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Thermal desorption of amino complex organic molecules. Effect of the substrate

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Poster number: 13

Formamide (NH₂CHO) and methylamine (CH₃NH₂) are complex organic molecules of great relevance in prebiotic chemistry. They are the most abundantly amine-containing molecules observed in many astrophysical environments, mainly in prestellar and protostellar objects, hot corinos, massive hot cores and comets [1-2]. The presence of these molecules in the gas phase may result from thermal desorption of interstellar ices. We present the experimental and the simulating results for thermal desorption of formamide and methylamine from analogues of interstellar dust grain surfaces (graphite HOPG and np-ASW ice). The aim of this work is to understand the interaction of these amino molecules with the water ice and compare their desorption energies [3]. Adsorption-desorption experiments of formamide and methylamine ices were performed in the sub-monolayer and monolayer regimes at temperatures 40-240 K using the cryogenic FORMOLISM setup located in the astrophysical laboratory LERMA at the university of Cergy. The desorption energy distributions of these two molecules were derived from TPD data using a set of independent Arrhenius equations. Results showed that the desorption of formamide from graphite and ASW ice surfaces occurs after the sublimation of the water ice at 150 K, whereas the desorption profile of methylamine depends strongly on the substrate. This latter desorbs before and during the desorption of H₂O, and even later at T>160 K. In addition, solid NH₂CHO fully diffuses through the ASW ice surface towards the graphitic substrate and releases into the gas phase with higher desorption energies that exceed that of the crystalline water ice (4930 K). Implications of these high binding energies are discussed.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

Research Area(s)
• Experimental laboratory astrophysics

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A new MALDI technique for the investigation of biomolecules in extraterrestrial environments

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Poster number: 14

Whether life has emerged on places other than Earth is still an open question and is intensively discussed in current Astrobiology. Over the past decades, a number of space exploration missions have been conducted, mainly to Mars, to detect traces of life, extinct or extant, in extraterrestrial environments [1]. The detection of indicators of life is extremely challenging as it depends on many different parameters, such as selection of appropriate field site, measurement capabilities of instrumentation, among many others. As of today, various spectroscopic and mass spectrometric (mainly GC-MS) techniques have been used on Mars and have proven to be unable to detect biomolecules, such as amino acids, peptides, and lipids. Therefore, in line with Hays et al. [2], for future space missions more sensitive measurement techniques are needed, or different measurements have to be performed, with a high spatial resolution compatible with the size of the expected life form. In this talk we will present a novel high-sensitive Matrix Assisted Laser Desorption / Ionization - Time-of-Flight Mass Spectrometry (MALDI - TOF MS) technique, specifically adapted to in-situ space-based applications. For the measurements discussed, a porous parylene surface is used, onto which molecules can be deposited. This circumvents the difficult sample preparation normally associated with MALDI (e.g. mixing of the sample with an appropriate matrix) and avoids contamination of the mass spectrum by matrix molecules. A miniature TOF MS, originally designed for in-situ chemical analysis of solids on planetary surfaces, is used for the mass spectrometric analysis [3]. Preliminary results of the first set of measurements of amino acids drop cast on the sample holder are presented, focusing on fundamental parameters such as laser pulse energy and concentration effects to obtain reliable detections of bio-relevant molecules. Finally, future applications to space missions are discussed in more detail.

References

Scientific Theme(s)
• Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
• Experimental laboratory astrophysics

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Laboratory simulation of light scattering from regolith analogue: Effect of porosity and particle size

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Poster number: 15

The surfaces of most of the atmosphereless solar system objects are referred to as regolith or layers of usually loosely connected fragmentary debris, produced by meteorite impacts. Measurement of light scattered from such surface provide information about the composition and structure of the surface. A suitable way to characterize the scattering properties is to consider how the intensity and polarization of scattering depend on the particle size, composition, porosity, roughness, wavelength of incident light and the different geometries of observation. Here in Assam University, Silchar, India we have set up a laboratory to simulate the light scattering properties of such surfaces in terms of intensity as well as polarization. For the laboratory simulation a goniometer is used with a CCD as a detector and a He-Ne gas laser as a source having wavelengths 543.5 nm and 632.8 nm. For imaging the surface, a thick lens [converging] is mounted in front of the CCD camera. For measuring degree of polarization an additional Polaroid has been mounted in front of the thick lens. The Polaroid can be rotated in many discrete steps. The light scattered from the regolith surface is detected by the CCD camera at three different positions of Polaroid. The intensity and polarization values of slight scattered by the surface are measured by varying phase angle. In the present work, the effect of porosity and particle size, on reflectance is studied for a diverse collection of regolith like samples with a wide range of albedo. Results obtained by the above experiment will be discussed.

Scientific Theme(s)
- Solar System formation and the pre-solar nebula

Research Area(s)
- Experimental laboratory astrophysics

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High resolution rotational spectroscopy of elusive molecules at the Center for Astrochemical Studies (CAS@MPE)

Spezzano, S.\textsuperscript{1}, Lattanzi, V.\textsuperscript{2}, Laas, J.\textsuperscript{3}, Chantzos, J.\textsuperscript{4}, Caselli, P.\textsuperscript{5}

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Poster number: 16

The Centre for astrochemical Studies (CAS) group includes experts in observations, theory, and the laboratory. The gas-phase spectroscopic characterisation of molecular species of astrophysical relevance is one of the main goals of the laboratory sub-group. In my talk I will focus on our experiments on unstable molecules, such as ions and radicals. We currently have two experiments for this task: the CASAC (CAS Absorption Cell), and the sub-millimetre free-unit jet experiment. The CASAC is a sub-millimetre-absorption spectrometer equipped with a negative glow-discharge cell with two stainless steel, cylindrical hollow electrodes separated by 2 m. The cell is cooled by liquid nitrogen. A 2m-long solenoid is wrapped around the cell to produce a coaxial magnetic field up to $\sim 300$ G and enhance the production of ions [1]. The molecular jet experiment is characterised by a supersonic free-jet expansion that allows to achieve a rotationally cooled molecular beam (about 10 K), and by a collision-free environment, which is particularly suitable when studying unstable molecules such radicals and ions. It is equipped with a pulsed valve, and large diffusion and mechanical pumps. The radiation source for both experiments is an active multiplier chain providing continuous coverage in the 75 - 1600 GHz frequency range. A liquid-Helium cooled InSb hot electron bolometer is used as a detector. In my talk I will present these techniques, and underline how their complementarity allows us to investigate different kind of molecules, as well as different part of the spectrum of the same molecule. I will also report on the different projects that have already been undertaken with these experiments, a. o. the extension of the frequency coverage of HCCO and DCCO up to 600 GHz and $K = 4$ [2], and the first detection of the b-type spectrum of protonated carbonyl sulfide (HSCO\textsuperscript{+}) [3]. Future developments and plans will also be discussed.

References


Scientific Theme(s)

- Star formation and the cosmic matter cycle in the near universe

Research Area(s)

- Experimental laboratory astrophysics

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Adsorption of volatile molecules on interstellar carbonaceous dust analogs

Herrero, V. J.\textsuperscript{1}, Maté, B.\textsuperscript{2}, Tanarro, I.\textsuperscript{3}, Jiménez-Redondo, M.\textsuperscript{4}, Peláez, R.\textsuperscript{5}, Escribano, R.\textsuperscript{6}
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Poster number: 17

The adsorption of molecules on the surface of dust grains is crucial for the physics and chemistry of interstellar clouds. Binding, diffusion and reaction of these molecules are determinant for the chemical inventory in many astronomical environments. Different groups have investigated the low-temperature interaction of small molecules with various solids like water-ice or silicates present in interstellar grains (see for instance \cite{1-3} ). In this work we study the adsorption of interstellar volatile molecules like H\textsubscript{2}O, CO\textsubscript{2}, CO, CH\textsubscript{4}, on solid deposits of amorphous hydrogenated carbon (HAC) which are taken as analogs of the carbonaceous component of interstellar dust grains. Our experiments are designed as a two step process. First we generate different HAC samples through deposition on Al substrates in RF plasmas of suitable precursors (CH\textsubscript{4}, C\textsubscript{2}H\textsubscript{2}). In the second step we transfer the substrates with HAC deposits to our UHV chamber (base pressure $1 \times 10^{-10}$ mbar) and place them in the cold head of He cryostat. We then introduce the volatile species into the chamber trough multichannel arrays and deposit them on the HAC samples at selected temperatures down to 15 K. We apply reflection absorption IR spectroscopy (RAIRS) and line-of-sight thermal programmed desorption (TPD) to determine binding energies and HAC specific surface areas by application of simple theoretical models. We will discuss at the meeting the astronomical implications of the results.

References
\begin{enumerate}
\item Herrero, V. J., Gálvez, O., Maté et al. 2010, PCCP, 12, 3164
\end{enumerate}

Scientific Theme(s)
\begin{itemize}
\item Star formation and the cosmic matter cycle in the near universe
\end{itemize}

Research Area(s)
\begin{itemize}
\item Experimental laboratory astrophysics
\end{itemize}
Anharmonic Aromatics

Lemmens, A. K.\textsuperscript{1}, Rap, D. B.\textsuperscript{2}, Thunnissen, J. M.\textsuperscript{3}, Rijs, A. M.\textsuperscript{4}, Buma, W.\textsuperscript{5}

\textsuperscript{1}University of Amsterdam, Netherlands, \textsuperscript{2}Radboud University, \textsuperscript{3}Radboud University, \textsuperscript{4}Radboud University, \textsuperscript{5}University of Amsterdam

Poster number: 18

We investigate the effects of anharmonicity in the IR spectra of gas-phase polycyclic aromatic hydrocarbons (PAHs). The photophysical properties of these aromatics are of key interest to the astronomical community, since it is hypothesized that they are abundant in interstellar space [1]. Using molecular beam laser spectroscopy IR absorption spectra of isolated PAHs at near-zero Kelvin temperatures have been obtained. Direct comparison of these high-resolution spectra to the widely used harmonic calculations reveals significant shortcomings in theory. These discrepancies can have far-reaching consequences as they are prone to lead to a misinterpretation of astronomical data. We therefore also present second-order vibrational perturbation theory anharmonic spectra [2] that reveal the effects of anharmonicity in the IR spectra of aromatic systems including combination bands, Fermi resonances and anharmonic shifts. A wide range of systems have been studied including the full range of acenes (linear PAHs), the grand-PAHs coronene, dicronylene and hexabenzenocoronene, as well as homo- and hetero-complexes of PAHs [3]. For all of these systems we show that anharmonicity is key to understanding and assigning the IR spectra.

References

Scientific Theme(s)
• Solar System formation and the pre-solar nebula

Research Area(s)
• Experimental laboratory astrophysics

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Gas-phase reactivity of CH$_3$C(O)CH$_3$ with OH radicals at interstellar temperatures (T = 11.7-64.0 K) using the CRESU technique

Blázquez, S.$^1$, Ocaña, A. J.$^2$, García, A.$^3$, Ballesteros, B.$^4$, Canosa, A.$^5$, Antiñolo, M.$^6$, Albaladejo, J.$^7$, Jiménez, E.$^8$

$^1$University of Castilla-La Mancha, Spain, $^2$University of Castilla-La Mancha, $^3$University of Castilla-La Mancha, $^4$University of Castilla-La Mancha, $^5$University of Rennes 1, $^6$University of Castilla-La Mancha, $^7$University of Castilla-La Mancha, $^8$University of Castilla-La Mancha

Poster number: 19

Hydroxyl (OH) radicals and acetone (CH$_3$C(O)CH$_3$) have been detected in cold dense molecular clouds. The gas-phase kinetics of the reaction of COMs with OH radicals has not been extensively investigated at temperatures of star-forming regions of the interstellar medium (T = 10-100 K). At those temperatures, the CRESU technique is the most suitable one to cool down gases below the freezing point without gas condensation. The CRESU system in Ciudad Real (Spain) allows us to study the OH+CH$_3$C(O)CH$_3$ reaction in the range of 11.7 - 64.0 K by using different Laval nozzles and buffer gases. Up to now, the title reaction has been studied at temperatures of the atmosphere (down to 202 K) [1] and at interstellar temperatures (79-148 K) [2]. At atmospheric temperatures, was observed a slight upward curvature in the Arrhenius plot (ln $k$ versus 1/T) below room temperature, indicating that the rate coefficient ($k$) for the reaction of OH with acetone would increase at T<200 K. Shannon et al. confirmed it [2], reporting an increase of almost 2 order of magnitude between 146 K and 79 K. Moreover, these authors observed a strong pressure dependence of $k$ at around 80 K, while at 140 K the p-dependence of $k$ was less pronounced. In this work, we have extended the temperature range (11.7-64 K) of the kinetic study in order to verify if $k$ continues increasing below 80 K. The CRESU technique coupled to the PLP-LIF technique was employed to perform the kinetic study. This technique has been described elsewhere in studies of some OH reactions of interstellar interest [3]. The loss of OH radicals was monitored by LIF under pseudo-first order conditions ([CH$_3$C(O)CH$_3$] and [OH-precursor] $\gg$ [OH]). Additionally to the investigation of the temperature dependence of $k$, the potential p-dependence of $k$ has been explored at 20 and 50 K. The astrophysical implications of our results will be discussed at the conference.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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Low Temperature Gas Phase Reaction Rate Coefficient Measurements: Toward Modeling of Stellar Winds and the Interstellar Medium.

West, N. A.\textsuperscript{1}, Rutter, E.\textsuperscript{2}, Douglas, K.\textsuperscript{3}, Blitz, M. A.\textsuperscript{4}, Decin, L.\textsuperscript{5}, Heard, D. E.\textsuperscript{6}

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Poster number: 20

Stellar winds of Asymptotic Giant Branch (AGB) stars are responsible for the production of $\sim 85\%$ of the gas molecules in the interstellar medium (ISM), and yet very few of the 10 - 300 K reaction rate coefficients needed to model the production and loss of these molecules in stellar winds have been experimentally measured. If measured, the value of the rate coefficient has often only been obtained at room temperature, extrapolating to lower and higher temperatures using the Arrhenius equation. However, non-Arrhenius behavior has been observed often in the few measured rate coefficients at low temperatures. This behavior is often caused by the formation of long-lived pre-reaction complexes and quantum mechanical tunneling through the barrier to reaction.

Reaction rate coefficients that were predicted to produce the largest change in the production/loss of Complex Organic Molecules (COMs) in stellar winds at low temperatures were selected from a sensitivity analysis. Here we present measurements of rate coefficients using a pulsed de Laval nozzle apparatus with the Pump Laser Photolysis- Laser Induced Fluorescence (PLP-LIF) technique. Gas flow temperatures between 30 - 134 K have been produced by the University of Leeds apparatus through the controlled expansion of N\textsubscript{2}, Ar, or He gas through Laval nozzles of a range of Mach numbers between 2.49 and 4.25.

Reactions of interest include those of $^1$CH\textsubscript{2}, OH, CN, and CH with volatile organic species, in particular formaldehyde, a molecule which has been observed in the ISM. Kinetics measurements of these reactions at low temperatures will be presented using the decay of the reagent. Since formaldehyde and the formal radical (HCO) are potential building blocks of COMs in the interstellar medium, low temperature reaction rate coefficients for their production and loss can help to predict the formation pathways of COMs observed in the interstellar medium.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe, Stars, stellar populations, and stellar explosions

Research Area(s)
- Experimental laboratory astrophysics

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Asteroid surfaces: irradiation and spectroscopy, in laboratory and in space

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Poster number: 21

Primitive extraterrestrial materials are characterized by a large heterogeneity of composition at small scales. This heterogeneity is observed in the laboratory on meteorites and interplanetary dust with different techniques. Among these, IR micro-spectroscopy has the advantage of being totally non-destructive and allowing a direct comparison with the astronomical observations of the minor bodies of the Solar System. In this presentation I will show some recent measurements of FTIR spectral imaging on different extraterrestrial materials, obtained in collaboration with the SMIS beamline of the SOLEIL synchrotron (France). In the second part I will present new spectral imaging data of meteorites irradiated in the laboratory with 40 keV ions, as a simulation of solar wind irradiation of the asteroid surfaces. Together with the irradiation effects measured in the particles of the asteroid Itokawa (collected by the Hayabusa mission), these experiments support the spectral interpretation of the observations of asteroids, to establish a link between asteroids and meteorites and to understand the energetic processes that modify the surfaces of the small bodies. In samples irradiated in the laboratory we observe spectral variations of organic and mineral components, as well as variations in albedo. These irradiation effects as a function of the dose are then compared on a micron-scale with the compositional heterogeneity of the original materials, to determine which spectral bands are more sensitive to the effects of space weathering. The results will be discussed in the context of the asteroid sample return missions Hayabusa2 (JAXA) and OSIRIS-REx (NASA).

References


Scientific Theme(s)

• Protoplanetary disks, debris disks, and the Solar System

Research Area(s)

• Experimental laboratory astrophysics

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Molecular Line Emission from Planet-Forming Disks

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Poster number: 22

Observations with the Atacama Large Millimeter Array (ALMA) have already revolutionized our understanding of protoplanetary disk evolution. At millimetre-wavelengths molecules, e.g. CO, HCO\textsuperscript{+}, HCN, SO, have bright detectable rotational transitions observable with ALMA. As a result of chemistry, these molecules will have different radial and vertical abundance distributions in disks. During the process of giant planet formation cavities form in the dust and gas disk and material will cross through this cavity to accrete on to the forming planet. These changes in disk structure will significantly alter the disk chemistry and hence are observable. We present ALMA observations of different molecular species in three nearby planet-forming disks and discuss their specific kinematics and abundance distributions showing the potential power of molecular lines as tracers of planet formation.

Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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The Belgian repository of fundamental atomic data and stellar spectra (BRASS): Quality assessing atomic data for unblended lines in FGK-type stars

Laverick, M.\(^1\), Lobel, A.\(^2\), Royer, P.\(^3\), Merle, T.\(^4\), Martayan, C.\(^5\), van Hoof, P.\(^6\), Van der Swaelmen, M.\(^7\), David, M.\(^8\), Hensberge, H.\(^9\), Thienpont, E.\(^10\)

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The Belgian Repository of fundamental Atomic data and Stellar Spectra (BRASS) aims to provide a large systematic and homogeneous quality assessment of atomic data for stellar spectroscopy by comparing state-of-the-art synthetic spectrum calculations with extremely high-quality observed benchmark spectra. We critically evaluate the atomic data, such as line wavelengths and oscillator strengths, of thousands of transitions found in the literature and across several major atomic data repositories. BRASS provides all quality assessed data, theoretical spectra, and observed spectra in a new interactive database under development at brass.sdf.org.

In this talk we present our recent quality assessment work for unblended spectral lines present in the wavelength range 4200-6800A for FGK-type stellar spectra. Atomic data for over 82000 transitions, previously collected by [1], is systematically synthesised and compared against several FGK-type stellar spectra at a resolution of R\(\sim\)85000 and signal-noise ratios of S/N\(\sim\)1000. We discuss our line selection and quality assessment procedures, paying special attention to the associated uncertainties of our work, and present our quality assessment findings for the atomic data of 1091 spectral lines belonging to 28 different species.

References

Scientific Theme(s)
- Stars, stellar populations, and stellar explosions

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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Photoprocessing of large PAH cations

Wenzel, G.¹, Rodriguez Castillo, S.², Mulas, G.³, Ji, M.⁴, Bonnamy, A.⁵, Sabbah, H.⁶, Giuliani, A.⁷, Nahon, L.⁸, Joblin, C.⁹, & EUROPAH

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Poster number: 24

As a part of interstellar dust, polycyclic aromatic hydrocarbons (PAHs) are processed by the interaction with VUV photons that are emitted by young stars. After absorption of a VUV photon, an isolated PAH can undergo different relaxation processes: ionization, dissociation and radiative cooling, including IR fluorescence which results in the aromatic infrared bands (AIBs) observed in many astronomical objects. Following an earlier work on smaller PAHs [1], we investigate the two relaxation processes of ionization and dissociation of large PAH cations ranging from 30 to 48 carbon atoms. The ions are trapped in the LTQ linear ion trap of the DESIRS beamline at the synchrotron SOLEIL and energized by VUV photons in the range of 8 - 20 eV. All resulting photoproducts are mass-analyzed and recorded as a function of photon energy. Ionization is found to be the dominating relaxation channel, with the photoionization yield increasing with number of carbon atoms. Action spectra are obtained from the photoproducts’ relative intensities and compared to the photoabsorption cross sections. The latter have been computed using the real time, real space implementation of TD-DFT from the OCTOPUS code [2]. Models of the chemical evolution of PAHs in HI photodissociation regions have shown that the dissociation of large PAHs may require multiple photon absorption [3]. To further investigate this process, we use the PIRENEA setup which combines cryogenic trapping and laser interaction. We show how this sequence of experiments can give insights into the photoprocessing of PAHs in different astronomical environments. Acknowledgements: We acknowledge funding from the European Union under the Horizon 2020 framework for the Marie Skłodowska-Curie action EUROPAH, Grant Agreement no. 722346, and support from the European Research Council under the EU’s Seventh Framework Programme ERC-2013-SyG, Grant Agreement no. 610256 NANOCOSMOS.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

Research Area(s)
• Experimental laboratory astrophysics

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Spontaneous polarisation charge on CO ice mantles accelerates ion recombination reaction rates in cold dark clouds.

Cassidy, A.\textsuperscript{1}, Rosu-Finsen, A.\textsuperscript{2}, Lasne, J.\textsuperscript{3}, McCoustra, M. R.\textsuperscript{4}, Field, D.\textsuperscript{5}

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Poster number: 25

We propose a new role for CO ice mantles in ion recombination reactions, and will demonstrate how the subsequent fall in the degree of gas phase ionization decreases the time required for cloud collapse under gravitational pressure. Laboratory experiments, using IR and VUV absorption spectra from thin CO films prepared at cryo-temperatures, show that CO ices spontaneously harbours electric fields immediately upon growth. CO ices can be considered as so-called spontelectric materials; a class of molecular materials that spontaneously assemble to generate static internal electric fields that permeate the film and can exceed $10^8$ V/m.$^[1]$ This internal electric field produces residual polarisation charge at the surface of a dust grain and the degree of charge increases with the CO ice thickness.$^[2]$

We provide experimental evidence for this effect and explain how it relates to the problem of cloud collapse using B68 as an example.$^[3]$ The rate of expulsion of the magnetic field in a molecular cloud can dictate the timescale for gravitational collapse. Ion recombination reactions are promoted by the spontaneous charge that develops at the surface of a CO ice layer and this decreases the degree of ionization in the gas phase by a factor of between 5 and 6. The magnetic field retarding gravitational collapse is reduced by a similar factor and the lifetime for cloud collapse is significantly accelerated.

This contribution combines new experimental laboratory measurements with what is known from observations about cloud conditions in B68, and introduces an analytical model to demonstrate the proposed reduction in cloud collapse time.

References


Scientific Theme(s)

- Star formation and the cosmic matter cycle in the near universe

Research Area(s)

- Experimental laboratory astrophysics

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VAMDC and Data Citation

Dubernet, M.\(^1\), Zwolf, C.\(^2\), Moreau, N.\(^3\), BA, Y.\(^4\), & VAMDC Consortium

\(^1\)Paris Observatory, France, \(^2\)Paris Observatory, \(^3\)Paris Observatory, \(^4\)Paris Observatory

Poster number: 26

The “Virtual Atomic and Molecular Data Centre Consortium” (VAMDC Consortium, http://www.vamdc.eu) [1] is a worldwide consortium which federates Atomic and Molecular databases through an e-science infrastructure and an organisation to support this activity (http://www.vamdc.org/structure/how-to-join-us/). About 90% of the 36 inter-connected atomic and molecular databases handle data that are used for the interpretation of astronomical spectra and for the modelling in media of many fields of astrophysics. VAMDC offers a common entry point to all connected databases through the VAMDC portal (http://portal.vamdc.eu) and VAMDC develops also standalone tools in order to retrieve and handle the data. VAMDC provides software and support in order to include new databases within the VAMDC e-infrastructure. One current feature of VAMDC e-infrastructure is the constrained environment for the description of data, in particular the XSAMS schema and other standardized protocols (http://www.vamdc.org/standards) that ensure a higher quality for the distribution of data. Recently VAMDC, commissioned by the Research Data Alliance (https://www.rd-alliance.org/groups/data-citation-wg.html), has implemented the recommendations of the RDA data citation group. Within this context a first work has been done on provenance of datasets (CM Zwolf et al., J. Mol. Spec. B, 327 (2016) 122) which impacts the XSAMS schema, and a second work, for which RDA provided funding to VAMDC Consortium, has implemented the concept of Query Store [2]. The talk will briefly present the VAMDC Consortium, the VAMDC e-infrastructure with the current status of its underlying technology (some of it inherited from IVOA), its services, the new feature of Query Store related to data citation, as recommended by the Research Data Alliance (RDA). It underlines how usage of VAMDC can increase the impact factor of A&M producers [3] and can offer a reliable citation of A&M datasets included in application fields.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe, Solar System formation and the pre-solar nebula, Protoplanetary disks, debris disks, and the Solar System, Stars, stellar populations, and stellar explosions

Research Area(s)
- Experimental laboratory astrophysics

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Modelling the Anharmonicity of Polycyclic Aromatic Hydrocarbons

Candian, A.\(^1\), Mackie, C. J.\(^2\), Lee, T. J.\(^3\), Tielens, A. G.\(^4\)

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Poster number: 27

Dusty, ultraviolet-irradiated regions of the interstellar medium show strong emission bands in their infrared spectra, the so-called Aromatic Infrared Bands (AIBs), generally attributed to Polycyclic Aromatic Hydrocarbon (PAH) molecules. PAHs absorb UV photons and relax through a collision-less cascade of IR photons, producing the AIBs. Emission spectroscopy experiments in interstellar conditions are incredibly challenging \([1]\), thus theoretical approaches are widely used. In the past years ([2] and references therein) we have calculated the anharmonic infrared spectrum of a sample of small PAHs using second order vibrational perturbation theory (VPT2) applied to Density Functional Theory-level quartic force fields. Comparison with high-resolution, low-temperature, gas-phase absorption spectra validated our methods. Building up on these results, we developed \([3]\) a fully theoretical IR cascade spectra of PAHs including: an anharmonic VPT2 treatment; the inclusion of Fermi resonances through polyads; and the calculation of anharmonic temperature band shifts and broadenings (including resonances) through a Wang-Landau approach. We also suggest a simplified scheme to calculate vibrational emission spectra that retains the essential characteristics of the full IR cascade treatment and can directly transform low temperature absorption spectra in IR cascade spectra. Additionally we show that past astronomical models were in error in assuming a 15 cm\(^{-1}\) correction was needed to account for anharmonic emission effects. This work will be crucial to interpret the AIB spectrum once the James Webb Space Telescope comes online.

References


Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

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On the correlation of the abundances of HNCO and NH$_2$CHO: Dehydrogenation of formamide by H atoms at low temperatures

Tarczay, G.$^1$, Haupa, K.$^2$, Lee, Y.$^3$

$^1$Eötvös University, Hungary, $^2$National Chiao Tung University, $^3$National Chiao Tung University

Formamide (NH$_2$CHO) is the smallest molecule that contains the biologically important peptide bond. Therefore, both its observation in the interstellar medium (ISM) and the laboratory experiments on its formation and destruction mechanisms are important from astrochemistry and astrobiology aspects. Since recent astronomical observations revealed that there is a tight linear correlation between the abundances of isocyanic acid (HNCO) and formamide in 10 low- and intermediate-mass pre-stellar and protostellar objects, it was suggested that formamide might be synthetized by hydrogenation of HNCO [1] in astrophysical ices. In contrary to this hypothesis, Nobel et al. have found that formamide does not form by hydrogenation in a pure HCNO ice at a low temperature [2]. They supposed that the reaction of a hydrogen atom with formamide produces carbamoyl (NH$_2$CO) radical, and its attack by a second H atom leads to the back formation of HNCO and H$_2$, instead of formamide. Investigating the reactions of formamide with atomic H in solid $p$-H$_2$, we demonstrate that at low temperatures the two-step destruction of formamide by non-thermal H atoms, leading to the formation of HNCO and H$_2$, can. These results explain both the correlation between the abundances of HNCO and formamide, and why formamide formation by hydrogenation of HNCO in low-temperature ices is not effective. We propose that hydrogen atom abstractions by non-thermal H atoms can be a general, important reaction mechanism in astrochemical ices. We also demonstrate that $p$-H$_2$ matrix isolation [3] is an excellent and perspective method for exploring the mechanisms of astrochemically relevant H atom reactions at low temperatures.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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A history of ice and gas: the case of Serpens SVS 4

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Poster number: 29

Astrochemists are faced with major unanswered questions associated with the interplay between ice and gas chemistry. In fact, a better understanding of the desorption processes at the interface between ice and gas provides vital information on how the thermal history of star-forming regions influences the ice complexity and evolution. To constrain the desorption processes and efficiency observationally, a combination of ice and gas-phase observations is required. If both ice and gas-phase maps are available for a specific region, it is possible to go one step further, to combine and compare those maps and thereby bring together the information obtained from gas-phase observations, ice observations, and laboratory databases. The combination of ice-gas maps allows to identify the ice constituents present just before the collapse phase and to set the initial chemical conditions for star formation. We here present such an analysis of the SVS 4 cluster, a dense region of deeply embedded low-mass protostars located in the Serpens Molecular Cloud. Infrared observations (VLT) have provided abundances of the icy inventory for ten young stellar objects located in the SVS 4 cluster. Submillimeter observations (SubMillimeter Array and Atacama Pathfinder Experiment) of the same region and comparable resolution have supplied abundances of the gas-phase molecules. A simplified chemical network has been developed to model the observed abundances and to better constrain the most dominant desorption channels (desorption efficiency, binding energy). This study also serves as a pathfinder for future James Webb Space Telescope and Atacama Large Submillimeter Array observations that will provide ice and gas-maps of complex organics for several regions. The simplified chemical network developed in this study and the combination of ice and gas-observations will be essential tools to investigate the formation and destruction channels of such complex molecules.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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Diffusion and Desorption Kinetics in the Apolar Ice Phase

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Poster number: 30

Diffusion of species within ices and their desorption from ice surfaces are important processes that influence the chemistry of astrophysical regions; yet, laboratory measurements of these kinetic parameters are scarce, particularly for the apolar (CO- and CO₂-rich) ice phases. Here we present measurements of CO diffusion into CO₂ ice at low temperatures using CO₂ longitudinal optical phonon modes to monitor the level of ice mixing. We model the diffusion kinetics with Fick’s second law and find that the temperature-dependent diffusion coefficients are well fit by an Arrhenius equation, giving a diffusion barrier of 300 ± 40 K. The low diffusion barrier, along with supporting experiments, suggests that CO diffuses through CO₂ along pore surfaces rather than via bulk diffusion mechanisms. We then measure the desorption energy of CO from CO₂ ices deposited at various temperatures and find that the desorption barrier ranges from 1240 ± 90 K to 1410 ± 70 K depending on the CO₂ deposition temperature and resultant ice porosity. We find that the CO desorption energy from compact CO₂ is identical to that from compact H₂O [1], which has implications for the modelling of snow-lines in protoplanetary disks (e.g. [2]). This combined diffusion-desorption study allows us to extract the diffusion-desorption barrier ratio, a key parameter for astrochemical models (e.g. [3]). We find E_{diff}/E_{des} ranges from 0.21 to 0.24 dependent on the ice morphology. The low diffusion-desorption ratio supports the hypothesis that the diffusion is a surface process and adds to previous experimental evidence in water-rich ices that have shown that surface diffusion is important for the mobility of molecules within ices in star-forming regions.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe, Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Experimental laboratory astrophysics

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Propagating Atomic Uncertainties to Infer Coronal Plasma Properties


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Poster number: 31

It is critical to understand how uncertainties in underlying atomic physics propagate to uncertainties in inferred plasma parameters in solar coronal structure analysis. We apply model-generated uncertainties in Fe XIII emissivities from lab measurements and different calculation schemes to interpret density-sensitive spectral lines observed with the EIS (Extreme-ultraviolet Imaging Spectrometer) on Hinode. Besides the Bayesian methodology that considers atomic uncertainties as fully specified (pragmatic Bayesian method), we allow observed intensities to update atomic uncertainties (fully Bayesian method). The former increases uncertainties on inferred density compared with models that incorporate only statistical uncertainties. The latter reduces uncertainties on inferred densities. We use two ways to incorporate atomic uncertainties into highly structured statistical models. A discrete analysis where atomic realizations are considered individually and a continuous analysis where principal component analysis (PCA) is used to fully summarize atomic uncertainties. The former suggests a different realization of emissivities is more likely than the default CHIANTI calculation and identifies areas of possible systematic problems with either atomic physics or observed intensities. The latter mitigates the gaps among the sparse atomic realizations. The fully Bayesian does include atomic information, while PCA based on it does not allow feedback to adjust atomic parameters. This methodology is used to infer both density and temperature in spectral analysis, e.g., with the temperature-sensitive Fe XVII, the H-like O VIII resonance, and the He-like O VII density-sensitive triplet lines in X-ray regime. Future improvements to the methodology and the structure of atomic databases allow realistic density estimation and the determination of the thermal structures of solar and stellar coronae. We acknowledge the generous support from the ISSI, RISE Grant, and Imperial College.

References

Scientific Theme(s)
• Stars, stellar populations, and stellar explosions

Research Area(s)
• Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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Laboratory rotational spectroscopy of interstellar isomers

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1 Institut des Sciences Moléculaires d’Orsay, CNRS, France, 2 Harvard-Smithsonian Center for Astrophysics, 3 Harvard-Smithsonian Center for Astrophysics

Poster number: 32

New laboratory investigations of the rotational spectrum of postulated astronomical species are essential to support the assignment and analysis of spectral line surveys in rich astronomical sources. In particular, considerable interest surrounds structural isomers of known interstellar species because they can serve as invaluable tools for probing the chemical dynamics and physical properties of astrophysical environments. While the minimum energy principle has been invoked to rationalize molecular abundances in space [1], chemical kinetics is also an important factor in molecule formation [2]. For this reason, high-lying, transient isomers of known astrophysical molecules may exist in space, but their astronomical detection is often hindered by the lack of available laboratory data. These energetic isomers are often challenging to characterize in the laboratory compared to their stable, often commercially available, counterparts and consequently relatively little is known about the spectroscopy of reactive isomers of relatively large astrophysical species (5 atoms and more).

We apply the recently developed experimental methodology of spectral taxonomy [3] to measure the pure rotational spectrum of transient isomers of known oxygen-containing interstellar molecules and their sulfur analogs from the centimeter to the submillimeter bands, the latter where high-altitude, high-sensitivity radio facilities such as ALMA operate. We will report results on several species among the isomeric families C₂H₂O and C₂H₂S (isomers of ketene and thioketene), and C₂H₄S (isomers of thioacetaldehyde), in particular results on hydroxyacetylene (HCCOH), ethynethiol (HCCSH), and vinyl mercaptan (C₂H₃SH).

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

Research Area(s)
• Experimental laboratory astrophysics

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The importance of being stable: new results about the survival of PAHs and hydrocarbon nanoparticles in extreme astrophysical environments.

Micelotta, E. R.¹
¹University of Helsinki, Finland

Poster number: 33

There is an increasing observational evidence that a non-negligible fraction of the cosmic carbon is locked into macromolecules, like Polycyclic Aromatic Hydrocarbons (PAHs), and in hydrocarbon nanoparticles. These species have been proposed as possible carriers of the dominant astronomical emission features in the mid-infrared and they play an active role in the cosmic matter cycle. Interstellar PAHs and nanoparticles live in extreme environments where they are processed by energetic photons (UV and X-rays) and by ions and electrons accelerated in hot shocked plasma and arising from cosmic rays. It is therefore important to quantify the capability of PAHs and nanoparticles to survive under these extreme conditions and to determine the structural modifications induced by such energetic processing. I will present some novel results on this topic, focusing on the bombardment by photons and ions and emphasizing the differences and similarities between PAHs and nanoparticles [1]. This work shows the importance of pairing an appropriate physical description of the interaction between target and projectiles with updated laboratory measurements of the relevant physical parameters. The results from physical modeling allowed to derive updated astronomical lifetimes for PAHs and nanoparticles under different conditions, which in turn have been used to interpret observations of selected test objects. This research exemplifies the mutual gain resulting from the synergy between theorists, experimentalists and observers. The first works on the stability of PAHs in space [2, 3] have stimulated the physics community to pursue experimental studies, which have provided laboratory measurements necessary for the better determination of the survival rate of these species presented here.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

Research Area(s)
• Theoretical calculations or simulations in laboratory astrophysics

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Selective mid-IR and THz Free-Electron Laser irradiation of water ice probed by FTIR spectroscopy

Ioppolo, S.\textsuperscript{1}, Noble, J. A.\textsuperscript{2}, Cuppen, H. M.\textsuperscript{3}, Coussan, S.\textsuperscript{4}, Redlich, B.\textsuperscript{5}, Mason, N. J.\textsuperscript{6}  
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Interstellar ice grains play a central role in the catalysis of prebiotic molecules that were essential for the development of life on Earth [1]. Tracing the physical-chemical evolution of ice grains is one of the main targets of the next NASA’s space mission JWST. Hence it is important to explore in the laboratories the morphology and dynamics of such ices and how they influence the pathways to chemical synthesis. Water is the most abundant solid species found ubiquitous on interstellar grains and icy bodies in the Solar System. We have measured the irreversible structural changes induced in pure water ices of different initial structures (i.e., porous amorphous, compact amorphous, cubic crystalline, and hexagonal crystalline) by means of selective THz and mid-IR coherent, tunable pulsed radiation from the free-electron laser FELIX-1 and -2 at FELIX Laboratory in the Netherlands. The ultimate aim of this work is the study of energy relaxation dynamics at the surface and in the bulk of solid water layers. The advantage of using a free electron laser for this study is the possibility of resonantly pumping specific modes, which is a much better, selective probe for the local structure of the ice than thermal heating. Table-top laser systems (e.g., OPOs) are not adequate for this project because of their limited spectral and energy ranges [2-3]. Molecular dynamic simulations are also used to provide insight in the experimental results.

References
[3] Coussan et al. 2015, PCCP, 17, 9429

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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Ion irradiation of astrophysical relevant frozen mixtures and characterization of organic refractory residues

Urso, R.1, Brunetto, R.2, Alemanno, G.3, Baklouti, D.4, Borondics, F.5, Maupin, R.6, Djouadi, Z.7, Mivumbi, O.8

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Poster number: 35

The comparison between laboratory experiments and astronomical observations is fundamental to spread light on the properties of frozen surfaces in space. During their lifetime, ices are exposed to cosmic rays and UV photons that modify their chemical composition and physical structure (e.g., [1]). In order to study the effects induced by low-energy cosmic rays, we carried out various experiments of ion irradiation (with 40 keV H+) up to few tens of eV/molecule of astrophysical relevant frozen mixtures containing water, C- and N-bearing species. Thanks to a new experimental setup, the samples were analyzed by means of in-situ transmission and reflection spectroscopy in the visible, NIR and MIR ranges. After the irradiation, the samples were warmed up to obtain organic refractory residues (e.g., [2,3]) that have been further characterized by means of ex-situ micro-IR and micro-Raman spectroscopy. This study contributes in the analysis of data collected by observations and space missions on primitive solar system small bodies. Also, they will support the interpretation of spectra that will be collected by the James Webb Space Telescope.

References

Scientific Theme(s)
• Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
• Experimental laboratory astrophysics

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Examining the chemistry Ophiuchi Diffuse Region using a rate sensitivity analysis

Tomassi, J.¹
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Poster number: 36

This project represents the work undertook as part of my masters degree. In this project we used the chemical software package Krome which is used to simulate chemical networks to be embedded in astrophysical simulations. For this project we looked at the Ophiuchi Diffuse Region, specifically the chemical effects on the presence of Polycyclic Aromatic Hydrocarbons (PAHs). The network that was used in based on the KIDA database and was simulated using Krome, first without the presence of PAHs then with them included. Once the network is complied a rate sensitivity analysis was conducted, details of which will be found below, to determine which reactions in the network had the biggest impact upon the rest of the network. The results between the two versions of the network are then compared.

Scientific Theme(s)
- Reaching beyond our galaxy: from extra galactic chemistry to dark matter

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

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Photofragmentation of coronene cations

Panchagnula, S.¹
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Poster number: 37

Polycyclic aromatic hydrocarbons (PAHs) lock up 15% of all interstellar elemental carbon and are known to play a crucial role in the physics and chemistry of the interstellar medium as they control the energy and ionisation balance of interstellar gas. [1] Recent laboratory studies have shown that extensive photo-processing of PAH cations causes them to dehydrogenate and ultimately form charged species that are comprised of only carbon atoms organized in a ring- or cage structure. [2,3] We present our latest experimental results recorded on our ion-trap time of flight mass spectrometer. We show that the key photodissociation fragment of the coronene cation (C\textsubscript{24}H\textsubscript{12}\textsuperscript{+}) is a carbon cluster of C\textsubscript{11}\textsuperscript{+} composition. We discuss potential dissociation pathways and energies and propose possible structures of the C\textsubscript{11}\textsuperscript{+} fragment. We use density functional theory to guide our interpretation of the experimental data and identify a link between the fragmentation dynamics of the coronene cation and its molecular properties in an astronomical context.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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H$_2$ photochemistry in interstellar ices: the formation of HCO in UV irradiated CO:H$_2$ ice mixtures


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Poster number: 38

The formation of formyl radical (HCO), a fundamental precursor of interstellar complex organic molecules (COMs), has been extensively studied in the solid state via hydrogenation (H-atom addition reactions) of carbon monoxide (CO) under prestellar core conditions. [1,2] However, the role of molecular hydrogen (H$_2$) with an abundance four orders of magnitude higher than that of H-atom in dense clouds, is still not clear due to the high activation energies required for ‘non-energetic’ association reactions. In this work, we investigated the potential contribution of H$_2$ to the hydrogenated species (H$_n$CO) formation on dust grains when the ‘energetic’ processing is involved. The goal is to test whether additional hydrogenation pathway is possible upon UV irradiation of a CO:H$_2$ ice mixture, i.e., mimic the case of the non-reacted interstellar molecules condensed/trapped in the ice bulks, which cannot be reached by the newly accreted H-atom from the gas phase. The photolysis experiments of CO:H$_2$ ice mixture were performed at 8-20 K under dense cloud conditions. After UV irradiation of a pre-deposited CO:H$_2$ ice mixture, the newly formed photo-products, HCO and H$_2$CO are unambiguously detected by Reflection Absorption Infrared Spectroscopy (RAIRS). It is proposed that the electronically excited carbon monoxide (CO$^*$) induced by UV-photons can react with a ground-state H$_2$ to form HCO and a free H-atom for further addition reactions. The kinetic study of HCO yields as function of UV fluence shows a strong temperature dependence for the investigated regime, which is most likely due to the H-atom diffusion rate and H$_2$ sticking coefficient. [3] The interaction between CO$^*$ and H$_2$ enhances the production of H$_n$CO species in the ice mantle and introduces a new solid-state chemistry involving abundant H$_2$ in dense clouds. Additional experiments are being carried out with ice mantles formed on interstellar dust grain analogues.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

Research Area(s)
• Experimental laboratory astrophysics

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Learning mid-IR emission spectra of polycyclic aromatic hydrocarbon populations from observations.

Foschino, S., Berné, O., Joblin, C.

IRAP - University of Toulouse, France, IRAP - University of Toulouse, IRAP - University of Toulouse

Poster number: 39

The James Webb Space Telescope (JWST) will deliver an unprecedented quantity of high-quality spectral data over the 0.6-28 \( \mu \)m range. Specific tools are required to provide efficient analysis of such large data sets. In this study, we aim at illustrating the potential of unsupervised learning methods to get insights into the chemical evolution of the populations that carry the aromatic infrared bands (AIBs), more specifically polycyclic aromatic hydrocarbon (PAHs) species and very small carbonaceous grains (VSGs).

Previous studies made use of spatial information on a few reflection nebulae, using Spitzer-IRS. In this study we consider ISO-SWS spectra which contain a richer spectral information. The lack of spatial resolution is compensated by including several sources in the sample. The selected objects include HII and compact HII regions, planetary nebulae, reflection nebulae, one post-AGB star and one starburst galaxy. After extracting the AIB contribution from the observed spectra, we applied a non-negative matrix factorization algorithm initialized by a geometric method to retrieve elementary spectra.

Four elementary spectra were extracted. Their main characteristics are those of populations dominated by cationic PAHs (PAH+), neutral PAHs (PAH0) and evaporating VSG [1] and large ionized PAHs [2], as previously identified [3]. We find that the improved spectral resolution reveals additional chemical information whose interpretation is however limited by the lack of spatial information.

The upcoming JWST data will allow us to overcome this limitation. The large hyperspectral datasets it will provide combined with the proposed method, which is fast and robust, opens promising perspectives for our understanding of the chemical evolution of the AIB carriers.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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A new chirped pulse microwave spectrometer dedicated to the measurement of reaction product branching ratios for astrochemistry

Hays, B. M.\textsuperscript{1}, Hearne, T.\textsuperscript{2}, Guillaume, T.\textsuperscript{3}, Abdelkaderkhedaoui, O.\textsuperscript{4}, Cooke, I.\textsuperscript{5}, Gupta, D.\textsuperscript{6}, Sims, I.\textsuperscript{7}

\textsuperscript{1}Universite de Rennes 1, France, \textsuperscript{2}Universite de Rennes 1, \textsuperscript{3}Universite de Rennes 1, \textsuperscript{4}Universite de Rennes 1, \textsuperscript{5}Universite de Rennes 1, \textsuperscript{6}Universite de Rennes 1, \textsuperscript{7}Universite de Rennes 1

The study of chemical reactions at temperatures relevant to the interstellar medium has often provided data only on the overall rate of reaction, rather than on the products formed from the reactions. Hardly any experimental measurements of product branching ratios in the gas phase at low temperatures exist. We have designed and built a new microwave spectrometer operating between 60-90 GHz to study product formation within the cold uniform supersonic (CRESU) flows in Rennes. This uses chirped pulse microwave (millimeter wave) spectroscopy to observe a wide variety of molecules. The experimental setup and challenges of these experiments will be discussed, especially in relation to the collisional dephasing observed when recording chirped pulse spectra at higher pressures, such as those in the CRESU flows. A study of this collisional dephasing will be presented, as well as initial results towards measuring reaction branching ratios at cold temperatures.

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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Amorphous Mg-Fe silicates via sol-gel: method, structure, spectroscopy and thermal evolution

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¹Diamond Light Source, United Kingdom, ²Diamond Light Source

Poster number: 41

Inorganic sol-gel provides a simple and highly reproducible means of producing amorphous pyroxene and olivine silicates with a wide range of relative compositions. Incorporating Fe into the silicate network requires avoiding the formation of oxide phases and can be problematic [1], while the influence the silicate structure, thus formed, has on spectroscopic behaviour requires extensive characterisation [2]. In this talk, we present the use of fast microwave drying as a method of producing amorphous pyroxene and olivine silicates with incorporated Fe, along with comparative characterisation measurements using the synchrotron structure-probing techniques of small angle X-ray scattering, X-ray pair distribution function analysis, X-ray absorption spectroscopy and FTIR spectroscopy in the mid-IR to identify relationships between production and properties. Results [3] from in situ thermal annealing, monitored by fast X-ray powder diffraction, show multi-phase, temperature and composition dependent, crystallisation of enstatite, forsterite and cristobalite phases. The crystallisation temperature of forsterite from bulk Mg-pyroxene composition is higher than for bulk Mg-olivine, while cristobalite appears as a high temperature diagnostic for Mg-pure compositions. The incorporation of Fe pushes the forsterite crystallisation temperature even higher. Activation energies derived from the diffraction data are used to place constraints on both the temperatures and locations within protoplanetary disks where grain mineralisation can occur. Although this work largely focusses on stoichiometric compositions, the use of our technique for the production of non-stoichiometric compositions will also be considered.

References

Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Experimental laboratory astrophysics

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The Titan Haze Simulation Experiment: Investigating Titan’s Low-temperature Atmospheric Chemistry in a Pulsed Plasma Jet Expansion

Sciamma-O’Brien, E. M.¹, Raymond, A. W.², Dubois, D.³, Mazur, E.⁴, Salama, F.⁵
¹NASA Ames Research Center, United States, ²Harvard University, ³NASA Ames Research Center/Bay Area Environmental Research Institute, ⁴Harvard University, ⁵NASA Ames Research Center

Poster number: 42

The THS experiment, developed at the NASA Ames COSmiC facility, is a unique experimental platform that allows us to simulate Titan’s complex atmospheric chemistry at Titan-like temperature (200 K) by cooling down N₂-CH₄-based mixtures in a supersonic expansion before inducing the chemistry by plasma. Both the gas and solid phase can be characterized.

Gas phase: Because of the accelerated gas flow in the jet expansion, the residence time of the gas in the active plasma region is less than 4 µs. This results in a truncated chemistry, enabling us to control how far in the chain of reactions the chemistry is processing. By adding heavier molecules in the initial gas mixture, it is then possible to study the first and intermediate steps of Titan’s atmospheric chemistry as well as specific chemical pathways (including production of aromatic species), as demonstrated by mass spectrometry and comparison to the Cassini Plasma Spectrometer data¹. A new model was recently developed to simulate the plasma chemistry in the THS. Calculated mass spectra produced by this model are in good agreement with the experimental THS mass spectra, confirming that the short residence time in the plasma cavity limits the growth of larger species².

Solid phase: Scanning electron microscopy, infrared- and x-ray absorption near edge structure spectroscopy have been used to investigate the effect of the initial gas mixture on the morphology of the THS Titan aerosol analogs as well as on the level and nature of the nitrogen incorporation into these aerosols. A comparison to Cassini VIMS observational data has shown that the THS aerosols containing more nitrogen are more representative of Titan’s aerosols³. A new study has been initiated to determine the THS aerosols’ optical constants from the visible to Far IR (0.4-45 µm) using a new optical constant facility recently developed at NASA Ames.

Acknowledgements: This research is supported by the SSW Program of NASA SMD.

References

Scientific Theme(s)
• Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
• Experimental laboratory astrophysics

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Heavy element abundance in the spectrum of the primary component in an extremely rare eclipsing binary HD66051

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Poster number: 43

The rare eclipsing binary HD66051 with an orbital period of about 4.75 d hosts as a primary a HgMn-related star, and an A-type star as a secondary component (Niemczura et al. 2017). The abundance analysis of the HARPS spectrum of the primary indicates a highly peculiar composition with an overabundance of the iron-group, heavy (e.g. Xe, Hg and Pt) and REE elements. However, the recent work by Kochukhov et al. (2018) using the ESPaDOnS data characterizes the primary as a classical Si-strong Bp star with a longitudinal field of the order of 50–100 G. In contrast to HgMn stars, the presence of heavy elements (e.g. Xe) is not expected in magnetic Si-strong Bp stars, nor are such stars members of very close SB2 systems. The high-resolution, high signal-to-noise UVES spectrum of HD66051 is used to firmly establish the type of peculiarity of the primary which could be the first HgMn star with a definitely detected magnetic field.

References

Scientific Theme(s)
• Stars, stellar populations, and stellar explosions

Research Area(s)
• Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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Water ice photodesorption by VUV photons and X-rays investigated with synchrotron radiation

Fillion, J.\textsuperscript{1}, Dupuy, R.\textsuperscript{2}, Bertin, M.\textsuperscript{3}, Féraud, G.\textsuperscript{4}, Michaut, X.\textsuperscript{5}, Putaud, T.\textsuperscript{6}, Philippe, L.\textsuperscript{7}, Cimino, R.\textsuperscript{8}, Baglin, V.\textsuperscript{9}, Romanzin, C.\textsuperscript{10}

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Poster number: 44

Water ice is ubiquitous at the surface of planets in our solar-system and in the interstellar medium (ISM). It is the main component of the ice mantles covering the dust grains in various cold regions of the ISM. Interaction between condensed water and high energy radiation - such as Vacuum UV photons (VUV) and X-rays - are key processes in space. They play an important role in the balance between the gas phase and the solid phase through photodesorption. This phenomenon is indeed central to the understanding of the surface erosion of ices in many regions irradiated by UV/X photons. We present, for the first time, an investigation of the photodesorption of amorphous solid water using monochromatized synchrotron radiation from the SOLEIL facility in the VUV (7 -14 eV) and in the O 1s range (520 - 600 eV). The approach combines neutral and ion quantitative detection as a function of photon energy, and kinetic energy filtering of the ionic species. In the VUV, the desorption of neutral molecules (H\textsubscript{2}, O\textsubscript{2}, OH, H\textsubscript{2}O) involving the first electronic excited band, which has been previously studied (see for example \cite{1,2}), can be compared to that observed at higher energies. Isotopic effects observed from the comparison between H\textsubscript{2}O and D\textsubscript{2}O samples will be shown. In the X-ray domain, neutral species are also found to be by far the most abundant species desorbed \cite{3}. The energy relaxation and desorption processes that follow the valence electronic excitation in the VUV or the core excitation in the X-ray domain are discussed qualitatively and quantitatively. The importance of these new results for modelling protoplanetary disks is also highlighted.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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PAH Clusters as Interstellar Very Small Grains

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Poster number: 45

PAH clusters are one candidate species for the interstellar ‘very small grains’ or ‘VSGs’, i.e., dust grains small enough to be stochastically heated and contribute to the aromatic infrared emission bands (AIBs). This possibility motivated laboratory experiments on the infrared spectroscopy of PAH clusters using matrix isolation spectroscopy. The spectral shifts due to PAH clustering in argon matrices provide clues for the AIB contribution from PAH clusters in the interstellar medium. Here we review results from a number of small PAH species, extrapolation to the much larger PAHs believed to be present in the interstellar medium, and the implications for a PAH cluster contribution to the VSG population.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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Laboratory Studies of the Radiolytic Destruction of Nucleobases in Icy Environments

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Poster number: 46

Biological nucleobases have been identified in extraterrestrial samples such as meteorites [1] and may be present in a wide range of Solar System ices. Since the irradiation of organic compounds such as nucleobases or amino acids embedded in ices results in their modification or destruction [2,3], quantifying these radiolytic processes should allow better prediction of the survivability of organic species under a range of conditions. Since these compounds are of astrobiological interest, they likely will be target molecules for future sample-return missions.

The Cosmic Ice Lab at NASA Goddard Space Flight Center is studying the radiolytic destruction of nucleobases and determining their decay rate constants by subjecting biological nucleobases embedded in ices (H₂O or CO₂) to ∼ 1 MeV protons over a range of temperatures and relative concentrations. We use infrared spectroscopy to monitor the destruction of nucleobases after each radiation dose. We find that ice composition and irradiation temperature play significant roles in the radiolytic decay. Here, we present our results and their implications for the detection of nucleobases in different environments.

References

Scientific Theme(s)
• Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
• Experimental laboratory astrophysics

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Formation of NH$_2$CHO and CH$_3$CHO upon UV processing of interstellar ice analogs

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Poster number: 47

Complex organic molecules (COMs) are detected in a wide variety of astrophysical environments spanning all stages of star formation, and may have played a role in the formation of life in the early Earth[1]. In particular, formamide (NH$_2$CHO) is the simplest molecule containing the peptide bond, and acetaldehyde (CH$_3$CHO), with a similar structure, is also thought to play an important role in astrobiology. Pure gas-phase chemical models fail to reproduce the observed abundances of formamide in any region of the interstellar medium (ISM), and even when they reproduce the abundance of acetaldehyde in cold molecular clouds, an additional contribution of thermally desorbed CH$_3$CHO molecules from ice mantles is also needed in star-forming regions. These molecules are thus thought to be produced by energetic processing of interstellar ice mantles[2,3]. This process can be experimentally simulated in the laboratory under astrophysically relevant conditions using ultra-high vacuum chambers, and useful parameters such as apparent formation rates can be subsequently incorporated into theoretical models used for the interpretation of observations. I will present the formation of both formamide and acetaldehyde upon vacuum-ultraviolet (VUV) irradiation of CO:NH$_3$ and CO:CH$_4$ binary ice mixtures, simulating the UV processing of interstellar ices in the interior of dense clouds. The formation yield of formamide is high enough to build growth curves that can be used to compare the apparent kinetics of the formation process for different experimental conditions. For example, the apparent formation rate does not vary for temperatures in the 8-24 K range, which indicates that diffusion does not participate in the formation process of formamide molecules at those temperatures. NH$_2$CHO is more probably formed by barrierless radical-radical reactions of neighboring HCO and NH$_2$ radicals formed upon absorption of the VUV photons.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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Decomposition of infrared ice features using genetic modelling algorithms

Rocha, W. R.\textsuperscript{1}, Kristensen, L. E.\textsuperscript{2}, Jørgensen, J. K.\textsuperscript{3}
\textsuperscript{1}University of Copenhagen, Denmark, \textsuperscript{2}University of Copenhagen, \textsuperscript{3}University of Copenhagen

Poster number: 48

Ice mantles covering dust grains record the chemical heritage of star-forming regions and dense cores in Interstellar Medium. In order to understand how this ‘chemical memory’ is related to the physical evolution of Young Stellar Objects, several laboratory experiments have been performed by combining different compounds, proportions, and ionising sources as attempt to explain the observed ice features in the infrared spectrum as can be seen in [1] and [2]. Deciding which laboratory data provides the best fits to the IR spectra is challenging, however, due to resolution power of the observations and the huge number of combinations among the data to fit a specific feature. To get closer in solving this problem, a computational code using the principles of genetic algorithms is in development. We have present the first results applying this code to IR data of protostars in the nearby Ophiuchus Molecular Cloud. The code provides good fits to the IR features, and quantitative constraints as the relative abundances of different species and various pure and mixed ices.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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Galactic and Extragalactic ices with JWST

Rachid, M. G.\textsuperscript{1}, van Scheltinga, J. T.\textsuperscript{2}, Marcandalli, G.\textsuperscript{3}, Koletzki, D.\textsuperscript{4}, Linnartz, H.\textsuperscript{5}

\textsuperscript{1}Leiden University, Netherlands, \textsuperscript{2}Leiden University, \textsuperscript{3}Leiden University, \textsuperscript{4}Leiden University, \textsuperscript{5}Leiden University

Poster number: 49

It is generally accepted that complex organic molecules (COMs) can form in molecular clouds and protoplanetary disks on icy dusty grains, e.g., upon hydrogenation or VUV/cosmic-rays irradiation. The detection of solid COMs, however, are very limited. With the upcoming launch of James Webb Space Telescope (JWST) this will change, but in order to identify solid state features of COMs, accurate laboratory data are needed \cite{1}. The IR spectra of a molecule change with the ice matrix, temperature, morphology and other characteristics such as the degree of porosity \cite{2}. In this work, we present high resolution (0.5 cm\textsuperscript{-1}) infrared spectra of acetone and methyl formate. Acetone (CH\textsubscript{3}OCH\textsubscript{3}) is the smallest ketone and it can be involved in a number of reactions in the ISM \cite{3}, but it has not yet been detected. Methyl formate (HCOOCH\textsubscript{3}) was detected in the gas phase, but not in the solid phase. Methyl formate detection in solid phase and its quantification can be the key of a number of questions that have been raised concerning its relative large abundances in hot molecular cores \cite{4}. Here, we show the most important changes in the spectra of these molecules in different ice environments (H\textsubscript{2}O, CO, CO\textsubscript{2}, CH\textsubscript{3}OH) and at different temperatures (15 K - 150 K). All the IR data that has been collected and shown here will be available at Leiden Ice Database, a large collection of infrared spectra of ice mixtures in a range of temperatures. The Leiden Ice Database (see http://icedb.strw.leidenuniv.nl/) can be used by the astronomical community to better guide and interpret future infrared observational data.

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Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

Research Area(s)
• Experimental laboratory astrophysics

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Laboratory investigation of the formation of methoxymethanol in the CO-rich layer of the ice mantle

He, J.¹, Chuang, K.², Qasim, D.³, Fedoseev, G.⁴, Cuppen, H.⁵, Linnartz, H.⁶

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Poster number: 50

In the CO-rich layer covering dust grains in dense molecular clouds, atomic hydrogen addition and abstraction reactions as well as recombination of radicals were shown to form new complex organic species (COMs), including methanol, methyl formate, glycolaldehyde, ethylene glycol [see e.g. 1,2]. Methoxymethanol, which is also likely to be formed in the CO-rich layer, has recently been detected by ALMA in the high-mass star-forming region NGC 6334I [3]. So far, however, laboratory study of its formation in an interstellar ice analogue is lacking, causing ambiguities about its formation mechanism. In this contribution we present laboratory experiments using the SURFRESIDE2 apparatus to study the chemistry taking place when frozen formaldehyde is bombarded by atomic hydrogen, showing that for the conditions investigated the formation of methoxymethanol is efficiently enough to explain at least a significant fraction of the observed methoxymethanol abundance. We also show that at the detection limit of our experimental setup, the hydrogenation of methyl formate in the solid state does not seem to result in the production of any methoxymethanol. Based on these results we expect that the recombination of CH₂OH and CH₃O radicals is the most likely formation mechanism of methoxymethanol in the CO-rich layer.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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Modelling the properties of interstellar dust using the Si K-edge

Zeegers, S. T.¹, Costantini, E.², Rogantini, D.³, de Vries, C. P.⁴, Mutschke, H.⁵, Tielens, A. G.⁶, de Groot, F. M.⁷

¹ ASIAA (Academia Sinica Institute of Astronomy and Astrophysics), Taiwan, ² SRON Netherlands Institute for Space Research, ³ SRON Netherlands Institute for Space Research, ⁴ SRON Netherlands Institute for Space Research, ⁵ Astrophysikalisches Institut und Universitats-Sternwarte Jena, ⁶ Leiden Observatory, ⁷ Debye Institute for nanomaterials Science

Poster number: 51

The properties of interstellar dust (ID) can be studied in great detail by making use of X-ray spectroscopy techniques. The radiation of X-rays sources is scattered and absorbed by dust grains in the interstellar medium. The X-ray band is especially suitable to study silicates - one of the main components of ID -since it contains the absorption edges of Si, Mg, O and Fe (e.g., [1,2]). In the Galaxy, we can use absorption features in the spectra X-ray binaries to study the size distribution, composition and crystalline structure of grains ([2,3]). In order to derive these properties, it is necessary to acquire a database of detailed extinction cross sections models, that reflects the contents of the dust in the interstellar medium. We present the extinction profiles of a set of newly acquired measurements of 15 dust analogues at the Soleil Synchrotron facility in Paris, where we focus on silicates and the Si-K edge in particular, which is modelled with unprecedented accuracy. These models are used to analyse ID in the dense environments of the Galaxy (Zeegers et al. 2018, in prep.).

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

Research Area(s)
• Experimental laboratory astrophysics

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Zigzag and armchair PAH subpopulations as probes of the local radiation environment

Ricca, A.\textsuperscript{1}, Roser, J. E.\textsuperscript{2}, Peeters, E.\textsuperscript{3}, Boersma, C.\textsuperscript{4}
\textsuperscript{1}\textit{SETI Institute/NASA Ames Research Center, United States, \textsuperscript{2}\textit{SETI Institute/NASA Ames Research Center, University of Western Ontario, \textsuperscript{4}\textit{NASA Ames Research Center}}

Poster number: 52

As is unequivocally evident from observations, Polycyclic Aromatic Hydrocarbons (PAHs) pervade the Universe. PAHs are easily detected through their vibrational IR emission bands at 3.3, 6.2, 7.7, 8.6 and 11.2 micron. They are found in a wide variety of environments, including post-AGB stars, planetary nebulae, young stellar objects, HII regions, reflection nebulae, the interstellar medium, and galaxies out to redshifts of $z \sim 3$. To date, PAHs are among the largest and most complex molecules known in space. They emit up to 10\% of the total power output of star-forming galaxies and harbor a significant fraction of the cosmic carbon. Being so abundant and widespread, PAHs play a crucial role in several astrophysical and astrochemical processes such as the heating of the diffuse ISM and surfaces of molecular clouds and proto-planetary disks, gas-phase abundances and surface chemistry.

The Infrared Space Observatory (ISO) and the Spitzer Space Telescope showcased the richness and complexity of the astronomical PAH spectra. The PAH features exhibit significant variability and depend on several parameters such as radiation field, object type and metallicity. These variations thus reflect both the physical conditions in the emission zones and the composition of the PAH population, i.e. the different PAH sub-populations which each respond differently to the local environment. The interpretation of current infrared spectra from ISO and Spitzer and future IR spectra from JWST requires infrared spectroscopic data of relevant PAH subpopulations. Here we compute the IR spectral characteristics of zigzag and armchair PAH subpopulations and assess their relevance for the PAH band profile classes.

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

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A quantitative approach to measuring VUV-triggered processes in icy (solid-state) COMs

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Poster number: 53

Vacuum UV irradiation of interstellar ice analogues comprising of relatively simple components was shown to result in the formation of a large number of rather complex species. The initial experiments focused on the chemical enrichment of bulk ices, analyzing the resulting residues using gas chromatography. More recently, cryogenic VUV ice studies use ultra high vacuum setups in which photo-products are monitored using spectroscopic (e.g. RAIRS) and mass spectrometric (e.g. TPD QMS) techniques. Such experiments allow to study ices in situ and also for more controlled conditions, but suffer from the fact that it becomes harder and harder to unambiguously identify larger complex species. For this reason, a few years ago, a new technique was introduced in Leiden in which the VUV irradiation of ices was combined with time-of-flight mass spectrometry [1,2]. In this contribution, we extend on this work, introducing a new method to measuring, quantitatively, photodesorption, photodissociation and recombination rates upon VUV processing of frozen complex organic molecules. It is possible to determine the rates of the three processes mentioned above by looking at how the depletion rate of the parent species changes in different experiments. First comparison is based on VUV processing of a pure thin ice with and without a non-reactive layer (argon) on top. The role of the top layer, here, is to quench any photodesorption processes. Furthermore the recombination rates can be limited by embedding the species of interest in the water matrix which upon irradiation yields highly reactive OH radicals. We demonstrate this method on the example of CO, confirming earlier data available from the literature [3] and present our first results for acetonitrile.

References


Scientific Theme(s)

- Star formation and the cosmic matter cycle in the near universe, Protoplanetary disks, debris disks, and the Solar System

Research Area(s)

- Experimental laboratory astrophysics

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Prebiotic chemistry under a simulated young sun

Rimmer, P. B.\textsuperscript{1}, Thompson, S.\textsuperscript{2}, Xu, J.\textsuperscript{3}, Sutherland, J. D.\textsuperscript{4}, Queloz, D.\textsuperscript{5}

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Poster number: 54

I discuss the design of a novel experimental apparatus that accurately reproduces the ultraviolet spectrum of the young sun impinging on the surface of the Early Earth. The apparatus consists of a D\textsubscript{2} and Xe lamp, a container filled with H\textsubscript{2}O used to control the sample temperature, with a loading bay for the sample at the top. The sample is irradiated, during which the D\textsubscript{2} lamp focus can be shifted to simulate flares, and liquid filters can be included in the path of the light beams to simulate different atmospheric conditions or aqueous environments. Prebiotic chemistry is explored using these samples, for the first time incorporating accurate broadband UV light. I will reveal the results from this experiment: new pathways for prebiotic synthesis of nucleotides and amino acids, as well as constraints for the environmental conditions under which life may have arisen on the Earth’s surface. I will finish with a brief discussion on the implications for the search for life on exoplanets.

Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Experimental laboratory astrophysics

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Quenched Nitrogen-included Carbonaceous Composite (QNCC): a powerful candidate of the carriers of the UIR bands in classical novae

Endo, I.\textsuperscript{1}, Sakon, I.\textsuperscript{2}, Onaka, T.\textsuperscript{3}, Lau, R. M.\textsuperscript{4}, Helton, A. L.\textsuperscript{5}, Kebukawa, Y.\textsuperscript{6}, Kimura, S.\textsuperscript{7}, Wada, S.\textsuperscript{8}, Ogawa, N.\textsuperscript{9}, Ohkouchi, N.\textsuperscript{10}

\textsuperscript{1}University of Tokyo, Japan, \textsuperscript{2}University of Tokyo, \textsuperscript{3}University of Tokyo, \textsuperscript{4}Jet Propulsion Laboratory, California Institute of Technology, \textsuperscript{5}SOFIA Science Center, USRA, NASA Ames Research Center, \textsuperscript{6}Yokohama National University, \textsuperscript{7}The University of Electro-Communications, \textsuperscript{8}The University of Electro-Communications, \textsuperscript{9}Japan Agency for Marine-Earth Science and Technology, \textsuperscript{10}Japan Agency for Marine-Earth Science and Technology

Poster number: 55

The Unidentified infrared (UIR) bands have been ubiquitously observed in various astrophysical environments. Many studies have been conducted to identify the band carriers based on combined approaches among infrared observations, theoretical calculations and laboratory experiments. Polycyclic aromatic hydrocarbon (PAH) hypothesis has been commonly used to interpret the nature of the UIR bands. However, the true nature of the carriers has not been fully understood so far. Recently, mixed aromatic aliphatic organic nanoparticles (MAON), which contain hetero atoms in addition to hydrocarbon models, has been proposed as a more realistic interpretation of the band carriers \cite{1}. Further experimental approaches to examine the influence of nitrogen inclusion into hydrocarbons are crucial for the better understanding of the band carriers. In this presentation, we report the success in synthesizing organics, ‘Quenched Nitrogen-included Carbonaceous Composite (QNCC)’, via plasma chemical vapor deposition (CVD) method, whose infrared spectral properties reproduce the characteristics of the UIR bands observed around classical novae \cite{2}. Past studies have shown that the UIR bands observed around novae appear somewhat differently from those observed in other astrophysical environment and are predominantly characterized by the presence of broad 8\textmu m feature \cite{3}. We found that N/C ratio (atom) of the QNCC is 4-5% based on the measurement with EA/IRMS. X-ray Absorption Near Edge Structure (XANES) analysis of QNCC indicates that amine structures are contained in the QNCC. We concluded that the broad feature at 8\textmu m is arising from amine structures in addition to aromatic C-C structures. The remarkable similarity between the infrared properties of QNCC and the UIR bands in novae indicates that organics containing amine structures should be the strong candidate of the carriers of the UIR bands in novae (Endo et al. in prep).

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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Laboratory Astrophysics Studies with the COSmIC Facility at NASA Ames

Salama, F., Sciamma-O’Brien, E., Bejaoui, S., Gavilan, L., Dubois, D.
1NASA Ames Research Center, United States, 2NASA Ames Research Center, 3NASA Ames Research Center & Bay Area Environmental Research Institute, 4NASA Ames Research Center & NPP/USRA, 5NASA Ames Research Center & Bay Area Environmental Research Institute

Poster number: 56

The COSmIC facility was developed at NASA Ames to study interstellar, circumstellar and planetary analogs in the laboratory [1]. COSmIC stands for ‘Cosmic Simulation Chamber’ and is dedicated to the study of neutral and ionized molecules and nanoparticles under the low temperature and density conditions that are required to simulate space environments. COSmIC integrates a variety of instruments that allow generating, processing, and monitoring simulated space conditions in the laboratory. It is composed of a Pulsed Discharge Nozzle (PDN) expansion that generates a plasma in a free supersonic jet expansion, coupled to high-sensitivity, complementary in situ diagnostic tools used for the detection and characterization of the species present in the expansion: Cavity Ring Down Spectroscopy (CRDS) and fluorescence spectroscopy systems for photonic detection and a Reflectron Time-Of-Flight Mass Spectrometer (ReTOF-MS) for mass detection. Recent advances achieved in laboratory astrophysics using COSmIC’s laboratory data in synergy with observational data will be presented. These results include (1) the diffuse interstellar bands (DIBs) with applications to the ESO Diffuse Interstellar Bands Large Exploration Survey (EDIBLES [2]), (2) the formation of dust grains and aerosols from their gas-phase molecular precursors in environments as varied as (i) circumstellar outflows [3] and (ii) planetary atmospheres [4]. Plans for future laboratory developments and techniques to study cosmic molecules and grains (including NIR-MIR CRDS, laser induced fluorescence (LIF) and incandescence (LII)) will also be addressed as well as their astronomical applications.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe, Solar System formation and the pre-solar nebula, Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
• Experimental laboratory astrophysics

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Electronic Spectroscopy of PAHs and PAH derivatives in Supersonic Jet. Astrophysical Implications

Bejaoui, S.\textsuperscript{1}, Salama, F.\textsuperscript{2}

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Poster number: 57

Polycyclic Aromatic Hydrocarbon (PAHs) molecules are thought to be ubiquitously present in space because of their ability to survive in the harsh environmental conditions of the interstellar medium. PAHs are proposed as the carriers of the IR emission bands and have been suggested as plausible carriers of the still unassigned diffuse interstellar bands (DIBs) for more than two decades now. The so-called PAH-DIB proposal has been based on the abundance of PAHs in the ISM and their stability against photo and thermo dissociation. PAH derivatives (PANs, polyynyl-substituted PAHs) exhibit spectral features similar to PAHs and may also contribute to the unidentified spectral bands. We present in this work high-resolution electronic spectra of interstellar PAH analogs. The measurements are performed in the cosmic simulation chamber (COSmIC) where the target molecules are seeded in argon carrier gas and expand through a thin slit into the vacuum chamber to generate a cold a supersonic jet expansion ($\approx 100$ K) \cite{1}. Using highly sensitive laser-based diagnostics such as the cavity ring down spectroscopy and the laser induced fluorescence techniques; we studied the absorption and the emission signatures of PAHs under astronomical relevant conditions. Electronic spectroscopy probes transitions that are unique for each molecule, and hence offers an exceptional tool for the assignment of signatures in astronomical spectra to specific molecules or ions. The intrinsic band profiles of the PAH molecules provide a conclusive and direct comparison with DIBs and serve as a guide for the astronomical search for new interstellar bands. Our approach, to assign PAH as carriers of some DIBs, and more generally to search for PAH signatures in the diffuse ISM, consists in recording the electronic spectra of the cold PAHs in the gas phase and performing a systematic search for possible correspondences with features in astronomical spectra \cite{2}.

References


Scientific Theme(s)

- Star formation and the cosmic matter cycle in the near universe

Research Area(s)

- Experimental laboratory astrophysics

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Vacuum Ultraviolet photoabsorption of molecules with astrochemical and astrobiological relevance: Benzonitrile and Hydroxylamine

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Poster number: 58

The recent detection of benzonitrile [1], as the first benzene derivative, in the ISM has attracted considerable interest across the astrochemical community. This detection also provides a potential indirect method to measure the abundance of the most basic aromatic species: benzene which is a building block for other PAHs known to be present in the ISM. However the source(s) of origin of benzonitrile and the mechanism for its formation in the extra-terrestrial environments, still remains an open question. To explore the routes leading the formation of benzonitrile and its reactions, it is necessary to characterize the molecule. Here, we present the VUV spectrum for benzonitrile in the ice phase. This is then linked with the VUV study of benzene [2] as a part of a wider study of polyaromatic hydrocarbons which may be influential in the photodesorption and photochemical process within the ice mantles.

The prebiotic molecules generate a significant astrobiological interest as they can lead to answering the mysteries on the origin of life. Nitrogen-containing molecules, including amino acids, form an important category within the wide range of the prebiotic molecules and hydroxylamine (NH₂OH) is one of the precursor candidates which can lead to their formation. The thermal desorption study [3] on the oxidation of ammonia leading to the formation of this species encouraged this VUV irradiation study where we present the photoabsorption spectrum of hydroxylamine.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe, Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
• Experimental laboratory astrophysics

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Microscopic simulations of laboratory and interstellar ice structure and chemistry

Garrod, R. T.¹, Clements, A. R.²
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Poster number: 59

Laboratory ice experiments play a crucial role in determining the behavior of dust-grain surface chemistry in interstellar and star-forming regions. An important determinant of this behavior is the structure of the ice in which the molecules exist, and thus the mechanisms and means by which the ices are formed (i.e. surface reactions, direct deposition, angle of deposition, surface temperature). Trapping of volatile molecules (e.g. CO) in porous structures within water ice is a particularly well-known phenomenon, and the extra surface area provided by pores may also lead to enhanced surface-chemical effects in cases where the ice constituents are chemically active.

In order to properly extrapolate these measurable effects from laboratory conditions and timescales out to those of the interstellar medium requires microscopic chemical kinetic models that can first explain the experimental data. Using the off-lattice Monte Carlo chemical kinetics model MIMICK, we have been working toward a self-consistent set of models that can be used to reproduce each stage of an astrophysical ice experiment, beginning with the simple deposition of water, and the build-up of porous structure. As well as calculating the porosities of simulated ices directly, we simulate typical laboratory methods of porosity determination such as N₂ deposition, making use of all available data to constrain the models. These models can then be directly translated from periodic boundary conditions to a three-dimensional simulation of an individual dust grain.

I will present a selection of simulations covering laboratory water ice deposition, temperature-programmed desorption of mixed ices, and chemical formation of surface molecules. I will demonstrate how different mechanisms affect the porous structures of the ices that are formed, and how we expect them to evolve over astrophysical timescales. These simulations provide a critical link between experimental and observational astrochemistry.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

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Fragmentation of neutral PAHs upon UV irradiation

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Poster number: 60

Polycyclic Aromatic Hydrocarbons (PAHs) are considered to be a major component of the interstellar carbon inventory. The (photo)chemistry or evolution of PAHs hence governs the carbon chemistry in the interstellar medium (ISM) significantly, yielding new species and playing an important role in processes such as fullerene formation [1], \( \text{H}_2 \) formation [2] and isotopic fractionation. The fragmentation patterns and processes are still largely unknown and many aspects are currently being investigated, including the evolution of PAHs into fullerenes [3] and the formation of molecular hydrogen in photodissociation regions (PDRs). Most of this work has focused on ionic species. In this work, we aim to investigate the dissociation patterns of neutral PAHs and H-PAHs upon photolysis and validate theoretical predictions. We use high-resolution spectroscopy techniques on cold molecular beams and to measure mass spectra as well as the UV/VIS spectra of small to large neutral PAHs and H-PAHs.

References

Scientific Theme(s)
• Reaching beyond our galaxy: from extra galactic chemistry to dark matter

Research Area(s)
• Experimental laboratory astrophysics

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Does the initial mixing ratio of an interstellar ice analogue affect the formation of products when it is processed with electrons?

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Poster number: 61

Numerous experimental studies show that mixtures of simple molecules (e.g. H₂O, CO₂, CO, CH₄, NH₃, CH₃OH) can produce bigger, more complex molecules after energetic processing (e.g. electrons, UV photons, ions) [1]. However, few studies systematically change the mixing ratios of the starting molecules and hence, we do not know whether the irradiation products formed are universal to all ratios. It is important to investigate what effect the initial mixing ratio has on product formation as observations of interstellar ice show that the composition and abundances of molecules can vary significantly between different interstellar clouds [2]. Additionally, varying the mixing ratio can help with the elucidation of formation pathways of some of the more complex irradiation products. A systematic, experimental study of electron irradiated CO₂:NH₃ and CH₃OH:CO₂ interstellar ice analogues as a function of initial ice ratio will be presented. A combination of mid-IR (4000 - 800 cm⁻¹) and vacuum-UV (110 - 340 nm) spectroscopy is used to determine how the initial mixing ratio of the ice affects product formation and the consequences of these results on astrochemical models and observations will be discussed.

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe

Research Area(s)
• Experimental laboratory astrophysics

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How to correctly model IR spectra of nanoclusters of astronomical interest

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We assess the accuracy of various computational methods for obtaining infrared (IR) spectra of silicate nanosized dust grains directly from the atomistic structure and their atomic motions. First, IR spectra for a selection of small nanosilicate clusters with a range of sizes and chemical compositions are obtained using density functional theory (DFT) within the harmonic oscillator approximation. To check if anharmonicity effects play a significant role in the IR spectra of these nanoclusters, we further obtain IR spectra from finite temperature DFT-based ab initio molecular dynamics (AIMD). For all these calculations we compare the performance of both the PBE0 and B3LYP hybrid exchange and correlation functionals. Finally, we also study the effect of temperature on the broadening of the obtained IR spectra peaks in a range of larger nanosilicate grains with a range of crystallinities. In this case, less computationally costly classical MD simulations are necessary due to the large number of atoms involved. In all cases we compare our results with relevant and available IR spectra from experiment and observation. Generally, we find that although DFT-based methods are more accurate, surprisingly good IR spectra can also be obtained from classical MD calculations.

Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

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Collision of centimeter-size water ice particles: impact of the surface roughness.

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Poster number: 63

Latest review report the detection of more than 3500 exoplanets and if we know that they are formed by accretion of kilometer-sized objects, the formation mechanisms of these planetesimals still raise tenacious questions. In a bottom-up scenario, the aggregation the nano- to micro-meter sized interstellar grains driven by van der Walls forces has been shown to be able to form milimeter sized particles. Arriving at this scale, the growth is still under question.

Beyond the snowline in protoplanetary disks, all the grains are covered by a layer of water ice whose composition, density and allotropic form are very dependant on the gas compositions and physical properties, but also vary with the history the ices underwent. Recently, collisional properties of crystalline icy particles have been studied at various velocities for centimeter particles have been carried out and reveal that the major collision outcomes are bouncing and fragmentation, and that the coefficient of restitution is very low \cite{Hill2015}. Moreover, Gaertner et al. \cite{Gaertner2017} recently showed that collisional properties of icy particles were strongly dependant on the surface properties. In that optics, we aim to study the influence of surface surface geometry and roughness on the collisional properties of these icy particles.

In order to conduct these experimental works, a cryogenically-cooled experimental setup described in Salter et al. \cite{Salter2009} will be used to collide centimeter-sized particles at velocities within $1 \text{−} 5 \text{ m s}^{-1}$. Ice particles with Various surface geometries will be produced and collided, and filmed by high-speed camera. Finally, the obtained results will be analyzed to understand how the collisional properties vary with the grain surface roughness, speed and with respect to temperature.

These results will be presented as preliminary studies aiming to prepare a parabolic flight campaign studying low-velocity collisions of amorphous icy particles in microgravity conditions.

References
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\end{enumerate}

Scientific Theme(s)
\begin{itemize}
\item Protoplanetary disks, debris disks, and the Solar System
\end{itemize}

Research Area(s)
\begin{itemize}
\item Experimental laboratory astrophysics
\end{itemize}
Gas-phase UV cross sections of radicals

Heays, A. N.\textsuperscript{1}, de Oliveira, N.\textsuperscript{2}, Lewis, B. R.\textsuperscript{3}, Stark, G.\textsuperscript{4}, Lyons, J.\textsuperscript{5}, van Hemert, M. C.\textsuperscript{6}, van Dishoeck, E. F.\textsuperscript{7}

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Radicals are certainly observationally important and their dissociation by UV radiation is closely integrated with the chemical cycles of the ISM and planetary upper-atmospheres. In some cases the detailed rovibrational structure of electronic transitions in the UV also leads to interesting isotope effects. However, the laboratory measurement and theoretical calculation of UV cross sections continues to be a challenge even for classical molecules.

With collaborators, I have been studying the photodissociation cross sections of small fundamental molecules, OH, S\textsubscript{2}, SO, and CN, and some of their isotopologues. The former three were measured at the DESIRS VUV beamline of the SOLEIL synchrotron, and CN was studied with a high-level ab initio calculation.

In this talk I will review the methods used, the challenges involved, the results obtained for these molecules, and their application to astrochemistry.

Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Experimental laboratory astrophysics

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H$_2$ Catalysis Through Superhydrogenation of Interstellar Polycyclic Aromatic Hydrocarbons

Simonsen, F. D.\textsuperscript{1}, Jensen, P. A.\textsuperscript{2}, Skov, A. W.\textsuperscript{3}, Hornekær, L.\textsuperscript{4}
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Poster number: 65

In the field of laboratory astrochemistry a primary objective is to identify and characterize effective catalysts in the interstellar medium (ISM). Molecular hydrogen (H$_2$) is the most abundant molecule in the ISM with well-established and efficient catalytic formation routes in many regions of inter-stellar space. However, in photodissociation regions (PDRs), the dissociation rate is so high that prevailing formation routes may not be efficient to explain the observed formation rates of H$_2$ \cite{1}. Here we examine a group of planar nanosized molecules called polycyclic aromatic hydrocarbons (PAHs) as possible catalysts. Using temperature programmed desorption (TPD) and scanning tunneling microscopy (STM) we study superhydrogenation of coronene (C$_{24}$H$_{12}$), pentacene (C$_{22}$H$_{14}$) and pentacenequinone (C$_{22}$H$_{12}$O$_2$). Density functional theory (DFT) reveals that coronene and possibly other PAHs will have 0eV barriers towards Hydrogen (H) addition and H$_2$ abstraction at low superhydrogenation degrees \cite{2}. The state of hydrogenation will depend on these competing processes and their relative cross sections for addition, $\sigma_{\text{add}}$, and abstraction, $\sigma_{\text{abs}}$. We expose the PAHs to atomic beams of deuterium (D) or H with temperatures of ca. 1000K. The PAHs reveal fully deuterated species, and hence the H/D exchange process reveals molecular HD formation \cite{3}. First addition cross sections, $\sigma_{\text{add}}(0)$ for D/H addition are found from the exponential decay in the pristine PAHs as a function of D/H fluence. Also observed from TPD are indications of preferred D/H-PAH configurations with high stability and increased barriers against further D/H addition. In addition, experiments have been carried out at the free electron laser facility, FELIX. H-PAH structures show indications of H$_2$ loss and C-C bond fragmentation which depend on the position of their aliphatic groups and on the IR wavelength which also reveal the vibrational modes of the molecules.

References
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Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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The chemistry of episodic accretion

Rab, C.\textsuperscript{1}, Elbakyan, V.\textsuperscript{2}, Vorobyov, E.\textsuperscript{3}, Güdel, M.\textsuperscript{4}, Dionatos, O.\textsuperscript{5}, Audard, M.\textsuperscript{6}, Kamp, I.\textsuperscript{7}, Thi, W.\textsuperscript{8}, Woitke, P.\textsuperscript{9}, Postel, A.\textsuperscript{10}

\textsuperscript{1}Kapteyn Astronomical Institute, Netherlands, \textsuperscript{2}Research Institute of Physics, Southern Federal University, \textsuperscript{3}University of Vienna, \textsuperscript{4}University of Vienna, \textsuperscript{5}University of Vienna, \textsuperscript{6}University of Geneva, \textsuperscript{7}Kapteyn Astronomical Institute, \textsuperscript{8}Max-Planck-Institut f"ur extraterrestrische Physik, \textsuperscript{9}University of St. Andrews, \textsuperscript{10}University of Geneva

Poster number: 66

Episodic accretion is an important process in the evolution of young stars and their environment. A consequence of an episodic accretion event are observed strong luminosity bursts which can last for 100s of years. The most prominent example showing such a burst is FU Orionis. Those bursts, which mainly heat the protostellar environment, likely have a long lasting (up to 10 000 years after the burst) impact on the chemical evolution of the disk and envelope of young stars.

We developed a new model for the chemistry of episodic accretion based on the two dimensional, radiation thermo-chemical disk code ProDiMo \cite{Woitke2016}. With this model we can follow the chemical evolution before, during and after the luminosity outburst including proper radiative transfer modelling to determine the temperature structure and radiation field.

We studied the chemical evolution of CO in the post-burst phase for a representative Class I protostar \cite{Rab2017}. In the post-burst phase CO freezes out from inside-out as the densities closer to the protostar are higher than farther out. This produces clear observational signatures such as rings and gradients in radial intensity profiles that can be observed with ALMA and allow to identify targets that experienced an outburst thousands of years ago.

We also present a model for the outbursting source V883 Ori where we fitted available observational data to get an accurate physical structure. This allows for a detailed study of the chemistry of episodic accretion. We can predict the location of the water ice line in the disk of V883 Ori and the abundance of molecules that sublimated from dust grains during the burst. Molecules such as methanol were recently observed with ALMA \cite{van2018}. V883 Ori is therefore an ideal testbed to study the sublimation, freeze-out and the chemistry of molecules which are otherwise difficult to observe in disks around protostars.

References

\cite{Woitke2016, Rab2017, van2018}

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe, Solar System formation and the pre-solar nebula

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data
Laboratory spectroscopy: from macroscopic molecular films to microscopic icy grains

Dawes, A.¹

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Poster number: 67

Carbonaceous material, ranging from polycyclic aromatic hydrocarbons (PAHs) to microscopic dust particles, is prevalent in the interstellar medium and the Solar System playing an important role in ice chemistry either by directly being involved in chemical processes or acting as condensation nuclei for ice mantle formation.

Benzene is a model aromatic molecule and a precursor to PAHs and its interaction with other molecules is of considerable interest in physical chemistry and astrochemistry. I will discuss the interaction between benzene and water ice from laboratory results of vacuum ultraviolet spectroscopy performed at the ASTRID2 synchrotron facility (Aarhus, Denmark) and infrared spectroscopy at the OU Molecular Physics Laboratory [1].

There is still much we do not understand about the physical and chemical properties of ices formed on microscopic dust particles, as opposed to vapour deposited ices grown on flat cm-sized substrates in the laboratory. There exist discrepancies between observational and laboratory spectra. One key problem is the infrared band profile of the 3 micron (O-H) stretch ‘ice band in the observational spectra of star forming regions that exhibits a characteristic extended ‘red wing’ excess [2]. Since Smith et al. [3] first suggested that interstellar grain size and shape could explain this extended ‘red wing’, this issue has been widely debated but remains unresolved and to date has not been reproduced in the laboratory. I will show some of my recent work on developing an ultrasonic trap and give a sneak peek at some recent preliminary results investigating the optical properties of levitated microscopic icy soot particles.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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Investigation of rotational state-changing collisions of CCN$^-$ ions with helium

Franz, J.¹, Gianturco, F. A.²

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Poster number: 68

Molecular anions which contain carbon chains, like C₄N⁻ and C₆N⁻, have already been found in the interstellar medium [1]. There is still no evidence for the existence of C₂N⁻ in interstellar medium. However, it is well known, that the molecule C₂N can form stable anions [2]. Because of their large dipole moments, these species have large rotational cross sections for rotational inelastic collisions with atomic species, like Helium [3]. Rotational inelastic collisions can accelerate the cooling of atomic gases by converting collisional energy into rotational energy, which can be emitted by radiation [3]. We are presenting results from quantum scattering calculations for the rotational inelastic collision process, C₂N⁻(J) + He → C₂N⁻(J) + He.

From our results we try to give some estimates for the cooling efficiency of the species C₂N⁻, C₄N⁻, C₆N⁻.

References

Scientific Theme(s)
• Reaching beyond our galaxy: from extra galactic chemistry to dark matter

Research Area(s)
• Theoretical calculations or simulations in laboratory astrophysics

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The gas structure of the HD 163296 planet-forming disk - Gas gaps or not?

Rab, C.1, Muro-Arena, G.2, Kamp, I.3, Dominik, C.4, Waters, R.5, Thi, W.6, Woitke, P.7
1Kapteyn Astronomical Institute, Netherlands, 2Anton Pannekoek Institute, University of Amsterdam, 3Kapteyn Astronomical Institute, 4Anton Pannekoek Institute, University of Amsterdam, 5SRON Netherlands Institute for Space and Research, 6Max-Planck-Institut für extraterrestrische Physik, 7University of St. Andrews

Poster number: 69

High spatial resolution observations have revealed stunning ring and gap features in the dust emission of several planet-forming disks, indicating that such features are quite common in disks around low and intermediate mass stars. Those gaps might trace ongoing planet formation, but also alternative theories for their origin exists (e.g. ice lines). Furthermore, it is not yet clear to what extent the gas follows the dust distribution; i.e. are the dust gaps also depleted in gas?

One example of such a gap/ring disk is the massive disk around the 5 Myr old Herbig Ae/Be star HD 163296. The dust disk was modelled in detail by [1], using high spatial resolution ALMA and SPHERE images, which provide strong constraints for both the large and small dust grain population.

On top of this azimuthally symmetric dust disk model, we model the gas structure using the 2D radiation thermo-chemical disk code ProDiMo (PROtoplanetary DIsk MOdel, [2]). We calculate besides the dust temperature also consistently the gas temperature, the chemical abundances and the resulting spectral line emission.

We show the impact of dust gaps on the gas temperature and chemistry and discuss to what extent a depletion of the gas inside the dust gaps is required to explain already available CO gas observations [3]. Furthermore, we show what kind of observations are needed to better constrain the gas density in the gaps (e.g. the gap width). Using multiple molecules such as CO, CN and CS allows to trace the different chemical processes within the gaps and consequently allow for a more accurate estimate of the possible gas depletion within the dust gaps. Such models, combined with high-quality observational data, provide crucial information for planet formation theories and constraints for the various proposed dust gap formation models.

References

Scientific Theme(s)
• Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
• Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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The latest spectral analysis on asteroids at NAO Rozhen

Vchkova Bebekovska, E.\textsuperscript{1}, Apostolovska, G.\textsuperscript{2}, Borisov, G.\textsuperscript{3}, Donchev, Z.\textsuperscript{4}

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Poster number: 70

By virtue of the physical, chemical and dynamical properties of asteroids, researchers gain insight into the formation and evolution of our Solar system. These objects are carrying important information regarding the formation of our planetary system and its evolution. Knowing the spectral class of an asteroid is one of the first steps for determining its chemical properties. Furthermore, for detailed analysis of the spectrum we have used mineralogical diagnosis with RELAB database of NASA. In our work the spectral classification of several asteroids was done by comparing their spectra with the laboratory spectrum. We determined spectral types of the asteroids \[1\] by the overall shapes of the spectra between 450 nm and 700 nm. In our spectral analysis we have used public software tool M4AST \[2\], which covers aspects related to taxonomy, curve matching with laboratory spectra, space weathering models, and mineralogical diagnosis. The wavelength calibration of asteroid spectra was made by measuring the pixel position of the lines in the spectrum of neon calibration lamp and fitted them with their laboratory wavelengths. Increasing the number of asteroids with known rotation period, shapes and spectral classification enrich the database of physical and dynamical properties of asteroid population.

References

Scientific Theme(s)
- Solar System formation and the pre-solar nebula

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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Asteroid collisions as origin of debris discs - asteroid shape reconstruction from BNAO Rozhen photometry

Apostolovska, G.\(^1\), Vchkova Bebekovska, E.\(^2\), Kostov, A.\(^3\), Donchev, Z.\(^4\)

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Poster number: 71

As a result of collisions during their lifetimes, asteroids have a large variety of different shapes. The Hubble image of the main belt active asteroid P/2010 A2 is very rare act of catching asteroid collision. High velocity collisions or rotational spin-up of asteroids continuously replenish dust to debris discs around extrasolars [1]. Knowledge of the spin and shape parameters of the asteroids is very important for understanding collision asteroid processes. Lately photometric observations of asteroids shown that variations in brightness are not accompanied by variations in colour index which indicate that the shape of the lightcurve is caused by variable illuminated surface of the asteroid rather than albedo variegation over the surface. It was confirmed when photometric investigations were combined with laboratory experiments [2]. The lightcurve inversion technique [3] introduced at the beginning of the last decade provide shape model represented by a convex polyhedron which approximates the real nonconvex shape of an asteroid. In order to reconstruct the asteroid shape and spin axis direction using lightcurve inversion technique we need a set of dense lightcurves obtained at different geometric conditions during several oppositions. Our photometric observations of asteroids were performed at Bulgarian National Astronomical Observatory (BNAO) Rozhen with 2m RCC telescope, 50cm/70cm Schmidt and 60cm Cassegrain telescope. About fifteen main belt asteroids were observed during four or more oppositions since 2002. Using convex lightcurve inversion method we obtained the sense of rotation, pole solutions and preliminary shape of few asteroids. Due to the lack of space missions, information about morphology and dynamical characteristics of asteroids have be found mostly from lightcurves, obtained from photometric observations with ground-based telescopes. This situation will dramatically be changed with the new space mission GAIA.

References

Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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Census and Modeling of Molecular and Gas-Dust Clouds in Galaxies

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Poster number: 72

The hydrogen and re-condensed dust are implicated in the formation and chemistry of molecular and gas-dust clouds (ISC). These point the importance of census and survey of ISC populations in galaxies in attempt to solve some problems of physics and evolution of ISC system in the Galaxy (MW) and external galaxies (EG), their impact on the dynamics and evolution of host galaxies. Based on data available in databases (as well as in previous catalogs like Fukui et al. 2010, Dobashi 2011) and using the data mining technology (aka, KDD) the cross-identified all-sky catalogs (l, b, d, D, M, n, T, vr, pm, etc.) of ISC were created for MW and 19 EG. Albeit the mass fraction of atomic and molecular gas contained not so much (0.001-0.3 in EG, 0.02 in MW) they localize wider than stellar content. The MW catalog has about 7000 entries (more than 1064 entries in Rice et al., 2016) with 200 large, >2500 smaller ISC (> 5000 objects including clumps and cores) observed at D < 11 kpc. For EG they belong to giant or hyper-giant ISC type according the range of their masses and sizes as well as other physical parameters. 3-D spatial distribution and physical properties of ISC in MW and several EG were drawn and analyzed. The statistical and physical correlation analyses were performed on ISC features in MW and compared with ISC in EG. The theoretical modeling of dynamical evolution and the physical model of ISC systems in MW and EG are discussed. ISC mass and angular moment (AM) follow a linear relationship for galaxy disks of rich in gas, where active star formation (SF) occurs. AM range extends by three orders of magnitude. Thus, the gas disks of both giant spirals and dwarf irregular galaxies are apparently located near the boundary of gravitational instability that promotes active SF. The complex program of ISC observations to cover the gaps in observed physical parameters using the 70 meter Suffa radio telescope reestablishing in Uzbekistan is also prepared.

References


Scientific Theme(s)

• Star formation and the cosmic matter cycle in the near universe, Reaching beyond our galaxy: from extra galactic chemistry to dark matter

Research Area(s)

• Observations showing use of laboratory astrophysics in the interpretation/understanding of data
A final-state resolved merged-beam experiment of mutual neutralization of Li\(^+\) and D\(^-\) at stellar photospheric temperatures at DESIREE

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Poster number: 73

We report on a merged beam experiment on the mutual neutralization (MN) of Li\(^+\)/D\(^-\) at low energies (0–0.6 eV), performed at the new double electrostatic storage ring national facility DESIREE in Sweden [1]. The aim is to demonstrate the ability to resolve the Li(3s) and Li(3p+3d) final channels, and compare the relative production to theory, and ultimately investigate the impact on current stellar atmospheric models.

Measurement of Li abundances in stars is an important problem in astrophysics. For example, as primordial Li was produced in the Big Bang, the relationship between the amount of Li observed in old, metal-poor stars and the primordial abundance is important to understand. Accurate Li abundances in such stars tell us about the Big Bang, stellar evolution, and physical processes in stars.

Li abundances in old, metal-poor stars are likely sensitive to Li+H collisions [2]. However, early work was based on a classical atomic collision model, known as the "Drawin formula" in stellar astrophysics. It has since then been demonstrated that quantum models differ from the classical results by orders of magnitude, and that MN of Li\(^+\) and H\(^-\) is the most important process in stellar atmospheres, which cannot be described by the classical model [3]. This experiment probes this process through the equivalent MN of Li\(^+\)/D\(^-\). The only previous measurements of this system were performed for collision energies higher than what is of interest in cool stellar atmospheres at 2000–6000 K (0.2–0.6 eV), and thus the energy regime of most importance has not been examined.

Our eventual goal is to map the absolute MN cross sections from meV energies to several tens of eV. This would provide strong constraints on both the theoretical collision models, as well as the astrophysical modelling and ultimately on the Li abundance in old stars.

References

Scientific Theme(s)
- Stars, stellar populations, and stellar explosions

Research Area(s)
- Experimental laboratory astrophysics

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Radiation Chemistry in Astrochemical Models: From the Lab to the ISM

Shingledecker, C. N.1, Ivlev, A.2, Kaestner, J.3, Herbst, E.4, Caselli, P.5, Vasyunin, A.6

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Poster number: 74

Most interstellar and planetary environments are suffused by a continuous flux of several types of ionizing radiation, including cosmic rays, stellar winds, x-rays, and gamma-rays from radionuclide decay. There is now a large body of experimental work showing that these kinds of radiation can trigger significant physico-chemical changes in ices, including the dissociation of species (radiolysis), sputtering of surface species, and ice heating [1].

Even so, modeling the chemical effects that result from interactions between ionizing radiation and interstellar dust grain ice mantles has proven challenging due to the complexity and variety of the underlying physical processes. To address this shortcoming, we have developed a method whereby such effects could easily be included in standard rate equations-based astrochemical models [2].

In this poster, we review recent work by us on the methods of incorporating radiation-chemical processes into astrochemical models, as well as the effects of non-thermal, non-diffusive cosmic ray-driven ice chemistry on the abundances of several astrochemically interesting species [3]. Moreover, we describe how such models, thus improved, can fruitfully be used to simulate experiments in order to better understand bulk chemistry at low temperatures.

References

Scientific Theme(s)
• Solar System formation and the pre-solar nebula

Research Area(s)
• Theoretical calculations or simulations in laboratory astrophysics

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H atom irradiation of formamide ice at 12 K

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Poster number: 75

Icy mantles exist on the interstellar and circumstellar dust grain surfaces and on the primitive bodies of our solar system such as comets and satellites. Spectroscopic observations by instruments on board space based telescopes reveal a continuous detection of new species in the water rich icy mantles. Formamide (HCONH\(_2\)), one of the simplest molecules containing H, C, N and O atoms, has gathered significant attention as a prebiotic ice due to the presence of a peptide-like bond. In addition, formamide is considered as a starting material for the synthesis of biomolecules in the course of chemical evolution. Formamide has been detected in a number of astrophysical environments such as cometary comae [1] and a variety of star forming regions [2,3].

The icy mantles undergo a series of physical and chemical changes induced in a number of ways such as heat, atom addition, UV photons and cosmic rays. Given the higher abundance of H atom in comparison to other atomic species, the H atom addition is one of the most important solid state processing mechanisms. This study is concerned with the effects of H processing on formamide ice at 12 K using IR spectroscopy. The aim is to examine the stability of formamide ice and understand the possible formation routes retrosynthetically. During irradiation, the infrared bands arising due to formamide are reduced, and new bands have appeared which are assigned to carbon monoxide (CO), carbon dioxide (CO\(_2\)), isocyanic acid (HNCO). Even after prolonged H atom irradiation, no synthesis of complex molecules is observed. The analysis of hydrogenation cross-section of formamide will be useful to understand the stability of formamide in an astrophysical environment.

References

Scientific Theme(s)
- Solar System formation and the pre-solar nebula

Research Area(s)
- Experimental laboratory astrophysics

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Deuteration of C\textsubscript{60} on a Highly Oriented Pyrolytic Graphite surface

Pantazidis, G.\textsuperscript{1}, Scheffler, M.\textsuperscript{2}, Cassidy, A. M.\textsuperscript{3}, Simonsen, F. D.\textsuperscript{4}, Jensen, P. A.\textsuperscript{5}, Hornekær, L.\textsuperscript{6}, Thrower, J. D.\textsuperscript{7}, & EUROPAH

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Poster number: 76

In interstellar space, the surfaces of nanoscale dust grains provide the opportunity for surface reactions. This, for example, provides a route to form molecular hydrogen. Buckminster Fullerene - C\textsubscript{60} - has been observed in the interstellar space, in regions near hot stars \cite{1}. The hydrogenation of C\textsubscript{60} and subsequent strain induced unzipping has been proposed as a route to form Polycyclic Aromatic Hydrocarbons \cite{2}, which are observed to be ubiquitous in interstellar space where they are proposed to act as catalysts for H\textsubscript{2} formation \cite{3}. Hydrogenated C\textsubscript{60} has been investigated in gas phase experiments and theoretical ab initio studies suggest that the strain on the molecule increases after the addition of about 36 hydrogen atoms to the C\textsubscript{60} molecule. However relevant experimental investigations of hydrogenation of C\textsubscript{60} on interstellar dust grain analogue surfaces along with the necessary theoretical support are still lacking. In this poster we present an experimental study of the deuteration of C\textsubscript{60} adsorbed on Highly Oriented Pyrolytic Graphite (HOPG), an analogue of interstellar carbonaceous dust grain surfaces. Deposition of C\textsubscript{60} was performed via a Knudsen cell on HOPG, held at a temperature of 360K. Subsequently, the C\textsubscript{60} film was exposed to a flux of D-atoms with a temperature of 1950K. Temperature programmed desorption (TPD) measurements were used to identify the different species existing on the surface through mass spectrometry. The TPD data reveal an increasing degree of deuteration, with increasing D-atom fluence. Moreover, the increased degree of deuteration shifts the desorption temperature of C\textsubscript{60} mass to higher values. The TPD spectra of the D\textsubscript{2} emitted from the samples can be divided in three temperature regions, each associated with different desorption processes from the surface. Scanning Tunneling Microscopy (STM) measurements were performed to investigate the adsorption structures of the adsorbed pristine and deuterated C\textsubscript{60} molecules.

References

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\cite{2} O. Berné, A. G. G. M. Tielens, PNAS, 109 (2) 401-406, (2012)
\cite{3} J. D. Thrower et al., The Astrophysical Journal, 752:3 (6pp), (2012)

Scientific Theme(s)

\begin{itemize}
  \item Solar System formation and the pre-solar nebula
\end{itemize}

Research Area(s)

\begin{itemize}
  \item Experimental laboratory astrophysics
\end{itemize}

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Are SiO molecules the seed of silicate dust around evolved stars?

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Poster number: 77

The SiO molecule is one of the candidates for the seed of silicate dust in the circumstellar envelope of evolved stars, but this opinion is challenged. In this work we investigate the relation of the SiO maser emission power and the silicate dust emission power. With both our own observation by using the PMO/Delingha 13.7 m telescope and archival data, a sample is assembled of 21 SiO $v=1, J=2-1$ sources and 28 SiO $v=1, J=1-0$ sources that exhibit silicate emission features in the ISO/SWS spectrum as well. The analysis of their SiO maser and silicate emission power indicates a clear correlation, which is not against the hypothesis that the SiO molecules are the seed nuclei of silicate dust. On the other hand, no correlation is found between SiO maser and silicate crystallinity, which may imply that silicate crystallinity does not correlate with mass-loss rate.

References

Scientific Theme(s)
- Solar System formation and the pre-solar nebula

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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Surface diffusion of OH radical on amorphous solid water

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Poster number: 78

Surface reactions on interstellar grains play an important role in molecular formation in dense clouds. Surface reactions proceed via elementary processes: adsorption, diffusion, and reaction with another adsorbate [1]. Therefore, diffusion process on dust grain surface is crucial to surface reactions and should be clarified experimentally. We study diffusion of OH radicals on amorphous solid water, because surface reactions with OH radical would contribute to the formation of complex molecules or those precursors [2]. Using the combination of photostimulated desorption and resonance-enhanced multiphoton ionization [3], we succeeded in detecting OH radicals on the ice surface. The intensity of OH radical was found to depend on the substrate temperature and decreased rapidly between 60 and 80 K. Assuming that the decrease of OH results from OH-OH recombination to form H₂O₂, the activation energy of recombination was determined by Arrhenius equation. Because the recombination would be a radical-radical barrierless reaction, it would be limited by the surface diffusion of OH radical. Diffusion activation energy of OH radical on the ice surface is derived to be 0.13 ± 0.01 eV.

References

Scientific Theme(s)
• Solar System formation and the pre-solar nebula

Research Area(s)
• Experimental laboratory astrophysics

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The origins of two distinct halo populations revealed from the nucleosynthesis of barium

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Poster number: 79

We present the abundances of Ba in 40 halo stars selected from the sample of Nissen & Schuster (2010), including of 13 low-\(\alpha\) halo stars and 27 high-\(\alpha\) halo stars. Taking into consideration of the hyperfine splitting of the Ba resonance line \(\lambda 4554\)Å result from the individual isotopes (Mashonkina & Gehren 2000), we determined the relative contributions from \(r\)- and \(s\)-processes to the Ba abundances by fitting the line profile of Ba \(\lambda 4554\)Å. Our results indicate that the abundance of Ba has a negative NLTE effect with an average the correction of -0.06 dex in [Ba/Fe] compared to the LTE abundance, and there is no systematic distinction between the two halo populations. For most of the low-\(\alpha\) halo stars, Ba is synthesized both from the \(r\)- and \(s\)-processes, but the contribution from the \(r\)-process is greater than that of the \(s\)-processes. Furthermore, for a few of low-\(\alpha\) halo stars, Ba is fully produced by a pure \(r\)-process. For the high-\(\alpha\) halo stars, the nucleosynthesis mechanism of Ba is more complex, in the most case, Ba is synthesized by both the \(r\)- and \(s\)-processes with a random relative contribution. While, for several high-\(\alpha\) halo stars, Ba can be produced by only a pure neutron-capture either the \(r\)-process or the \(s\)-process. We suggested that either the high-\(\alpha\) or low-\(\alpha\) halo stars is not originated from a single site. They are more likely formed in multi-situations, such as the in situ, kicked-out, and accreted, as well as some other origins.

References

Scientific Theme(s)
- Stars, stellar populations, and stellar explosions

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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Complex organic molecules tracing the comet-building zone in protoplanetary disks

Walsh, C.\textsuperscript{1}

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Poster number: 80

High sensitivity observations with the Atacama Large Millimeter/submillimeter Array (ALMA), have allowed the first detection of complex organic molecules (COMs) towards protoplanetary disks around nearby young stars. The successful detections of cold gas-phase CH\textsubscript{3}OH \textsuperscript{[1]}, CH\textsubscript{3}CN \textsuperscript{[2]}, and HCOOH \textsuperscript{[3]} towards TW Hya provide the first constraints on the ice composition of the comet-building zone towards our closest planet-forming neighbour. These observations have also highlighted the importance of non-thermal desorption mechanisms in releasing large molecules into the gas-phase in the cold outer disk, where we would otherwise expect non-volatile species to be depleted from the gas phase. Protoplanetary disks are thus a useful astrochemical laboratory to directly investigate the role of non-thermal desorption by stellar UV photons and X-rays in setting the gas-ice balance in cold astrophysical environments.

Presented are new high-angular resolution ALMA observations of gas-phase CH\textsubscript{3}OH in the TW Hya protoplanetary disk. These data reveal the compact nature of the emission (< 60 au), and suggest that the bulk of the observable ice reservoir is hosted on large mm-sized grains that have a similar radial extent. The detection of emission from transitions with low-lying upper energy levels only (< 38 K) suggests that the emission is coming from cold gas close to the midplane. Possible mechanisms for the non-thermal release of gas-phase methanol in this region of the disk are discussed.

References

Scientific Theme(s)
- Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Observations showing use of laboratory astrophysics in the interpretation/understanding of data

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Low-temperature condensation of polyaromatic carbon grains from PAHs


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Poster number: 81

Our goal is to condense laboratory analogs to interstellar carbonaceous dust and to shed light on the origin and molecular structure of the infrared aromatic band carriers. We present the results of a study using the COsmic SImulation Chamber (COSmIC) experimental facility at NASA Ames. The COSmIC setup includes as Pulsed Discharge Nozzle (PDN) used in grain condensation. The PDN is fed by a supersonic jet of Argon seeded with organic molecules of increasing size (i.e., increasing ring number), that include benzene, naphthalene, anthracene and pyrene. High voltage pulses generate a plasma discharge in the stream of the jet-cooled supersonic expansion (50 - 150 K). Grains are condensed within the cold plasma and are collected in-situ onto substrates placed a few centimeters away from the electrodes. The grains are extracted from the COSmIC chamber and characterized ex-situ via infrared microscopy and mass spectrometry. Infrared absorption spectra in the 3 - 16 µm range exhibit stretching and bending modes associated to CC bonds within the rings and CH groups attached to the rings and are also accompanied by aliphatic group vibrations, broad bands and plateaus, suggesting the presence of a mixed aromatic-aliphatic backbone. The solid grain samples are further characterized via the laser desorption mass spectrometry technique at UCSB. In this technique, laser desorption volatilizes low vapor pressure molecules from a surface into the gas phase without fragmentation or thermal degradation. Jet cooled molecules are excited and photo-ionized and the ions are detected in a time-of-flight mass spectrometer. Mass spectra reveal the rich molecular complexity within the grains and show the presence of molecules larger in mass than the seed for all PAH precursors. These results allow us to propose a new picture of stable molecular pathways in PAH-grain condensation.

References

Scientific Theme(s)
- Star formation and the cosmic matter cycle in the near universe

Research Area(s)
- Experimental laboratory astrophysics

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Plume profile studies of Nanosecond laser-induced desorption of water ice - amorphous versus crystalline -

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Poster number: 82

In the interstellar medium and within our solar system, ice is present in diverse locations ranging from molecular clouds to the Jovian moon Europa. There have been various efforts to develop new techniques to replicate these environments and study these ices in the laboratory. From an astrochemical point of view, the development is key for understanding how the energetic processing of ice can lead to molecular complexity. From a planetary science point of view, the development is driven to investigate novel instrumentation for future space exploration missions. The Jovian moon Europa is of particular interest for the search of extraterrestrial life within our solar system.

At NASA’s Jet Propulsion Laboratory, we have used the two-color Laser Ablation Ionization Mass Spectrometer system to study such ice-surface analogue [1,2]. The system has the capabilities to simulate relevant conditions, encountered in relevant environments. The structure of the ice depends on the deposition temperature. IR laser desorption combined with multi-photon ionization mass spectrometry, provides insights in the desorption dynamics of the plume. We are capable of varying the wavelength of the IR laser, from 2700-3100 nm. By introducing different species in low abundances into the ice structure, we can study if these molecules follow the same trend in extraction time as the water molecules. These fundamental investigations are essential for understanding the processes at play, and gaining insights into the nanosecond laser-induced desorption process.

References

Scientific Theme(s)
- Solar System formation and the pre-solar nebula, Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
- Experimental laboratory astrophysics

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Kinetics of the reaction between the CN radical and methanol at low temperatures using the CRESU technique

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Poster number: 83

The interstellar medium is host to a rich chemistry that produces a variety of species, including those with six or more atoms that have been named complex organic molecules (COMs). Methanol is one of the simplest COMs detected in various astrophysical environments, e.g., protoplanetary disks [1], comets and the interstellar medium. Studying the reactivity of methanol at low temperatures will aid our understanding of the formation of other complex, and potentially prebiotic molecules. Neutral-radical reactions are an important route of destruction for many neutral species, and given the widespread abundance of the CN radical in space, the reaction between methanol and the CN radical is of significant interest.

Here, we study the kinetics of the reaction between methanol and the CN radical using the well-established CRESU technique (a French acronym standing for Reaction Kinetics in Uniform Supersonic Flow) [2] combined with Pulsed Laser Photolysis-Laser-Induced Fluorescence (PLP-LIF). Our results display a negative temperature dependence, typical of what has been seen previously for other radical-neutral reactions that do not possess potential barriers. The values obtained at room temperature display a strong disagreement with the previous study conducted at room temperature by Sayah and colleagues [3].

While the PLP-LIF technique provides us with the overall reaction rate coefficients, it is unable to identify the reaction products. Electronic structure calculations were performed for this reaction in order to provide a theoretical perspective. We are also developing a new setup integrating chirped-pulse broad-wave microwave spectroscopy with continuous flow-CRESU (CRESUCHIRP), which will allow us to identify the products and provide the branching ratios for the multiple channels.

\[ \text{CN} + \text{CH}_3\text{OH} \rightarrow \text{CH}_2\text{O} + \text{HNC} \]
\[ \text{CN} + \text{CH}_3\text{OH} \rightarrow \text{CH}_2\text{OH} + \text{HCN} \]

References

Scientific Theme(s)
• Star formation and the cosmic matter cycle in the near universe, Protoplanetary disks, debris disks, and the Solar System

Research Area(s)
• Experimental laboratory astrophysics

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Natural transportation routes in the Solar System

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Poster number: 84

In the last few decades, powerful computers enabled the implementation of numerical methods that gave new understanding to the transportation mechanism in our Solar system. This is especially important in our attempt to explain the possible mechanism in the early Solar System, by which water-rich asteroids may have been delivered to Earth. Knowing that carbonaceous (C-type) asteroids, with a large fraction of water molecules, dominate in the outer part of the asteroid belt and that the possibility of their migration toward Earth is still not well explained, we use sophisticated numerical techniques and we search for transportation mechanism and transportation routes that may have brought a large amount of carbonaceous material from the outer part of the main belt in the close neighborhood of Earth.

Scientific Theme(s)
- Solar System formation and the pre-solar nebula

Research Area(s)
- Theoretical calculations or simulations in laboratory astrophysics

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