

# Solid-state astrochemistry in star-forming regions

Surface-catalysed chemical reactions, the molecules they form, and the implications for star formation were key themes in an international workshop on “Solid-state chemistry in star-forming regions” at the Lorentz Centre, Leiden University, the Netherlands from 14–17 April 2003. **Helen Fraser, David Williams, Ian Sims, Anita Richards and Jeremy Yates** report.

**W**ith the advent of new technologies in the laboratory, and 8 m class telescopes at the disposal of observers, we are gradually probing deeper into the role of surface chemistry in generating a number of molecular species detected in star-forming regions. Surface processes play a vital role in the molecular evolution from diffuse to dense clouds, and in the collapse of clumps within these clouds to form protostellar objects, which themselves eventually evolve into planets, comets and life. More than 60 astronomers, physicists and chemists gathered together for this week-long meeting held at the Lorentz Centre, Leiden, the Netherlands, and organized on behalf of the Astrophysical Chemistry Group of the RAS and RSC. Delegates gathered from across Europe, the USA and Japan to present their latest results and discuss the hottest topics, covering diverse fields from theoretical chemistry, astrochemical modelling and observational astronomy, to surface catalysis and experimental molecular physics.

The meeting opened with a Plenary Lecture from **Ewine van Dishoeck** (Leiden, Netherlands) who reviewed heterogeneous processes in

astronomy. She presented all the observational evidence for the existence of dust in astronomical situations including extinction, polarization and continuum observations. From such data astronomers can derive that interstellar dust grains are asymmetric, have a range of sizes but probably (at least in diffuse and dense clouds) less than 150 nm across, and may be aggregates of smaller grains (down to about 5 nm). Only around 1% by mass of a dense cloud is granular, primarily refractory elements such as C, Mg, Si and Fe, whose abundances are depleted from the gas phase. IR observations show that silicate grains dominate and both amorphous and crystalline features have been observed. Most carbon is thought to be “locked-up” in graphitic or amorphous carbon grains, or in polycyclic aromatic hydrocarbon molecules, observed in emission.

## Interstellar grains

The Infrared Space Observatory mission led to the realization in the mid-1990s that ices were prevalent in dense clouds and the disks around young stellar objects. This led astronomers to their core–mantle picture of interstellar grains,

**1: Astronomers, chemists and physicists get reactive over surface chemistry in interstellar space... The Carina Nebula is a giant star-forming region, 8000 light years away from the Earth. (NASA, The Hubble Heritage Team [AURA/STScI])**

with bare grains dominating in the diffuse medium, and ices building-up on the cold grain surfaces in dense clouds and protostellar disks, as atoms and molecules “freeze-out” from the gas phase. Grain-surface chemistry at the surfaces of both the bare and ice-covered grains is a key mechanism in astrochemical models to provide increasing molecular complexity as star formation progresses.

Many assumptions are made in modelling the grain-surface chemistry, so there is a real need for laboratory work to confirm or refute the theories underpinning astrochemical models (luckily for the delegates at this meeting!). Spectroscopy is the only tool available to astronomers to probe the structure and evolution of grains and ice mantles – along different lines of sight the spectra look different! All the regions in which surface chemistry is important to astronomy are dynamically evolving, and ices and grains can be subjected to thermal heating, UV radiation fields, ion bombardment (in the keV–MeV range), and high-energy cosmic rays. Evidence already exists for systematic alterations to the ices and grains from such effects. Van Dishoeck summarized by stressing the data needs and requirements from astronomers to chemists, particularly from laboratory

measurements. Her final message: the astronomical laboratory is complex, but don't panic; there are regular trends and consistent facts wherever we look in the sky.

This was followed by **Serena Viti** (University College London/CNR-Istituto di Fisica dello Spazio Interplanetario, Italy) and **Jonathan Rawlings** (UCL) who spoke in detail about astrochemical models. Viti focused on how the models are constructed and how they work, illustrating her points with some of the latest results from her astrochemical models, which have already incorporated the latest experimental results from McCoustra and co-workers at Nottingham University. Generally, the output from an astrochemical model predicts the fractional abundances of different atomic and molecular species towards different astronomical objects, and is a good basis on which astronomers can compare what they think is happening with what they actually observe. But she stressed that most surface chemistry and surface reaction rates are missing from their data sets; there is a real need for such information to run models accurately, because what comes out of these models is only as good as what went in. This is where Rawlings took over, discussing the successes, problems and limitations of how far astronomers can get using astrochemical models. To illustrate the successes, he showed some beautiful examples of line-shape profiles derived from the abundance outputs of astrochemical models of young stellar objects, where in-fall on to the new star and outflows perpendicular to the protostellar disk confuse the observed line-shapes. Using his and others codes, astronomers have been able to identify where exactly along any line of sight most of their observed signal arises from. One problem, however, is that if he changes the sticking probability of the species (i.e. ability of a gas to be frozen out on to grains) by a factor of two or more, then clear changes in the predicted line-profiles result; without good laboratory data to tie the many model parameters down, it is almost impossible to know which factor is having the greatest influence in the observations.

Before the afternoon session set aside for discussions and interactions, **Martin McCoustra** (Nottingham) delivered a thought-provoking and powerful lecture on "Data use and validation in astrochemistry". Typically, astrochemical models contain up to around 4000 species participating in 400 or so chemical reactions, yet only around 20% of the data used in these models have been measured or calculated: the rest are guessed from extrapolation or intuition. McCoustra warned against such practice, citing results from the CRESU experiment by Sims and co-workers from Birmingham University, who have shown that the reaction rates of many low temperature neutral-neutral gas phase reactions

do not follow a simple Arrhenius law, and may actually be enhanced by many orders of magnitude over this extrapolation. He also warned astronomers to the limitations of laboratory data – every experiment has intrinsic errors and uncertainties, and sometimes experimentalists disagree. Experimentalists were reminded to ensure their data was reproducible and reliable before publication. He stressed that much of the data astronomers might require is already available in the literature, but perhaps outside the journals traditionally frequented by astronomers – producing a rush for pens as a few references flashed by. Even if data is in the literature, a number of different values may exist, and there is no easy way for non-specialists to determine the "best" value to use, for example for a binding energy, reaction rate or sticking probability. McCoustra then drew an analogy with the atmospheric chemistry community, comprising experimentalists and modellers, with a need for data validation and "best" values. The IUPAC Commission on Physical Chemistry has taken this role on board, and meets a few times year to review the literature and agree on "recommended" values, with reasons, for atmospheric model data sets. Data sets such as the UMIST database do already exist in astrochemistry, but their validation is not yet on the scale of the atmospheric community.

## H<sub>2</sub> formation

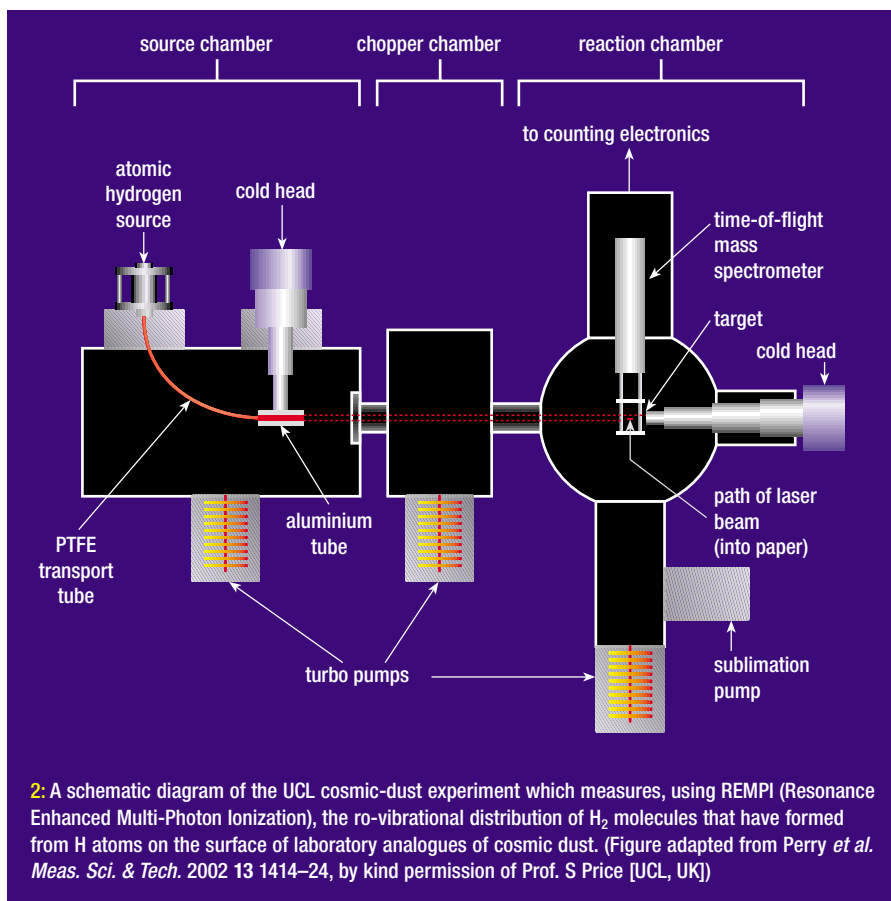
In the second plenary lecture, **Alex Dalgarno** (Harvard) explained observed formation rates of the simplest and most abundant molecule in our universe, H<sub>2</sub>. Although H<sub>2</sub> formation in the early universe, and ion-molecule reactions that produce H<sub>2</sub> in the gas phase, are well understood, the observed H<sub>2</sub> abundances in diffuse and dense clouds require additional H<sub>2</sub> formation mechanisms, surface reactions on bare dust grains, and even ice-covered dust grains. From an astronomy viewpoint, the reported H<sub>2</sub> formation rate, between 1 and  $4 \times 10^{-17}$  cm<sup>3</sup> s<sup>-1</sup>, is the same everywhere (except in photon dominated regions [PDRs] where the rate is one order of magnitude higher). From an astrochemical viewpoint, however, the question is how to account for this rate – what surface reaction mechanisms underpin H<sub>2</sub> formation?

**Valerio Pirronello** (Catania, Italy) and **Liv Hornaeker** (Odense, Denmark) are trying to answer exactly these questions and presented their latest laboratory results. Pirronello reviewed five years of work at Syracuse University in collaboration with Vidali and co-workers, studying H<sub>2</sub> formation on silicate, amorphous carbon and H<sub>2</sub>O-ice surfaces. The experiments are conducted under ultra-high vacuum conditions, and at very low surface temperatures (around 10 K), to mimic as closely as is possible the interstellar conditions. Even at pressures around a billion times lower than

atmospheric pressure, such experiments are affected by the background H<sub>2</sub> in the experimental chamber, so both groups actually studied HD formation. H and D atoms were delivered to the surface using triply differentially pumped molecular beams of H and D. In the Syracuse experiment HD formation was observed from all three surfaces; Pirronello presented the reaction rates and energy barriers associated with the formation and desorption of HD under pseudo-interstellar conditions. He also discussed methods developed in collaboration with Biham at the Hebrew University of Jerusalem to "convert" the laboratory timescales and doses to realistic interstellar conditions, where gas-grain collisions happen around once a day (compared to around  $10^{15}$  cm<sup>-2</sup> s<sup>-1</sup> in the laboratory) and the lifetime of a dense cloud is  $10^6$  years (plenty of time for chemistry but a little too long for a researcher wanting a career).

Hornaeker then continued to describe their newest and exciting results from the Odense laboratory. Luntz and co-workers have focused on HD formation at H<sub>2</sub>O-ice surfaces, specifically amorphous solid water (ASW), a porous ice formed by vapour deposition of H<sub>2</sub>O at very low substrate temperatures (described below). This session was a real highlight of the meeting, since the Odense and Syracuse groups vary quite considerably from each other in their interpretation of their results. A careful calibration of their background data showed how H<sub>2</sub>, D<sub>2</sub> and HD interact direct with ASW, and how their desorption profiles can be affected by the nature of the underlying ice structure, initial coverage of the molecule on the ice surface, and the binding sites they occupy at the ice surface. One advantage of the Odense experiment compared with the Syracuse experiment is the ability to use MIDS, a multiple ion detection system, to look for H<sub>2</sub>, HD and D<sub>2</sub> signals concurrently. From these, and another host of sequential dosing (H then D vs. D then H vs. H then H etc) experiments, they conclude that HD forms at very low temperatures in the ice, the H and D atoms being mobile in the ice, even at very low temperatures ( $\approx 10$  K), and then the reaction progresses via a "hot atom" diffusion mechanism. The excess enthalpy of formation is thought to dissipate in the ice, and the HD rapidly thermalizes with the surface. These two talks sparked lively debate and discussions throughout the week.

A further problem, also of concern to astronomers, is how energy is distributed after H<sub>2</sub> formation. The reaction  $H + H \rightarrow H_2$  is exothermic by around 3–4 eV. Is this excess energy simply used to heat the grain surface and desorb the H<sub>2</sub> as it forms, is it partitioned between the translational, rotational and vibrational states of the H<sub>2</sub> molecule, or is it both? Vibrationally excited H<sub>2</sub> could be even more



reactive than H<sub>2</sub> alone and, given that H<sub>2</sub> drives much of the gas phase chemistry in dense clouds, it is important for astrochemists to understand these issues. **Stephen Price** (UCL) spoke about an ambitious experiment that has been built at UCL to try to answer these questions (see figure 2). H<sub>2</sub> is formed during H atom recombination, at a cold (20–30 K), highly orientated polycrystalline graphite surface in an ultra-high-vacuum chamber. As the H<sub>2</sub> desorbs from the surface its ro-vibrational state is probed using resonance-enhanced multiphoton ionization spectroscopy. Results to date have shown H<sub>2</sub> leaving the surface in the first and second vibrationally excited state, possibly with some enhancement of the  $v=2$  vibrational state above the Boltzmann level. This could be the first experimental evidence for significant energy partitioning within the H<sub>2</sub> molecule. From the experimental data it was also possible to place an upper limit of 0.9 eV on the translational energy of the H<sub>2</sub>. Although the rotational energy distribution of the vibrationally excited states look to follow Boltzmann distributions, some results suggest statistically significant populations of the highly excited rotational states in the ground vibrational state. In a complementary piece of work, **Anthony Meijer** (UCL) and co-workers are attempting to make theoretical chemistry calculations of the H<sub>2</sub> formation on graphite surfaces, via Langmuir Hinshelwood and Eley–Rideal mechanisms, and then follow the

energy partitioning of the desorbing molecule. Theoretical results show that H<sub>2</sub> can leave the surface in rotationally and vibrationally excited states, and that isotope effects are important, so the formation of HD for example may not be identical to H<sub>2</sub>.

In the afternoon, time was set aside to focus on H<sub>2</sub> formation. Prior to this session **Junko Takahashi** (Yokohama, Japan) spoke on her “formation pumping” astronomical models, which include the latest laboratory data on H<sub>2</sub> formation, as well as the effects of the interstellar UV field, to predict the populations of gas-phase H<sub>2</sub> molecules in dense clouds, in vibrationally excited states. Her models suggest that different cascade transitions dominate, depending on whether the H<sub>2</sub> was excited during grain surface formation or by the UV field. This may give astrochemists another indirect probe of grain densities, and morphology, if the H<sub>2</sub> formation rate and excited-state distributions can be linked. Calculations suggest that the vibrationally excited states of H<sub>2</sub> should be detectable towards lines of sight without significant UV sources or dynamic shocks, but although attempts have been made to make the observations at the Japanese SUBARU radio telescope, no detections have been reported to date.

### Ices

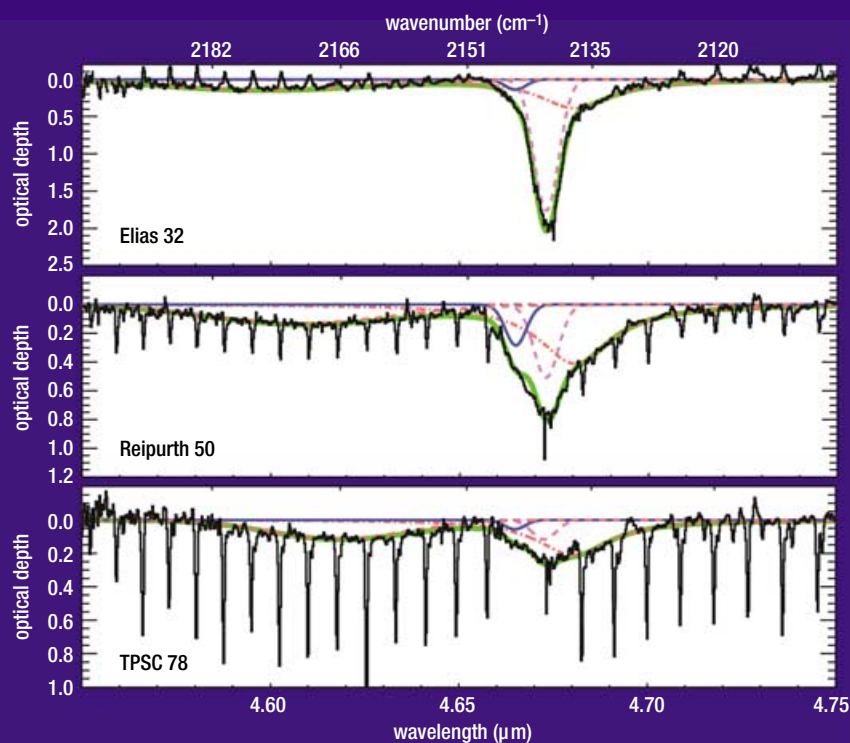
The third day began with **Emmanuel Dartois** (Orsay, France), who discussed in detail the evidence for ice-mantle formation and evolution in

dense clouds, around embedded objects, and in circumstellar disks. For the benefit of the chemists, he explained that observations are integrations along a line of sight, encompassing different pressure and temperature regions, so it is sometimes difficult to decipher whether the observed features are associated with specific grain populations, or different chemical environments on a “standard” interstellar grain. Evidence for interstellar dust grains and their icy mantles come from a range of wavelength regions, from the UV to the sub-mm: some observations are in absorption, some in emission, which makes it difficult to compare observations that were made at different wavelengths. However, the mid-IR region has been particularly useful as a tool to identify the chemical species present on the grains (or their functional groups at least). Substructure in the mid-IR solid-state bands can help astronomers to elucidate information on the prevailing temperature, molecular species and morphology of the ices. Dartois warned, however, against making direct comparisons between line profiles and molecular abundances – ices may be segregated into layers (or on different grains), or intimately mixed, even forming complexes, all of which affect the absorption cross-section. One other major problem is that we have to understand the light scattering properties of our grains (and mantles) before we can compare laboratory data with astronomical observations. He explained that understanding the nature and morphology of these icy mantles is significant because grain-surface reactions are thought to be a key chemical route towards the production of many species in star-forming regions, including more complex organic species. In fact even “simple” molecular species such as H<sub>2</sub>O, the most abundant molecular species in the solid state, must be formed in surface reactions on bare grain surfaces between OH and H or H<sub>2</sub> and O. There is also a strong coupling between the gas-phase and solid-state chemistry, and grain surfaces may have a significant influence on isotopic substitution. Grain-surface chemistry is thought to be driven by thermal processes, UV photons or chemistry induced by cosmic rays. Different processes dominate in different star-forming regions, accounting for discrepancies in observed abundances of ice molecules along various lines of sight.

**M Elizabeta Palumbo** (Catania, Italy) then summarized laboratory experiments in which ice mixtures, representative of the components thought to form icy interstellar mantles, were subjected to either UV photons or keV or MeV ions or electrons, to simulate the diffuse UV field and cosmic rays. Her experiments employ Raman and IR transmission spectroscopy to study the products generated in the ices, and the residues on the substrate once the ices have evaporated. She illustrated that qualitatively the



**3:** Absorption spectra of the CO stretching-vibration mode at 4.67  $\mu\text{m}$  towards three young stellar objects. The curves show the decomposition of the solid CO band into three distinct components. The centre and width of each component is fixed for all lines of sight and only the relative contributions were allowed to vary. The three CO components are centred on 2136.5  $\text{cm}^{-1}$ , 2139.9  $\text{cm}^{-1}$  and 2143.7  $\text{cm}^{-1}$ . The emission lines (for HH 100) and absorption lines (for RE 50 and TPSC 78) are ro-vibrational lines of gas-phase CO from the vicinity of the central stars. Broad and shallow absorption features in the CN stretching-vibration region around 2165–2175  $\text{cm}^{-1}$  are also visible. (Figure adapted from spectra recorded at VLT-ISSAC, by kind permission of K Pontoppidan *et al.* [Leiden Observatory], *A&A* 2003 in press)



products from both UV photon bombardment (between 1000 and 2000  $\text{\AA}$ ) and keV or MeV ions or electrons were the same, except when the ices contained CO or  $\text{N}_2$ . The degree of chemical complexity in an energetically processed ice was much greater if UV photons were used. **Allain Allouche** (Marseille, France) continued the theme, discussing theoretical chemistry models of amorphous and crystalline ices. He also showed results pertaining to the complexes formed in the bulk and at the surface of binary ice systems. He discussed the importance of the dangling “OH” bonds, freely oscillating OH bonds that “hang” out of ice surfaces, which are highly reactive surface sites where chemical reactions might take place, or species can adsorb (through hydrogen bonding). The theoretical predictions from his calculations have been used to elucidate laboratory data, obtained in IR and volumetric measurements, on a number of adsorbates at ice surfaces of astronomical and atmospheric relevance.

**Bruce Kay** (Pacific Northwest Laboratories USA), summarized the chemical physicists’ perspective on the current understanding of amorphous solid water (ASW), i.e.  $\text{H}_2\text{O}$  ices grown by vapour deposition from the gas phase on a cold substrate below around 140 K. These ices are a useful model for interstellar ices, although Kay’s motivation for his experimental work is to obtain a controllable model for liquid water. He explained that ASW is a metastable, glassy  $\text{H}_2\text{O}$  phase, and can be used as a model system for nanomaterials. Between the glass transition temperature (at around 136 K) and the crystallization temperature (at

around 145 K – assuming experimental system pressures around  $1 \times 10^{-10}$  mbar),  $\text{H}_2\text{O}$  behaves like a super-cooled viscous liquid. Laboratory studies on these systems have enabled his team to decipher many ASW properties. For example, ASW has a vapour pressure twice that of crystalline ice; crystallization is an activated process that commences in the bulk of the ice sample (regardless of the substrate); it requires more energy to crystallize the ice than to sublime it, therefore crystallization and desorption are competing processes in the laboratory. His experiments have also shown that if ASW is grown on a crystalline ice template, crystallization of the amorphous layer occurs more readily, from the interface between the two ices, as no energy is now needed to form nucleation centres in the bulk of the amorphous layer. Kay also showed experiments which illustrate that the morphology of ASW films can be affected by the growth conditions, such as angle between the impinging  $\text{H}_2\text{O}$  molecules and the surface, deposition rate and substrate temperature. For experiments to be reproducible, all these parameters must be taken into account. Background dosing of ASW films led to ice layers that are highly porous with large surface areas: dosing normal to the surface produces compact ices with surface areas similar to the geometric surface area of the dosing region. Recent results from this laboratory have shown that the surface area of an ice, grown on a  $1 \text{ cm}^2$  substrate, can reach  $3000 \text{ m}^2 \text{ g}^{-1}$  (of  $\text{H}_2\text{O}$  deposited). This sponge-like material has a broad distribution of binding-sites available at the surface, and empty “pores” within the structure, which affect chemical reactivity and

physical desorption of adsorbates.

The final talk before the afternoon discussion on ices and ice reactivity, was given by **Xander Tielens** (Groningen, Netherlands), who highlighted the importance of ices and reactions at the surfaces of (or within) the icy mantles, but also raised some of the difficulties facing astrochemical modellers when accounting for observations in solid-state grain models. One key problem is the rate at which ice mantles accrete: typically it is assumed that there is around one collision per day between the basic species in the gas phase in dense clouds, e.g.  $\text{H}_2$ , H, O,  $\text{O}_2$ , CO,  $\text{O}_2$ , C,  $\text{N}_2$  and N, yet mantles appear to build up to around 100 molecular layers thick, engage in chemistry and desorb again, all in the space of  $10^6$  years. It is also pretty difficult for laboratory experiments to truly recreate interstellar timescales: researchers don’t have  $10^6$  years to get a result, but they do have to produce enough of a component to be detected. Tielens highlighted a few of the species that must be produced through grain-surface reactions, such as  $\text{CH}_3\text{OH}$  and  $\text{CO}_2$ , simply because gas-phase processes do not produce enough of them for the observed abundances. He stressed that reactions with atomic H and atomic O were key to understanding the ice chemistry, and that for now we need to focus in the laboratory on the processes and mechanisms involved.

### Surface chemistry

The final day of the workshop was started by **Ed Bergin** (Harvard), who summarized current understanding of gas-grain chemistry, simply on the basis of observations and astrochemistry

## The means to the end: support for a successful conference

The meeting was generously sponsored by the Lorentz Center, NOVA (the Dutch Research School for Astronomy), the Tony and Angela Fish Bequest from the Royal Society of Chemistry, the Royal Astronomical Society, the Astrophysical Chemistry Group, Varian, Pfeiffer Vacuum, Hositrad Holland and Dutch Space.

Ten places were specially funded and competitively awarded to young researchers not yet in a permanent position, to allow them to benefit from attending this meeting at no cost to themselves.

Additional funds were made available to assist a further 10 PhD and postdoctoral scientists attending the meeting.

The Lorentz Centre is an international study and visitors' centre for research in astronomy, mathematics, physics and computer science. The aim of the centre is to bring scientists from different disciplines together in a congenial atmosphere for collaboration, discussions and stimulating interactions. In this respect, the meeting was a great success, crossing traditional boundaries between many disciplines: the research underpinning solid-state astrochemistry in star-forming regions looks an exciting area for new discoveries in the years to come.

models. He focused on a number of key species, such as H<sub>2</sub>O, CH<sub>4</sub>, NH<sub>3</sub>, CO<sub>2</sub>, CH<sub>3</sub>OH and OCN<sup>-</sup>, which have been identified in grain mantles, are not necessarily observed in the gas phase in star-forming regions, and must result from grain-surface reactions. Some of these species might be formed through energetic processing by UV or cosmic rays, but thermal reaction routes, replying only on grain heating, may also induce some of their production. Bergin highlighted the observational differences between low-mass and high-mass star-forming regions, including the prevailing physical conditions and rates at which evolution to chemical complexity appear to progress. Focusing on low-mass star formation, he showed that the grains clearly act as a passive sink for many molecular species, but no clear observation evidence yet exists for grain-surface chemistry there. But the grain-surface chemistry can be inferred indirectly from gas-phase abundances and evolution. By comparing models and observations, it is possible to establish that grain-surface reactions must also play a role in low-mass star-forming regions. In high-mass star-forming regions, hot cores are formed, where ices are rapidly evaporated and a diverse chemical complexity is observed. This is the astronomers' best chance to try and track down the chemicals made at grain surfaces and to understand the significance of such processes in the chemical evolution of star-forming regions.

The theme of surface reactions at ice surfaces was continued by **Helen Fraser** (Leiden, Netherlands) and **Dinko Chakarov** (Göteborg, Sweden). Fraser focused on interactions between CO and other ice constituents, such as H<sub>2</sub>O, CH<sub>3</sub>OH, CH<sub>4</sub>, HCOOH and CO<sub>2</sub>, with a view to understanding recent observations towards a sample of 38 protostellar objects, that show remarkably similar solid-CO features despite being at different evolutionary stages (see figure 3). Chakarov focused on substrate-induced chemistry, when thin ice films are bombarded with UV photons at energies below the H<sub>2</sub>O dissociation energy. Secondary electrons emitted from the graphite substrate can be used to induce many reactions in the ice overlayer, producing species such as CO<sub>2</sub> if CO is

doped into the ice layer.

**Kenzo Hiraoka** (Kofu, Japan) presented a summary of hydrogenation reactions in low-temperature ices, and their role in elucidating the formation of H<sub>2</sub>CO, HCOOH and CH<sub>3</sub>OH, via thermal reaction pathways. He showed that the yield of many of these species increases as the ice cools, possibly suggesting that H atoms are tunnelling through the ices. The most recent experiments, in which CO ices were bombarded with H atoms, seem to prove conclusively that CH<sub>3</sub>OH cannot be formed directly through H-addition reactions to CO. Some experimental evidence contradicts these results, but the observed abundances of CH<sub>3</sub>OH remain a key problem to gas phase and surface astrochemists alike. **Geert-Jan Kroes** (Leiden, Netherlands) then continued the ice reactivity theme, talking about his group's recent theoretical work, studying sticking and residence time of small molecules at crystalline and amorphous ice surfaces. He showed that the well-depth of the interaction between the adsorbate and the ice surface is key to the sticking and the residence time. For molecules such as HCl, impinging on the surface at collision energies greater than 1 eV, the adsorbate itself penetrates the ice surface. Theoretical studies show that the approach direction, energy and impact position were all key to this penetration. In similar molecular dynamics calculations with CO, no penetration was observed, and the ice surface was severely distorted on impact. Kroes's research shows that a range of binding energies exist between CO and crystalline ice, with a maximum theoretical value of around 10 kJ mol<sup>-1</sup>. On amorphous ices, studies just beginning show that this binding energy can be even greater if the CO is stabilized by having even more water molecules around it, and trapping of CO is observed as the CO penetrates the porous structure.

The final talk of the workshop was given by **Stephen Charnley** (NASA Ames, USA), who discussed the grain-surface reactions that are key to astrochemical models. In particular, he introduced the idea that many complex species could be made at grain surfaces, in chain-like addition reactions (involving O, C and H), then desorbed

to the gas phase, where they could undergo further reactions producing the stable complex species observed in the sub-mm region towards star-forming regions. It is important for modellers to understand which molecular rearrangements are possible, and whether any difference exists between chemical reactions within the icy mantle and those at the surface of the ice grain. Laboratory studies are required to establish rare reaction mechanisms, and reactive intermediates, that may never be detected in mid-IR observations. He also highlighted the need to understand isomerism – certainly where there are several competing pathways in grain-surface chemistry models it is difficult to establish which isomers will dominate, and whether or not conformational barriers between one isomer and another can be overcome.

### Summary

In addition to the varied lectures, more than 35 posters were displayed for the whole week, promoting discussion during coffee and lunch breaks. A dedicated poster session held on the Tuesday evening was well attended by delegates and local researchers from Leiden University alike. In such a culturally and scientifically diverse group, language or conceptual understanding was sometimes a challenge, but a stimulating scientific programme, and the odd social event or two, as well as the excellent conference facilities at our disposal, made it possible and fruitful. Even with a much larger group than was originally anticipated, the delegates worked together to identify the key existing facts, outstanding issues and future requirements: from astronomers to chemists and vice versa. ●

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Further information, copies of the talks and posters, photographs of the meeting and summaries of the discussions are available at [www.leidenuniv.nl/chweb/2003/20030414/info.php3?wsid=76](http://www.leidenuniv.nl/chweb/2003/20030414/info.php3?wsid=76)*