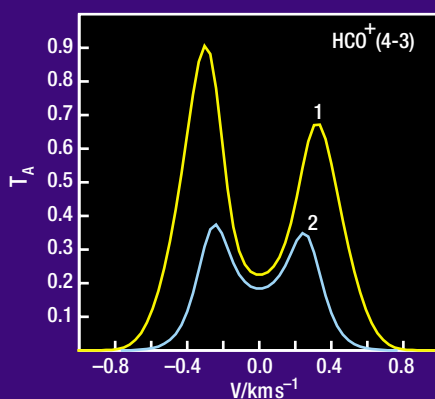


The chemistry of star formation

Understanding the chemistry of molecular clouds is now realized to be fundamental to our understanding of the whole star-formation process. A two-day meeting was held within NAM2002 to bring together chemists and astronomers to discuss this complex subject. Derek Ward-Thompson, Helen Fraser and Jonathan Rawlings report.

1: Results from a combined chemical, dynamical and radiative transfer model of a star-forming cloud undergoing gravitational collapse, where it is assumed that impacting molecular species “stick” to the surface of dust grains with an efficiency of (1) 30%, and (2) 50%. The graphs show the predicted submillimetre spectral line profiles of HCO^+ as a plot of antenna temperature versus velocity for each of the two cases. Note the very strong sensitivity of the profiles to small variations in sticking efficiency, highlighting the fact that it is impossible to diagnose the physics of the infall process without a full understanding of the molecular processes in star-forming regions. (From Rawlings J M C and Yates J A 2001 *MNRAS* 326 1423.)

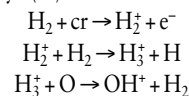


The meeting began with a review by Eric Herbst (Ohio State) of astronomers' current understanding of the chemistry that is important in molecular clouds – the birth-place of stars. He began by pointing out some of the main differences between low-mass and high-mass star formation. Low-mass stars form during the gravitational contraction of dense cores within molecular clouds. There is an ongoing debate about whether this is regulated by magnetic support or turbulent dissipation, but in either case the clouds are largely quiescent. High-mass stars tend to dissociate the molecules in their immediate surroundings rapidly

and ionize the gas, making chemistry less significant in these regions. There are exceptions to this, such as the region boundaries, known as PDRs (photon dominated regions), and regions undergoing the initial phases of collapse, known as “hot cores”. However, the meeting focused largely on low-mass star formation (0.2–2 solar masses).

The first step towards chemistry in the interstellar medium (ISM) is the formation of molecular hydrogen from atomic hydrogen on the surfaces of dust grains in dense regions within molecular clouds. Thereafter the molecular H_2 is released back into the gas phase, where it par-

ticipates in what is now known to be a rich chemistry. In general, ion-neutral reactions proceed faster than neutral-neutral reactions, and the primary reactions are believed to be initiated by cosmic rays (cr):



Thereafter the OH^+ drives the oxygen chemistry. A similar sequence occurs for the carbon chemistry. There are now known to be some 120 molecular species that have been identified in space, up to about 13 atoms in size. To build a chemistry that explains their existence we need to develop chemical models of networks containing some 400 species interacting in about 4000 chemical reactions. An understanding of these reactions is central to the interpretation of molecular line observations. Bill McCutcheon (British Columbia) and Les Little (Kent) gave examples of such observations in specific regions of star formation: NGC 6334 and HH24.

Surface chemistry

In star-forming regions the densities are higher than the average densities in the ISM. Under such conditions atoms and molecules collide with dust grains frequently, and interactions and reactions on dust grain surfaces can be as important as (or even more important than) gas-phase reactions. The formation of H_2 is an essential prerequisite for all gas-phase chemistry, and this is believed to take place on grain surfaces. Stephen Price (UCL) discussed two of the main laboratory experiments taking place to simulate the formation of H_2 on grain surfaces (figure 1).

Laboratory work has some problems in replicating the real physical conditions of clouds. For example, chemists shiver when astronomers talk of 30 K as warm! In addition, the laboratory-simulated grain surfaces are all much cleaner than those predicted to occur in the ISM. How much these factors affect the validity of the results remains to be determined. The Syracuse experiment fires atomic hydrogen and deuterium on to grain surfaces and measures the molecular HD coming off. The UCL experiment uses only atomic hydrogen and measures the relative ratios of the different ro-vibrational states of the emitted H_2 . They find ratios consistent with a high degree of rotational and vibrational excitation, broadly consistent with the predictions of theoretical models.

Richard Blackwell-Whitehead (Imperial) discussed the specific case of manganese, studied using the world's only dedicated vacuum UV Fourier transform spectrograph. Laboratory spectra can be measured with this to an accuracy of about 0.01 ppm. Despite significant progress, still fewer than half of the predicted lines have laboratory-measured values, and many lines are discovered first in space by the

HST before they are measured in the lab. **Janet Bowey** (UCL) discussed the specific case of the 69-micron band of crystalline Mg_2SiO_4 (forsterite) observed with ISO. She showed that changing the crystal's temperature causes a lattice contraction that shifts the peak wavelength of this band, allowing it to be used as a thermometer in the ISM.

Gas-phase chemistry

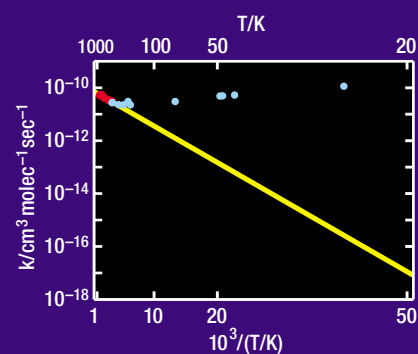
A rich mixture of gas-phase chemical reactions takes place in star-forming regions. **Ian Sims** (Birmingham) described how progress can only be made towards an understanding of this chemistry by the detailed interaction of laboratory measurements, theoretical predictions of quantum chemistry and astronomical observations. Things are made somewhat simpler in the ISM than in the laboratory, since three-body chemical reactions can be ignored, as the densities are just too low. However, even though the rate constants (k) of many relevant reactions have been measured, they have not always been measured at sufficiently low temperatures (10–20 K).

Extrapolation from higher temperature measurements is very dangerous (figure 2). Preliminary studies of a few k - T relations show that even those which are linear from room temperature down to 100 K can become very nonlinear thereafter. Much further work is needed in this field, and the message from the chemists to the astronomers is: if you give us a reaction, we'll measure it. **Jane Greaves** (ATC) described how observations of the polarization of some molecular line transitions (chiefly CO) can be used to measure the magnetic field direction in star-forming regions. **Derek Ward-Thompson** (Cardiff) described how the spectral line shapes of various transitions of HCO^+ in the in-falling envelopes of protostars can be used to measure levels of turbulence and hence shed light on the evolution of protostars. **Edward Polehampton** (Oxford) showed ISO observations of the Galactic Centre region, illustrating how the hydrogen/deuterium ratio varies with galacto-centric radius.

Gas-grain interactions

The gas and dust in molecular clouds interact in several ways. The dust shields the gas from interstellar UV that would otherwise dissociate the molecular gas back into its atomic state. In the centres of clouds, where stars are forming, the gas can freeze out on to the dust grain surfaces, causing observers of gas-phase molecules to underestimate molecular abundances. **Martin McCoustra** (Nottingham) reviewed laboratory measurements of gas-grain interactions, referring to dust grains as the “chemical factories” of the ISM. He pointed out that what an astronomer calls a “dense cloud”, a laboratory chemist refers to as an “ultra-high vacuum”. So

2: A rich mixture of gas-phase chemical reactions takes place in star-forming regions, and laboratory measurements help us to understand these reactions. However, even though the rate constants (k) of many relevant reactions have been measured, they have not always been measured at sufficiently low temperatures ($T = 10$ – 20 K), and extrapolation of k - T relations is dangerous. This graph plots k vs T for the reaction $\text{CN} + \text{C}_2\text{H}_6$ for a range of temperatures. A clear linear relation is seen from 1000 K down to 300 K but the relation becomes very nonlinear thereafter and the extrapolation incorrectly estimates k at 20 K, inaccurate by seven orders of magnitude. (Prof. I Sims, Birmingham.)



there are clearly language barriers to overcome in crossing the traditional boundaries between subjects. Laboratory measurements have entailed condensing H_2O at a cold surface and measuring desorption coefficients as a function of temperature. At temperatures around 10 K (typical of “dense clouds” in the ISM) ice layers grow by ballistic deposition. CO subsequently bonds well to the water-ice surface, migrating into the bulk ice structure as the temperature rises, producing characteristic spectral lines at 2138 and 2152 cm^{-1} , depending on the bonding structure.

Wing-Fai Thi (UCL) showed VLT observations of solid-ice features in the envelopes of young stellar objects. He found evidence for water ice, CO ice, solid methanol and solid OCN^- at wavelengths from 3 to 5 microns. This illustrates how various molecules freeze out under different conditions. There is some evidence for broader CO features in more evolved objects, perhaps indicating a build-up of ice layers over time. **Jamie Rae** (Leeds) presented the results of theoretical chemical modelling of CO, and how to reform it after it has been dissociated. This predicts levels of chemical ionization at odds with some previous work on magnetically regulated star formation that is sensitive to the ionization fraction. **Matt Redman** (UCL) showed how freeze-out of CO on to dust grains can make molecular cloud cores look very different in continuum emission when compared with molecular line emission. In addition, optical depth effects in molecular lines can also be misleading. He outlined a method for checking the optical depths of main-line CO transitions, starting from measurements of C^{17}O hyperfine structure lines and using known isotope abundance ratios.

The future

Serena Viti (UCL) presented a perspective of how she perceives the way forward in this field. Laboratory and theoretical chemists must work even more closely together with astronomers in future. Observations must have better calibration, involve quicker and larger-scale surveys, and have higher sensitivity and resolution. Laboratory experiments are required to provide more of the parameters needed to interpret the observations, such as rate coefficients and tran-

sition probabilities. Theoretical models must explore a larger parameter space if they are to tie together observations with experiments, and not just stick to steady-state chemistry, but pursue time-dependencies and other complicating factors.

One example of how these aspects interact is in observations of CS and NH_3 in star-forming cores. Both theoretically trace the same density regime, and yet typical maps of molecular cloud cores show CS being far more spatially extended. One explanation for this is that molecular clouds could be fragmented on much smaller scales than can currently be resolved, and these small-scale fragments could be transient short-lived features. In that case CS, which has a quicker theoretical formation rate, could form in the transient clumps while NH_3 , which has a much slower formation rate, would not have time to form before a clump dispersed. This would explain why CS is more widespread.

Recent satellites such as ISO, SWAS and HST have helped our understanding of these regions, but future telescopes such as Herschel and ALMA will be needed to make significant further progress. In addition, the increasing speed of available computers will allow more complex models of star-forming regions to be constructed. **Michael Smith** (Armagh) showed some impressive 3-D simulations of turbulence in molecular clouds. When such models can also include all of the chemistry discussed at this meeting, then we will be much closer to understanding star formation in molecular clouds.

In his summary of the meeting **Jonathan Rawlings** (UCL) emphasized both the active and the passive roles that molecular processes play in star-forming regions and how they may be used to diagnose the bigger picture of the dynamical evolution of the ISM. To make progress it is therefore imperative that we encourage stronger links between the various disciplines represented at this meeting: observers, astrochemical modellers and both laboratory and theoretical chemists. ●

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