Final report GR/S15273/01

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Background

In dense regions of the interstellar medium (ISM), astronomical observations have led to the detection of more than 140 different molecules¹. These molecules range from simple diatomics, such as H_2 and CO, through to complex long chain hydrocarbons. Interstellar dust grains have also been detected in space² and some of these molecules are believed to be formed on the surface of the grains.

Although the detected molecules make up less than 1% by mass of the observable universe, they have an important role to play in its evolution³, and it is now recognised that understanding the processes that lead to the adsorption, desorption and formation of these molecules leads to an understanding of some of the key aspects of star and planet formation⁴. In particular, knowledge of the interactions of the molecules found in molecular clouds with interstellar dust grains is crucial to our understanding of stellar and planetary evolution. However, surprisingly little is currently known about this interaction and about the chemistry of the adsorption, desorption and reactions of atoms and molecules on the surface of dust grains.

The composition of interstellar ices identifies the key molecules and surface reactions to study. The exact ice composition varies from one interstellar location to another, but includes H_2O with varying proportions of CO, CO₂, CH₃OH, NH₃ and other trace species. The dust grains themselves consist mainly of carbonaceous and silicaceous material and can be found bare or covered in films of molecular ices⁴. Highly oriented pyrolytic graphite (HOPG), and other carbon based surfaces, are therefore considered suitable analogues of dust grains and have been used previously in investigations of H₂ formation on dust grain surfaces⁵⁻⁸.

Desorption is a particularly important process in star-forming regions, where molecular ices are deposited on the surface of dust grains during the collapse of dense cores. Once the star is born, ices evaporate and return to the gas phase. Before desorption occurs, however, the composition of the molecular ices often alters as they undergo surface reactions on the dust grains, and it is these surface reaction processes that give rise to the rich chemistry observed in these regions. Desorption is also important in hot core regions^{9,10}. Hot cores are small, dense, relatively warm, objects detected in the vicinity of newly formed massive stars. Hot cores are rich in small unsaturated molecules and in large organic species due to the evaporation of thermally processed ice, formed during the star formation process. In the past, studies of hot core chemistry have assumed that desorption of the molecular ices is instantaneous. However, more recent studies¹¹ have shown that, in fact, desorption is not instantaneous. Studies have also shown that it may be possible to determine the age of a hot core from observations of molecular species found in the gas phase during the desorption process. Hence, in order to understand the chemistry of hot cores and of the star-forming process, it is important to obtain a thorough understanding of the desorption of icy mantles from dust grain surfaces.

With this in mind, we have undertaken detailed studies of the adsorption and desorption of pure H_2O , pure CH_3OH and pure NH_3 ices from an HOPG surface. We have also investigated the adsorption and desorption of binary layered CH_3OH/H_2O ices and of intimately mixed CH_3OH/H_2O ices from an HOPG surface. We have also begun preliminary studies of the formation of these species on HOPG.

Key advances

The key results that have been obtained during the course of this project concern the adsorption and desorption of molecules found in interstellar ices adsorbed on an HOPG surface¹²⁻¹⁹. The results of these studies have been incorporated directly into astrochemical models of hot cores and of the star-formation process²⁰. The results have also been used to predict desorption temperatures and residence times of the ices on a dust grain surface under astrophysical conditions²¹.

Studies were initially undertaken of pure H_2O , pure CH_3OH and pure NH_3 ices adsorbed on, and desorbing from, an HOPG surface. The two surface science techniques that were used to study these ices were reflection absorption infrared spectroscopy (RAIRS) and temperature programmed desorption (TPD). The initial aim of these studies was to provide an experimental "fingerprint" of these molecules so that when formation experiments were performed, we would easily be able to identify the reaction products using RAIRS and TPD. Prior to these investigations, no detailed studies of adsorption and desorption had been undertaken on a suitable dust grain analogue surface, although less detailed studies had been undertaken on HOPG^{22,23} and studies of the desorption of H_2O had been undertaken on a Au surface²⁴. Studies of the desorption of CH_3OH and NH_3 had also previously been undertaken on a Au surface²⁵ and a CsI^{26} surface, but not on a suitable dust grain analogue surface. All experiments were performed for ices adsorbed at ~ 80 K. Although this temperature is not as low as that found in the ISM, where temperatures are usually around 10-20 K, it still allows an understanding of the adsorption and desorption of these species to be obtained. This higher temperature is also important for studies of cometary ices and for hot cores. Particular care was taken only to investigate species that were known to desorb at temperatures above 80 K.

 H_2O is the most abundant species found in interstellar ices, accounting for 60-70% of the composition of such ices². Experiments investigating the adsorption and desorption of pure H_2O ice from the HOPG surface show that the behaviour of H_2O on graphite is complex¹³. RAIRS experiments show that H_2O is physisorbed on HOPG at all coverages. Experiments at higher surface temperatures show marked changes in the O-H stretching region of the infrared spectrum, which can be attributed to a phase transition from amorphous to crystalline H_2O ice. The infrared signature of both phases of solid H_2O on HOPG was determined and these can be used to identify the phase of the ice spectroscopically. The ability to distinguish between ice phases spectroscopically is especially important in the ISM, where H_2O ice acts as a catalytic surface for the formation of many molecules²⁸.

TPD spectra¹³ showed the desorption of physisorbed H_2O at all exposures, as seen in Figure 1. At very low coverages it was possible to distinguish the desorption of H_2O from 2D and 3D islands. The observation of island formation showed that H_2O does not wet the HOPG surface, and instead grows as hydrogen bonded clusters on the surface. As the H_2O coverage on the surface increased, the desorption of multilayers of H_2O was observed. At very high exposures, the amorphous to crystalline H_2O phase transition was observed as a bump in the TPD spectrum on the low temperature side of the main desorption peak. The crystalline ice to hexagonal ice phase transition was also observed as a separate peak at 175 K. Neither of these phase transitions had been observed in previous TPD investigations of water desorption from HOPG²³.



Figure 1: TPD spectra following increasing exposure of H_2O on an HOPG surface held at ~ 80 K¹³. (A) spectra recorded following doses of 0.04, 0.06, 0.1, 0.2, 0.3, 0.4, 1 and 2 L of H_2O ; (B) spectra recorded following doses of 2, 3, 7, 10 and 15 L of H_2O ; (C) spectra recorded following doses of 15, 20, 50, 100 and 275 L of H_2O^{13} .

To shed more light on the amorphous to crystalline phase transition of H_2O ice, isothermal TPD spectra were also recorded¹³. Isothermal spectra showed that, in contrast to previous studies of H_2O desorption from HOPG^{22,23}, perfect zero order desorption kinetics were not observed. Detailed analysis¹³ of the TPD spectra seen in Figure 1 allowed kinetic parameters for the desorption of H_2O from HOPG to be elucidated (see Table 1). Prior to this study, kinetic parameters for H_2O desorption from HOPG had not previously been determined, despite their importance for the development of accurate models of the chemistry of the ISM.

Experiments were also performed to investigate the adsorption and desorption of pure CH₃OH ice adsorbed on HOPG¹². CH₃OH is another important component of interstellar ices, with a composition of 5-50% relative to H_2O^{29} . As for H₂O, TPD spectra were also complex with several desorption peaks being observed as a function of increasing ice thickness. For very thin ices, the desorption of monolayer CH₃OH directly from the HOPG surface was observed. For thicker ices, the desorption of multilayers of CH₃OH was also observed and, for the thickest ices studied, the formation of crystalline CH₃OH was also detected at high enough temperatures. As for the H₂O ice, kinetic parameters for the desorption of CH₃OH ice were determined directly from the TPD data¹² (see Table 1). This was the first time that detailed kinetic parameters had been determined for the desorption of CH₃OH ice from a dust grain analogue surface. RAIR spectra were also recorded for CH₃OH adsorption and these showed that CH₃OH was physisorbed at all coverages investigated. When the adsorbed CH₃OH ice was heated, splitting of the O-H and C-O bands in the RAIR spectrum, characteristic of the formation of crystalline CH₃OH, was observed¹².

Table 1: Table showing the kinetic parameters derived for the desorption of pure H_2O^{13} , pure CH_3OH^{12} and pure NH_3^{14} ices from the HOPG surface.

	Desorption order, n	Desorption energy/kJ mol ⁻¹	Pre-exponential factor*/ molec m ⁻² s ⁻¹
H_2O^{13}	0.26 ± 0.02	39.9 ± 0.8	$1 imes 10^{27 \pm 1}$
NH_3^{14}	0.25 ± 0.05	23.2 ± 1.2	$8\pm3\times10^{25}$
CH ₃ OH multilayer ¹²	0.35 ± 0.21	33 - 48	$6 imes 10^{25 \pm 3}$
CH ₃ OH monolayer ¹²	1.23 ± 0.14	31 - 40	*9 × 10 ^{9±3}

The units given for the pre-exponential factors for H_2O , NH_3 and CH_3OH multilayers are those expected for zero order desorption, despite the fractional order desorption obtained from the data. ^{}The units given for the pre-exponential factor for monolayer CH_3OH are those for first order desorption (s⁻¹) despite the fractional desorption order obtained from the data.

 NH_3 has also been observed in interstellar ices²⁷, where it has an abundance of 5-30% with respect to H_2O^{30} . In contrast to the CH_3OH and H_2O ice films, pure NH_3 ice shows much simpler behaviour in both adsorption and desorption¹⁴. RAIR spectra show very sharp bands, characteristic of the formation of physisorbed crystalline NH_3 ice on the HOPG surface at ~ 80 K. TPD spectra also show the formation of physisorbed species. Unusually the monolayer of NH_3 is observed to desorb at a lower temperature than the multilayer. This can be attributed to the extensive hydrogen bonding that occurs in the multilayer. Kinetic parameters (see Table 1) were also determined for the desorption of NH_3 from HOPG¹⁴. Again, this was the first time that the parameters for NH_3 desorption from HOPG had been determined.



Figure 2: Simulated TPD profiles²¹ for NH₃, H₂O and CH₃OH desorption from HOPG as a function of heating rate. The spectra (from left to right) have heating rates of 1 K century⁻¹, 1 K year⁻¹, 1 K day⁻¹, 0.5 K s⁻¹ (0.2 K s⁻¹ for NH₃) and 10 K s⁻¹.

Once kinetic parameters for the desorption of the pure ices from the HOPG surface had been determined, we were then able to use these to predict the desorption temperature of ices from interstellar grains in the ISM²¹. These results can then be incorporated directly into astrochemical models. The desorption temperatures for pure H₂O, CH₃OH and NH₃ determined in our experiments¹²⁻¹⁴ cannot be directly incorporated into astrochemical models. This is because the temperature at which desorption occurs depends not only on the thickness of the ice, but also on the heating rate. During star formation, the rate at which the temperature of the dust grain rises is dependent on the mass of the star¹⁰. It has been shown that a dust grain in a hot core is typically heated at a rate of the order of 1 K century^{-1 10,31}, clearly impractical in laboratory studies. In order to determine the extent to which desorption temperatures vary between laboratory and astrophysical conditions, we simulated the desorption of pure H₂O, CH₃OH and NH₃ ices from an HOPG surface at a range of different heating rates²¹. The simulations use a method developed by Collings and co-workers³² and involve calculating the rate of change of gas phase concentration of the desorbing species as a function of temperature²¹. In this way, the simulations produce traces which resemble TPD peaks (Figure 2). The results of the simulations shown in Figure 2 are invaluable to astronomers as they give information about the expected desorption temperature of ices under real interstellar conditions. The data shown in Table 1 and Figure 2 were also used to determine gas depletion rates and residence times for pure ices adsorbed on grain surfaces²¹. This data is also of importance to astronomers, because molecules are depleted from the gas phase when they are adsorbed onto the surface of dust grains. The rate of depletion from the gas phase is an important consideration in modeling the true column density of molecules present in dark clouds such as H₂O, CH₃OH and NH₃. Residence times are also used by astronomers in models of grain-surface chemistry in a range of different interstellar environments including hot cores, star-forming regions and the surfaces and atmospheres of comets and planets.

As well as looking at the desorption of pure ices, we have also investigated the desorption of binary layered¹⁵ and intimately mixed¹⁹ H₂O/CH₃OH ices. Molecular ices found in the ISM are not generally pure, and combining studies of pure ices to give information on mixed ices is not always reliable. Hence studying layered and mixed ices is important to obtain an understanding of how CH₃OH and H₂O behave when mixed. The layered ices were formed by depositing CH₃OH ice of various thicknesses onto the surface of a pre-deposited layer of amorphous H₂O ice¹⁵. RAIRS shows that there is no detectable interaction between the layers on adsorption, however heating the layered ice leads to mixing of the H₂O and CH₃OH layers as seen in Figure 3. TPD data also show evidence of mixing of the layered ices when heating occurs, with a TPD peak being observed that can be assigned to the trapping of CH₃OH within the H₂O ice structure.

The TPD peak assigned to the trapped species increases in size as the thickness of the underlying H₂O layer increases, and is thought to arise due to entrapment of the CH₃OH at grain boundaries (or holes) that form in the H₂O ice as the amorphous to crystalline phase transition takes place. It is proposed that it is this trapped CH₃OH species that gives rise to the observed shift in the O-H band observed in the RAIR spectrum (Figure 3). TPD peaks are also seen for the desorption of monolayer and multilayer CH₃OH and, as seen with RAIRS, TPD cannot distinguish between monolayer CH₃OH desorbing from the H₂O surface and monolayer CH₃OH desorbing from the bare HOPG surface. Additional TPD peaks are also observed that can be assigned to the formation, and desorption, of crystalline CH₃OH and also to the desorption of CH₃OH that occurs as the H₂O crystalline to hexagonal ice phase transition occurs.



Figure 3: RAIR spectra for 50 L of pure H_2O annealed to 150 K, 50 L of pure CH_3OH annealed to 141 K and 50 L CH_3OH adsorbed on top of 50 L H_2O ice annealed to 155 K, all grown on HOPG at 90 K. The fit generated by the addition of the pure CH_3OH and pure H_2O spectra is shown as a dotted line. Clearly the data for the annealed layered ice cannot be fitted by the simple addition of the spectra for the pure ices, suggesting that mixing has taken place. The inset shows the fit shifted down by 50 cm⁻¹ to show the good overlap with the spectrum for the layered ice annealed to 155 K.

As expected, co-deposited H_2O/CH_3OH layers¹⁹, consisting of 10% CH₃OH in H₂O, behave somewhat differently to either pure¹² or layered ices¹⁵. TPD data shows that heating the mixed ice leads initially to desorption of CH₃OH molecules that are present on the surface of the ice. Further heating of the ice, beyond the amorphous to crystalline transition temperature of the H₂O, results in significant reordering of the ice which causes channels to open and close within the ice structure. These allow the percolation of CH₃OH molecules trapped in the bulk towards the surface of the ice where they then desorb. Once the crystallization of the H₂O ice is complete the channels become sealed and the remaining CH₃OH is trapped within the bulk of the H₂O ice and can only desorb when the H₂O desorbs, leading to the so called codesorption peak in the TPD spectra. The behaviour of the H₂O within the mixed ice is little changed from that expected for pure H₂O. The RAIR spectrum of the H₂O in the mixed ice is perturbed by the presence of H₂O in the ice, so that it is possible to distinguish CH₃OH trapped within the H₂O from that present on the surface of the ice¹⁹.

The data recorded for the desorption of layered and mixed ices is of relevance to studies of the desorption of interstellar ices in areas such as comets, star-forming regions and hot $cores^{9,10}$. Previous work has categorised the molecules found in interstellar ices according to their desorption characteristics³². These categories were then used to model the desorption of interstellar ices in hot core regions¹⁰. CH₃OH was categorised as a "H₂O-like" species³², meaning that it shows desorption characteristics similar to those of H₂O. CH₃OH desorbing from a H₂O layer was not observed to trap within the structure of the H₂O ice and only the desorption of monolayer and multilayer CH₃OH was observed. However, the peak assigned to the desorption of monolayer CH₃OH was coincident with the desorption of H₂O³². Our results suggest that this "monolayer" peak should actually be reassigned to the desorption of CH₃OH trapped within the bulk of the H₂O ice¹⁹. Since we are clearly able to distinguish the desorption of monolayer, multilayer and trapped CH₃OH^{15,19}. The apparent difference between our results and the previous results³² can be explained by the different exposure ranges of the two experiments. Our experiments^{15,19} were performed over a wide range of CH₃OH exposures, however the previous results only investigated the desorption of 5 L of CH₃OH adsorbed on the underlying H₂O ice surface³². Hence it is clear that the previous classification of CH₃OH was limited by the exposure range used. Indeed, the authors of the previous work³² pointed out that their study was an attempt at initial categorisation of astrochemically relevant molecular species and that more detailed studies were needed in order to give a full understanding of the relevant adsorption systems.

This data has recently been used in astrochemical models to observe the effect of the different categorisation of CH_3OH on the chemistry observed in star-forming regions, and also to observe the effect of the ice thickness and the nature of the dust grain surface on the chemistry observed^{20.} The results of the model suggest that the nature of the surface does not have a large effect on the results of the astrochemical models, at least for H_2O and CH_3OH . However the re-categorisation of CH_3OH causes different behaviour for low mass stars²⁰, with a fraction of the CH_3OH desorbing at lower temperatures than previously thought¹⁰. Hence in terms of predicting the age of a warming hot core, the observation of CH_3OH would be a useful indicator that the core had not yet reached the maximum temperature and that ice coated grains may still be present.

Project plan review

It was originally intended to spend the main part of this research project investigating the formation of the molecular species found in interstellar ices. However, the project plan was changed and most of the project has instead been spent investigating the adsorption and desorption of molecules found in interstellar ices from a dust grain analogue surface, as detailed above. There were two main reasons for this change of plan. The initial reason was scientific and the second reason was due to a problem with the liquid helium cryostat, detailed below. Preliminary studies were undertaken of the adsorption and desorption of pure H₂O, CH₃OH and NH₃ ices from the HOPG surface in order to provide a "fingerprint" of the infrared spectrum expected for these species, our target molecules, on the HOPG surface. TPD studies were also undertaken and kinetic parameters were determined for the desorbing ices. The data we obtained were extremely interesting and were also of great interest to astronomers - as detailed by our publication describing desorption temperatures and residence times under astrophysical conditions²¹. Once the investigations of the pure ices had been completed, it was intended to begin investigations of the formation of these species on the HOPG surface. At this point it was necessary to cool the sample to liquid helium temperatures, using a liquid helium cryostat that we already had. Unfortunately the cryostat was not able to regularly achieve temperatures of 10 - 20 K, as required for the formation reactions. After spending almost 6 months trying to solve this problem, we took the decision to replace the cryostat with a closed cycle helium refrigerator, as used by other researchers in this field^{24,25}. Our decision to do this was also influenced by the increasing cost of purchasing liquid helium that has been observed over the last few years. The decision to change to a different cryostat for cooling the sample caused a delay to the start of the formation experiments, since the new cryostat had to be designed, built and tested before it could be used. While the cryostat was being manufactured, it was decided to investigate the adsorption and desorption of mixed and layered H₂O/CH₃OH ices as this was a logical continuation of the experiments on pure ices. As described above, these experiments gave extremely interesting data which was of interest to astronomers - in fact Dr S. Viti (UCL Physics and Astronomy) incorporated our data into an astronomical model of hot core regions, as described above²⁰. The H atom source was designed and built at the beginning of the project, whilst the investigations on pure ices were taking place. The new cryostat has now been tested, and therefore experiments investigating the formation of these molecules on a dust grain analogue surface have recently begun.

Research impact

The main impact of the research described here has been in the astronomy and astrochemistry community and the full impact of the research is just beginning to be realised. The results provide much needed information about the adsorption and desorption of the species found in molecular ices from a dust grain analogue surface. Comparisons with other results, where adsorption of the ices has been performed on alternative surfaces, gives an indication of the effect that the nature of the dust grain surface has on the adsorption and desorption. The spectroscopic information about the ices that we have recorded, particularly for the layered and mixed ices, can also be used to identify species observed in the ISM. The kinetic parameters for the desorption of the ice species have also been determined and these are of crucial importance to astrochemists as they allow us to predict desorption temperatures and residence times of ices on a dust grain surface under astrophysical conditions²¹. The results have also been directly incorporated into astrochemical models²⁰ and give information about the species observed in the gas phase during the star formation process and during the evolution of hot cores.

The results are also of benefit to surface scientists, who are interested in the adsorption properties of the species found in molecular ices on an HOPG surface. In particular, the data that we have recorded gives crucial information about the role that hydrogen bonding places in adsorption on surfaces of this type.

Of course, all of the data recorded to date is also of crucial importance for providing a fingerprint for the products of the formation experiments, which are now underway.

Explanation of expenditure

Most of the funds for this project were spent as indicated in the original proposal.

Travel and subsistence: Funds were spent attending scientific conferences and meetings in the fields of surface science and astrochemistry, including those detailed in the dissemination section below.

Technical salaries: Time in both the electronics and mechanical workshops at UCL was used during the period of this grant and the technical salaries were therefore spent accordingly.

Studentship: A PhD student, Angela Wolff, was appointed and the allocated funds were spent on her fees and maintenance. Due to an increase in the fees and maintenance over the period of this grant, there was an overspend on both the student fees and the maintenance part of the grant. We were informed by EPSRC early in the project that this overspend was legitimate. The student submitted her thesis in August 2006 and was awarded her PhD on 30th November 2006.

Consumables: Consumables money was spent as detailed in the original proposal on samples, gaskets, solvents, gases, liquid nitrogen/helium and general consumables. Consumables money was also spent on various small repairs to the UHV apparatus, as required. A preventative maintenance contract for the infrared spectrometer was also purchased, as originally intended.

Equipment: The only area where there was a slight change in the planned expenditure was for equipment. As detailed in the original proposal, it was intended to purchase equipment to build an H atom source, to purchase electronics to convert our LEED optics to allow the performance of LEED/AES experiments and to purchase a source for metal evaporation. Electronics for the LEED/AES system were bought. A microwave cavity and a microwave generator with associated cables were also purchased to allow the generation of H atoms. A differentially pumped vacuum chamber for the H atom source, and associated pumps and gauging, were also purchased. Due to the problems encountered with the original liquid helium manipulator (detailed above), and due to the rising cost of purchasing liquid helium, it was decided to purchase a closed cycle helium refrigerator to allow the sample to be cooled to 10 - 20 K. This purchase used up the rest of the equipment funds and so a metal evaporation source was not bought. This will now be purchased with funds awarded by the Leverhulme Trust (see below).

Further research and dissemination activities

Further research: Several areas of further research have arisen as a direct result of the work described here. WAB has been awarded a grant by the Leverhulme Trust to continue this research and to undertake detailed investigations of the formation of the species found in molecular ices on dust grain analogue surfaces. The Leverhulme grant funds a post-doctoral researcher along with associated consumables. WAB has also been awarded an EPSRC DTA studentship from the UCL chemistry department to continue this research, and WAB and SDP have jointly been awarded (in collaboration with Dr S. Viti, UCL Physics and Astronomy) a faculty EPSRC DTA studentship for a project in which the student will take data in the laboratory and then incorporate this data directly into astrochemical models. As a direct result of the research described here, WAB has become a coordinator of an EPSRC funded network on Surface Science Applications in Laboratory Astrophysics (the AstroSurf network - see http://www.chem.ucl.ac.uk/astrosurf/home.html for details). WAB is a co-investigator on this ESPRC funded grant (GR/T05004) and regularly arranges scientific meetings for the network. Also as a direct result of the research described here, and the continuing studies of molecular formation reactions, WAB has been awarded an EPSRC grant (EP/D500524) to undertake theoretical investigations of the formation of molecules on dust grain analogue surfaces. These calculations are performed in collaboration with Prof. R. Catlow (UCL chemistry) and Dr A. Wander (Daresbury Laboratory). Finally, again as a direct result of the research described here, WAB has become involved in experiments at the Rutherford Appleton Laboratory Lasers for Science Facility (in collaboration with M.R.S. McCoustra, Heriot-Watt and H.J. Fraser, Strathclyde) to investigate the ultraviolet processing of interstellar ice mixtures. We have, so far, been awarded four periods of laser access time for these experiments, and another period of access for 2007 has recently been applied for.

Dissemination: A total of 10 publications in international peer-reviewed scientific journals have directly resulted from the work described here. Of these 5 are already published^{12-14,20,21}, 2 are currently in press^{15,16} and 3 more are in the final stages of preparation¹⁷⁻¹⁹. This research has been presented by WAB and by Angela Wolff, the PhD student employed on the grant, at numerous conferences and seminars in both the surface science and astrochemistry fields. Conference presentations include an invited talk by WAB at a workshop on "Carbon in space" in Italy in 2006; an invited poster by WAB at the Transatlantic Frontiers of Chemistry conference in New Hampshire, USA in August 2006; a talk and paper for discussion given by WAB at Faraday Discussions 133, France April 2006; a talk given by Angela Wolff and a poster given by WAB at ISSC-15, Cardiff June 2005; a poster given by Angela Wolff at the IAU symposium in Asilomar USA, June 2005; a talk given by WAB at the RSC Astrochemistry group meeting, Cardiff, January 2005; and an invited talk by WAB at the National Astronomy Meeting

Milton Keynes, March 2004. WAB has also given 5 invited university research seminars on this work over the period of the grant and will be giving 2 more university colloquia on this research in March 2007. The work described here has also been publicised via WAB's web site (www.chem.ucl.ac.uk/people/brown) and via the web site of the UCL centre for cosmic chemistry and physics, of which all of the investigators on this project are members. Regular meetings of all of the researchers involved in the UCL centre for cosmic chemistry and physics also ensures that the research described here is immediately disseminated to the end users of the data – the astronomers. In addition to this, as already described above, WAB is a coordinator of the AstroSurf network and regularly arranges conferences and research meetings for surface scientists and astronomers within the network. These meetings also facilitate the dissemination of data directly to the astrochemists. This research has also been described to a wider audience by articles in the EPSRC Newsline magazine (September 2003 and July 2005) and in the RSC magazine Chemistry World (August 2005).

As well as these more traditional dissemination routes, the research in this project has also been described to the general public and to school children via an exhibit, called "Stars 'R' Us!", which WAB became involved in as a direct result of the work undertaken in this project. Stars 'R' Us! (http://www.chem.ucl.ac.uk/cosmicdust/starsrus.html) is an exhibit which aims to show the connection between chemistry and astronomy via a series of hands-on displays. The exhibit is a collaboration between WAB and researchers at Heriot-Watt, Strathclyde and the Open University and was originally exhibited at the Royal Society Summer Exhibition 2004. Since then Stars 'R' Us! has also featured at exhibitions at the National Maritime Museum Greenwich (UK science week 2005 and 2006) at Villages des Sciences Paris 2005 (French science week, invited by the British Council), on an RSC shopping centre tour (Chemistry week 2005) and at the Royal Society Science exhibition in Glasgow in September 2006. Over the last 3 years, WAB has also given 3 public lectures on the role of chemistry in astronomy to school children and to interested members of the public. Stars 'R' Us!, and therefore indirectly the work undertaken on this grant, has also led to the publication of an article in Education in Chemistry³³ and to the award of several small grants for public understanding of science activities from the RSC, the IoP and from PPARC (PP/B501071/1) and the EPSRC (EP/E022081).

References

¹D.C.B. Whittet, W.A. Schutte, A.G.G.M. Tielens, A.C.A. Boogert, T. de Graauw, P. Ehrenfreund, P.A. Gerakines, F.P. Helmich, T. Prusti, E.F. van Dishoeck, Astron. Astrophys. 315 (1996) L357.

- ²D.A. Williams, S.D. Taylor, Quart. J. Rev. Astro. Soc. **37** (1996) 565.
- ³T.W. Hartquist, D.A. Williams, The Chemically Controlled Cosmos, OUP, Oxford, 1995.
- ⁴D.A. Williams in Dust and Gas in Astronomy, Eds. T.J. Millar, D.A. Williams, Institute of Physics Publishing, Bristol, 1993.
- ⁵J.S.A. Perry, S.D. Price, Astrophys. Space. Sci. 285 (2003) 769.
- ⁶V. Pirronello, C. Liu, J.E. Roser, G. Vidali, Astron. Astrophys. **344** (1999) 681.
- ⁷J.S.A. Perry, J.M. Gingell, K.A. Newson, J. To, N. Watanabe, S.D. Price, Meas. Sci. Tech. **13** (2002) 13.
- ⁸N. Katz, I. Furman, O. Biham, V. Pirronello, G. Vidali, Astrophys. J. 522 (1999) 305.
- ⁹D.A. Williams, Farad. Discuss. **109** (1998) 1.
- ¹⁰S. Viti, M.P. Collings, J.W. Dever, M.R.S. McCoustra, D.A. Williams, Mon. Not. Roy. Astron. Soc. **354** (2004) 1141.
- ¹¹S. Viti, D.A. Williams, Mon. Not. Roy. Astron. Soc. **305** (1999) 755.
- ¹²A.S. Bolina, A.J. Wolff, W.A. Brown, J. Chem. Phys. **122** (2005) 044713.
- ¹³A.S. Bolina, A.J. Wolff, W.A. Brown, J. Phys. Chem. B **109** (2005) 16836.
- ¹⁴A.S. Bolina, W. A. Brown, Surf. Sci. **598** (2005) 45.
- ¹⁵A.J. Wolff, C. Carlstedt, W.A. Brown, J. Phys. Chem. C (2007) in press.
- ¹⁶D.A. Williams, W.A. Brown, S.D. Price, J.M.C. Rawlings, S. Viti, Astronomy and Geophysics (2007) in press.
- ¹⁷R. Chen, M.P. Collings, M.R.S. McCoustra, A.S. Bolina, W.A. Brown, Mon. Not. Roy. Astron. Soc., to be submitted.
- ¹⁸W.A. Brown, Phys. Chem. Chem. Phys. invited article, in preparation.
- ¹⁹A. J. Wolff, W. A. Brown, in preparation.
- ²⁰W.A. Brown, S. Viti, A.J.Wolff, A.S. Bolina, Farad. Discuss. **133** (2006) 113.
- ²¹W.A. Brown, A.S. Bolina, Mon. Not Roy. Astron. Soc. **374** (2007) 1006.

²²R.B. Phelps, L.L. Kesmodel, R.J. Kelley, Surf. Sci. 340 (1995) 134; D.V. Chakarov, L. Osterlund, B. Kasemo, Vacuum 46 (1995) 1109; D.V. Chakarov, L. Osterlund, B. Kasemo, Langmuir 11 (1995) 1201.

- ²³D.V. Chakarov and B. Kasemo, Phys. Rev. Lett. **81** (1998) 5182; D.V. Chakarov, M.A. Gleeson, B.Kasemo, J. Chem. Phys. **115** (2001) 947.
- ²⁴H.J. Fraser, M.P. Collings, M.R.S. McCoustra, D.A. Williams, Mon. Not. Roy. Astron. Soc. **327** (2001) 1165.

²⁵M.P. Collings, M.A. Anderson, R. Chen, J.W. Dever, S. Viti, D.A. Williams, M.R.S. McCoustra, Mon. Not. Roy. Astron. Soc. 354 (2004) 1133.

- ²⁶S.A. Sandford, L.J. Allamandola, Astrophys. J. **417** (1993) 815.
- ²⁷D.C.B. Whittet in in Dust and Gas in Astronomy, Eds. T.J. Millar, D.A. Williams, Institute of Physics Publishing, Bristol, 1993.
- ²⁸P. Ehrenfreund et al, Rep. Prog. Phys. **65** (2002) 1427.
- ²⁹S.A. Sandford, Meteoritics and Planetary Science 31 (1996) **449**; C.J. Skinner, A.G.G.M. tielens, M.J. Barlow, K. Justtanont, Astrophys. J. 399 (1992) L79.
- ³⁰E.L. Gibb, D.C.B. Whittet, J.E. Chiar, Astrophys. J. 558 (2001) 702; E. Dartois, L. d'Hendecourt, Astron. Astrophys. **365** (2001) 144.
- ³¹S. Viti, D.A. Williams, Mon. Not. Roy Astron. Soc. **305** (1999) 755.
- ³² M.P. Collings, M.A. Anderson, R. Chen, J.W. Dever, S. Viti, D.A. Williams, M.R.S. McCoustra, Mon. Not. Roy. Astron. Soc. 354 (2004) 1133. ³³M.R.S. McCoustra, W.A. Brown, S. Viti, Education in Chemistry **42** (2005) 153.