Astrochemistry: Recent Successes and Current Challenges
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Future Directions in Astrochemistry

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Abstract. An account of a free-ranging Panel Discussion held during the Symposium.

1. Introduction

'Future Directions in Astrochemistry' was the title of a Panel Discussion held during the Symposium. The Panel members were selected to represent 'voices of experience' in the fast-moving field of astrochemistry, and were invited by the Scientific Organising Committee to discuss briefly their perceptions of the big questions facing modern astrochemistry or of the new directions, in which our subject should develop. It proved to be an interesting and entertaining evening, in which some useful scientific perspectives were gained and new prospects described. The Panellists were Lou Allamandola, John Black, Ewine van Dishoeck, Michel Guélin, Eric Herbst, Tom Phillips, Jonathan Rawlings, Xander Tielens, and Malcolm Walmsley. The proceedings were chaired by David Williams.

There was no prior collusion between the Panel members, nor were the discussions prepared or rehearsed in any way. Yet there was an interesting convergence of views as to some of the challenges facing astrochemistry today. These included:

- the high level of complexity of modern astrochemical models: are the model outputs realistic and credible?
- future observational data rates from facilities such as ALMA: will the future astrochemical community be able to cope?
- can we use the detailed mapping of entire galaxies now available to determine the implications for comprehensive understanding of galactic-scale physics and chemistry?
- are we able to develop useful treatments of non-equilibrium chemistry in weakly ionised, magnetic, and non-Maxwellian media?
- how should we account in our models for the interaction of gaseous atoms, molecules and ions with grain surfaces?
- do we properly understand the chemistry of interstellar water and the formation of water ice on dust grains?
- dirty ice chemistry; what is the role of stable ions in solids?
- can cosmic rays induce the ejection of all kinds of molecules from ices?
- can we constrain galactic astrochemistry by a comparison of interstellar regions of differing physical parameters?
- is deuterium fractionation the key to understanding the physics and chemistry of star-forming regions?
- have we made any progress in understanding long-standing pathological cases, such as interstellar CH^+?
- can astrochemistry contribute to the important astronomical question: the origin of planets?

Of course, as Mr Rumsfeld might say, such a list inevitably contains only the 'known knowns' and 'known unknowns'. There are sure to be the 'unknown unknowns', some of which will (we hope) become apparent at the next Astrochemistry Symposium. All these and other topics were discussed, but two areas were particularly emphasised and will be described in more detail here. These were, firstly, the ever-increasing complexity of the models by which we try to understand and interpret observations, and, secondly, the major gaps in our understanding of the interaction of atoms and molecules with surfaces, and the growth and processing of ices.

2. Complexity in Astrochemistry: are Astrochemical Models Reliable and do They Represent Reality in Some Limited Way?

Over the four decades in which astrochemistry has grown and matured, the models by which we try to understand and interpret astronomical observations have become vastly more complex. Initially, we simply computed steady-state chemical abundances for uniform and static regions to compare with molecular abundances deduced from observations. Now, our models may need to include time-dependence, temperature variability, gas dynamics, the role of magnetic fields, and spatial heterogeneity. The gas-phase networks we use have grown in size from a few tens to several thousands of reactions of many types. Thanks to the dedication and skill of laboratory scientists and theoreticians large numbers of these reactions have been studied experimentally and theoretically. It has been an astounding response to the needs of astrochemistry, though it is still true that many reactions (and their temperature dependences and products) are still poorly understood. New laboratory work continually reveals how deeply subject to error is our understanding of astrochemistry. Throughout this period in which our subject evolved, the importance of the gas/dust interaction has become gradually accepted, and there are many uncertainties to be associated with that interaction, as described below. In addition to these uncertainties, the improvements in observing facilities, particularly those affording high angular resolution, reveal ever-increasing spatial structure on smaller and smaller scales, with the implication of the relevance of shorter and shorter timescales. Thus, in many situations, the original concepts within which chemistry was explored are simply no longer valid. For example, the well-known object TMC-1 has been known since the beginnings of our subject to be exceptionally rich in carbon-chain molecules. The anomalous region was believed to lie in what was found to be a sub-component of TMC-1, known as Core D; but we now know that Core D is itself complex and has a very high degree of sub-structure within it (nearly 50 sub-units), with the implication that it may be evolving rapidly. Hence, the original models of polyyne formation inTMC-1 inevitably rested on a poor foundation.

Thus, complexity arises from incomplete knowledge of chemistry in the gas phase, on surfaces and in the solid state; it is compounded by a limited understanding (driven by ever-improving observations) of the physical situations we seek to explore and describe. The extent to which non-thermal processes or turbulence play a role is unclear. Can we believe the output of our models? Are they useful?

The Panel's discussion tended to stress the incremental approach. No, we could not, as we used to, simply 'put everything in the pot, stir gently, and serve' and hope to arrive at the truth. Computational complexity needs to be tested through simpler approaches. More limited chemical networks can highlight reactions that might have a crucial role, and which should therefore be examined in detail. Modellers must acknowledge that the background of chemical information is continually improving, and update their databases. But it is also important to recognise that the physical basis of any model is open to question, since densities and temperatures deduced from observations are volume-averaged quantities, where the volumes are so large that the important fine detail is lost. For example, the chemical processes determining the abundance of CH^+ molecules by gas-phase reactions in diffuse clouds appear to be well understood and and their rate coefficients well determined, but the physical description of the gas in which those processes play a part is evidently not well characterised or cannot be described sufficiently well.

So the conclusion offered by the Panellists from this part of the discussion might be: do not be disheartened by the slow emergence of the truth, nor make gross claims for one's own work. The enterprise is necessarily slow and iterative between laboratory, theory, observations, and modelling. And that's what makes it fun!

3. The Interaction of Gas and Dust: What are the Issues for Today?

The second area of extensive discussion was also related to concerns about complexity. It is now apparent that the interaction between atoms and molecules with dust grains is an important factor in astrochemistry, and one in which current knowledge is a seriously limiting factor. The scientific issues are the adsorption of atoms and molecules on grain surfaces, the mobility of surface species and their reaction on the surface, the deposition of mixed molecular ices, the chemical processing of such ices, and their removal by thermal or non-thermal means.

The present situation for our understanding of the gas/grain interaction is analogous to that of gas-phase chemistry when our subject began. While the general concepts were then broadly understood, the extent of reliable information on gas-phase reactions relevant to astrochemistry was very small indeed. For example, discussion in the literature from the 1960s and later on the formation of molecular hydrogen on the surfaces of dust grains considered the same issues as now: physisorption and chemisorption, mobility of adsorbed species, the reaction mechanism and the energy budget, and product desorption (either prompt or delayed). Those theoretical speculations have now been very greatly influenced by the results of several recent and sophisticated experiments on molecular hydrogen formation, some of which were described elswhere in the Symposium. Thus, technical advances in the laboratory and in computing power have made possible much more detailed and realistic studies of various surface and solid state processes.

Yet it is clear that we are only at the beginning of this process of learning. It is much easier to pose questions arising from astrochemistry on surfaces or in the solid state than to answer them. However, we have at least advanced from a state of denial of the importance of the gas/dust interaction (an early cause of contention). Molecular hydrogen and other species certainly form on grain surfaces in the interstellar medium, and under suitable conditions molecular ices are deposited on those surfaces. The consequent loss of species from the gas phase is measureable in dense cores in molecular clouds, and this demonstrates that time-dependent freeze-out of species occurs and is an interstellar clock that merely needs to be normalised by a laboratory determination of the relevant sticking probabilities. Detection of relatively complex species in the vicinity of star-forming regions indicates that relatively simple molecular ices may be converted to greater chemical complexity, and desorbed. Many laboratory experiments demonstrate how this chemical complexity may be induced by energy deposition from UV or fast particle irradiation. An important open question at present is desorption: what are the processes desorbing molecules from interstellar ices? Obviously, thermal desorption will be important where the ice temperature can be raised significantly above its normally low value, but even in this apparently simplest of cases recent laboratory work shows unexpected desorptive behaviour linked to the physical nature of ice itself. This is an important issue to address: what is the nature of the interstellar ice? Is it porous or compact? Is its structure dependent on its formation mechanism? Why is there at least partial separation between ice materials?

One area of current interest is the balance of reduction and oxidation reactions occurring within interstellar ices. For example, laboratory work indicates that carbon monoxide may be hydrogenated in some circumstances to formaldehyde, and ultimately to methanol. The relatively high fraction of methanol in interstellar ices indicates that such hydrogenation may be occurring. On the other hand, carbon dioxide, also detected to be abundant in interstellar ices, is surely the oxidation product of carbon monoxide. While it is evident that for gas-phase interstellar chemistry we have some understanding of how the network responds to changes in the physical or chemical conditions, for chemistry in the solid state such intuition eludes us. Nevertheless, it seems likely that simple addition and exchange reactions of neutral species are occurring. The actual situation may, however, be considerably more complex than that. Photolysis of laboratory ices has been shown to produce stabilized ions of polycyclic aromatic hydrocarbons. If such ions and ions of other species exist within interstellar ices, as seems likely, then they may certainly have important roles in cosmic chemistry and physics.

Panel members were confident that the interaction of gaseous atoms and molecules with interstellar dust grains was a very significant influence on interstellar chemistry and therefore on interstellar physics. The broad outlines of that interaction are clear, through surface reactions, ice deposition and processing, and the later ejection of ice molecules back into the gas phase. The details of the processes, however, are mostly obscure, but at least these processes are now capable of being studied with current laboratory techniques, and the next Astrochemistry Symposium should show a major step forward in our understanding. It is, however, at least as likely that new experiments will reveal gaps in our understanding of which we are currently unaware. As Charles Townes (echoing Donald Rumsfeld's words, but with greater clarity) said at the opening of this Symposium 'There is much that we don't understand; in many cases we don't even understand that we don't.' The audience of the Panel discussion seemed excited, rather than depressed, by the challenges outlined during the evening.

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