Summary

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1. Introduction

The quantity of scientific work in the area of astrochemistry is now enormous, and this meeting - in attempting to cover most of the aspects of our subject - has had problems in coping with it due to difficulty of reviewing very active, broad areas in a limited time. At this meeting we have had almost 40 hours of formal and informal discussion, and about 45 oral presentations at which I estimate that about 1500 transparencies and slides have been projected for our enlightenment. About 100 posters have been presented in three sessions. The posters were uniformly of a high standard and generated a great deal of interest and discussion. I think the prominence given in the programme to the posters has been particularly successful. The range of activity, and the enthusiasm with which it is pursued, demonstrate that astrochemistry is in a vigorous state. It has its own intrinsic interest, and in its present maturity is now making substantial contributions to understanding in astronomy.

The growth in the population of astrochemists is striking, and appears to be related to the number of molecular species identified in the interstellar medium. In 1965, the population was probably about a dozen, or several times the number of molecular species then identified. Today, the number of identified molecular species is about 100, and the number of astrochemists is approximately several hundred, of which about half are here. Given the advances in submillimetre and IR technology, and the imminence of several orbiting astronomical missions, we can confidently expect the number of identified interstellar species to rise dramatically. It will be interesting to observe whether the population of astrochemists rises in proportion.

There are few areas of present-day science which are so challenging and interesting as astrochemistry. We have, as the format of our meeting shows, the opportunity of addressing questions from the Early Universe to the Solar System, from the properties of tenuous quiescent gas to star formation, circumstellar envelopes, novae, and supernovae. To do this, we need acquaintance with a wide range of micro and macroscopic phenomena, from atomic and molecular physics to large scale dynamics. We need familiarity with the language of the quantum chemist, of laboratory chemical kinetics, of solid state physics and chemistry, of gas dynamics including hydrodynamic and magnetohydrodynamic shocks, flows, interfaces, and turbulence. We need to

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be aware of the value and limitations of observations made anywhere in the electromagnetic spectrum. We need especially to understand the astronomical context, and pose our questions appropriately.

Dalgarno, in his remarks at the IAU Symposium 120 on "Astrochemistry", Goa, 1985, gave what I believe is the first definition of astrochemistry. His opening remarks to this symposium illustrated the present state of knowledge and emphasised the developments since Goa. He also showed the first chemical equation at this meeting: exceptionally, it contained an error. This was surely not an accident, but a way of subtly reminding us that nothing is certain, and recommending caution and humility. This view was supported later in the meeting by Millar who, with disarming candour, said: "When I put the observational results in the left hand column, and calculated values in the right hand column, I want you to ignore both". Such scepticism was, however, short-lived in the enthusiasm of the meeting.

In this Summary it would be impossible to refer to every matter discussed at the Symposium. I can only give a personal view, and comment on some of the topics that have seemed to me to be particularly exciting. I conclude by highlighting important areas of activity, or themes, for the future.

2. Comments

It used to be a standard comment when discussing chemical networks that few of the relevant rate coefficients had been measured in the laboratory. This is no longer true: and is a testimony to the immense achievements of laboratory workers in Europe and the US over the last decade. Rowe emphasized especially the recent advances in low temperature ion molecular reactions, branching ratios and rate coefficients in dissociative recombination reactions. Recent results on the reaction of N^+ with H_2 and on CH_3^+ (via ternary reactions) radiation association have had immediate and significant impact on cloud models. A significant discrepancy between theory and experiment remains in ternary reactions and in dissociative recombination branching ratios. The most exciting and important single study reported by Rowe, was of the dissociative recombination of H_3^+, now believed to be fast in interstellar conditions.

Ellinger posed the question: Can Quantum Chemistry be a partner in Astrophysics Research? To which the answer was a resounding and emphatic: yes. The complexity of the systems that Quantum Chemistry is now confidently handling is very great. Ellinger illustrated this with work on IR intensity ratios in small PAH ions, and made the confident assertion that the DIBs arise from small ionized and partly dehydrogenated PAHs.

The chemistry of carbon molecules is an essential part of astrochemistry. Kroto discussed recent laboratory work and emphasised the discovery with which he has been associated of large closed structures such as C_{60} and C_{70}.

This is surely one of the most remarkable and important developments in chemistry today. Direct evidence of such structures may exist in observations of the Red Rectangle. The next few years should reveal whether these large molecules are widespread in the Galaxy.

The importance of both experiment and theory in determining data for astrochemistry cannot be overestimated. Great progress has been made. However, Tarafdar questioned whether enough effort is being put into the study of photoprocesses - echoed later by Glassgold in his discussion of circumstellar envelopes.

Good progress has been made in elucidating the role of chemistry in the Early Universe. The link between the details of the chemistry and the size of the collapsing region, to become a protogalaxy, a protocluster, or a protostar, was convincingly established by Shapiro. The discussions by Ferlet, Tielens and Owen of the abundance of deuterium in various locations are a useful pointer to the origin and evolution of matter. The concensus was that variations in the D:H ratio are real and are a consequence of different mixing processes. Owen presented data on deuterium abundances in the Solar System: these provided good evidence of both condensation and outgassing processes occurring in the protosolar nebula.

A large amount of information on External Galaxies is now available, as revealed in papers by Karawa, Guélin, Henkel and Millar. However, detail is missing - it is very large scale data. The scale size in studies of M82 discussed by Henkel and by Milllar is $\sim$ 100pc. One must assume, however, that the range of processes occurring in other galaxies is at least as complex as in our own.

Diffuse Clouds are one type of region in our own Galaxy which are still not fully understood, in spite of modelling efforts going back at least 40 years. van Dishoeck illustrated how the most precise and careful studies lead to some considerable successes; but there are also some failures in our understanding. The subject is, fortunately, receiving new observational input, particularly those involving high spectral resolution and high signal:noise, as described by Crane. Shocks are probably excluded as sources of CH^+. There seems to be a much greater variety of types of regions present in the diffuse interstellar medium than are normally considered (cf. Falgarone's remarks). The recent discovery of interstellar NH implies that dust is chemically active. Perhaps H_2 (high J) formation on dust will allow lower radiation fields to be possible. This area of research will become, with new instruments and techniques, once again observationally driven, and we can expect new developments and new understanding before the next astrochemistry symposium. Blitz reviewed the subject of high latitude clouds and created some order in what had been a very confusing situation. HLCs now include low extinction CO clouds, tiny little clouds, IRAS clouds without radio CO emission, and intermediate velocity clouds. Some of these are rich in molecules. How these objects are related to each other, and how they evolve is something to which astrochemistry will contribute much understanding in the next few years.

The study of Quiescent Clouds and regions of low mass star formation was by far the largest section, with 11 contributions. This is an area where much effort, both observational and theoretical, has been expended. Yet of all the areas discussed, this seems to be the area of least agreement between model and theory, or even between models. Falgarone's work illustrates the basis of the problem. Structures in the interstellar medium are generally found to be long and filamentary, with parameters that change rapidly with space and time. The description she proposes is one of fractal structure with which the tracers A_v, HI, 100μm, CO (3 lines) and H_2 (1-0) all agree, giving the fractal dimension 1.4. Until we understand better what is driving this system, our understanding is bound to be limited. Some new aspects have been developed in recent years: gas-grain interaction is now agreed to be important (as emphasized by d'Hendecourt, Tielens, and Charnley) and mantle limitation must occur, perhaps both continuously and intermittently. Dynamics must not be ignored; Prasad discussed the collapse of single entities, while Charnley described a class of cyclic models in which gas moves between high and low density phases. Shocks may play a role in some regions but not all; Wu showed that some stable cores exist. The interpretation of some NH_3 observational data as representing quiescence was questioned by Rawlings. The applicability of pseudo-time-dependent models as represented, e.g., by the work of Suzuki and collaborators in interpreting chemical differences between TMC-1 and L134N, and the adoption of so-called early-time abundances, are areas of some discussion. Newly detected molecules in these sources (cf. Ohishi's presentation) may throw much light on this crucial comparison. Zuirys' talk on shocked regions in regions of high and low mass star formation and in SNRs (given by Snyder) presented observations that are interesting but which do not always provide very clear evidence of shocks. SNRs provide best direct evidence of the impact of a blast wave with molecular clouds; SiO seems to be shock enhanced. It is difficult to draw any clear conclusions on the effects of interstellar shocks. The next few years should be instructive, and our understanding of these regions will surely improve.

In discussion of regions of high mass star formation the question of the gas-dust interaction again received attention. Walmsley discussed a number of regions of high density in which the freeze-out time should be short, yet in which gaseous molecules are clearly present. Though freeze-out occurs, the evidence suggests that either some return of mantle material to the gas is occurring, or that the freeze-out is less efficient than often assumed. Studies in these regions are being influenced by beautiful new observational work. Maillard illustrated this with high resolution observations of gaseous and solid CO in the 4 μm band, towards young stellar objects. The solid:gas

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CO fraction towards these sources is small, contrasting with the situation for H_2O. This suggests a differential mantle release mechanism is operating. Further work in the infrared was presented by Evans; high resolution observations at 13.4 μm of interstellar molecules such as C_2H_2 - previously thought to be undetectable - show what can now be achieved.

Interface regions were areas of some of the most successful activity and development in theory and observation described at this meeting. White, Stutzki and Jaffe in particular gave a coherent picture of interface regions with three nicely related talks. These showed that interfaces are clumpy, implying that clouds, too, are clumpy. The models of interfaces that have been developed by Tielens and Hollenbach, and by Sternberg and Dalgarno, are broadly successful. In the future, we shall expect significant refinements, such as time-dependence, shocks, dynamics, and realistic grain properties, to be included in the models. Stutzki's discussion of CI, CII, CO suggested that the brightest C^+ coincides with CS dense clumps so that C^+ follows molecular cloud material. The interpretation is that the C^+ observations delineate the cloud surface, if current models are correct. Stutzki also claims that CO surveys detect CO in PDRs around clumps, rather than the cool interiors, so the CO measurements merely count the clumps and hence give a measure of mass. Jaffe's conclusions also emphasized the general tenor of the meeting - that structure and dynamics are important. Warm gas is seen in many regions, and is heated in a variety of ways. Models must take account of this complexity. In the future we can expect observations in previously unexplored wavebands to enhance our knowledge and understanding. A sample of this enhancement was provided by Wright's description of the results obtained by the COBE satellite at wavelengths 200 μm to 0.5 cm. Positive first detections of several important interstellar species are reported, and whole-sky maps should reveal much about the energy balance in the interstellar medium.

The study of near stellar environments has been characterised by some beautiful new observational work, by good agreement between theory and observations, and by some successful exploratory calculations. Rawlings described recent work on novae and supernova. These models require a much greater degree of complexity than for any other type object discussed here: these regions are dense and hot, conditions are harsh, timescales rapid, yet molecules are observed. Models show conditions under which observed molecules can form, and constrain the picture we have of these dramatic events. Curiel, in his discussion of Herbig-Haro objects, presented some beautiful observations, together with very detailed modelling involving shocks, winds, jets, magnetism, etc. At last, an understanding of these fascinating objects is emerging. Glassgold and Lucas discussed observation and theory of circumstellar envelopes. In spite of some uncertainty concerning the rate of photoreactions, good agreement exists between observation and theory.

Interferometric work presented by Lucas illustrated very convincingly the contrast between pre-cursor and shell molecules.

The contribution of dust to interstellar chemistry now seems well established. Allamandola reviewed the large body of laboratory work on photo-induced reactions on ices, being carried out at Ames and at Leiden. The evidence that similar processes occur in mantles on interstellar dust is compelling.

There is enormous amount of recent data on cometary chemistry and A'Hearn, Snyder, Despois, and Delsemme gave us a flavour of this work. A'Hearn posed the interesting question: Can we put Humpty Dumpty together again? i.e. can we from reaction products infer the original pre-cursors and so define the chemistry in the cometary nucleus? Then, can we discuss the variations within cometary nucleus, and comet-comet variations. He showed that a tremendous amount is being achieved, and noted the similarity in many of the ideas with those popular in interstellar chemistry - especially grain-related phenomena. Snyder drew attention to the list of 15 molecular species identified in comets and compared it with the much larger list of identified interstellar species. He suggested that the cometary list incomplete, and his lists should stimulate further searches. Despois showed what can be done to explore the interstellar - Solar System connection through isotopic elemental and chemical abundances, the ortho:para ratio, and grain properties. The connection is indeed an important one. There are few astrochemists who have expertise in both areas, yet the benefits of strengthening the connection could be great.

3. Conclusions

After a week of intense activity one is forced to conclude that the subject of astrochemistry is in a very healthy state. There is a great deal of well-directed, purposeful activity. It is clear that the entire subject is so extensive that it cannot be covered in depth in a one-week meeting.

The subject is being observationally driven, and some excellent new work has been shown here, especially high spectral and angular resolution observations of high signal to noise. New wavebands, too, are becoming accessible. Future prospects for new discoveries and for detailed observations are most encouraging. To come, there will be ISO, SWAS, with more from HST, ASTRO, etc., and splendid ground-based developments. Theory is developing rapidly, too.

What are the lessons to take away from this meeting? Firstly, the importance of structure (fractals?) is indicated by all the measurements. Variations in density and temperature significantly affect the chemistry and all time scales. Secondly, dynamics is likely to be important in almost all situations. However the importance of shocks in chemistry in interstellar clouds is uncertain. One of the areas developing most rapidly is that of interfaces: Mixing, via turbulence, will need to be incorporated in our understanding. The importance of the gas-dust interaction is now confirmed; solid state chemistry does occur in the interstellar medium. Deposition and ejection (both continuous and intermittent) seem to be taking place. Much work on PAHs has been reported here. The role that they play, and their relation to interstellar dust will be clarified in the next few years. On data: astrochemists should challenge the quantum chemists with further problems. From the evidence presented here, any likely problem arising in astrochemistry is or will become amenable to theoretical attack. The response of laboratory workers to astrochemical needs has been magnificent. Yet, there is still more to do, with photo-reactions continuing to be an area for study. The value of making the connections between the branches of our subject is well illustrated in the discussion of cometary chemistry and the Solar System - interstellar dust relation. There, the benefits of such considerations are clear. There may be other connections whose study would bring similar rewards.