ASTROCHEMISTRY -- A SUMMARY

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ABSTRACT. A brief summary of the content of the papers comprising the symposium is presented.

Astrochemistry is the chemistry of astronomical entities in which molecular compounds exist. It embraces observations of molecular absorption and emission spectra and their use as diagnostic probes of the physical environment and the study of the influence of molecular composition on the behavior of the objects. Basic to astrochemistry are the elementary processes of molecular formation in the gas phase and on the surfaces of solid particles and the response of molecules to electromagnetic and corpuscular radiations and to dynamical interactions.

The symposium demonstrated forcefully that astrochemistry is an intellectually exciting area of research which will remain vital into the foreseeable future. It embraces many disciplines and enhances them by the mutual interactions that it stimulates. Astrochemistry addresses deeply significant issues arising in the formation of galaxies, stars and planets and ultimately perhaps the origin of life. There are many more questions than answers but progress is clearly possible in several directions. There exists already an impressive array of observational data and yet we can look forward to major improvements in spectral range, sensitivity and resolution. Of particular value will be the expected enhancements in spatial resolution. The challenges to theoretical interpretations are formidable but real progress is being made, if only in some areas, of providing a more explicit definition of the problems.

New interstellar molecules continue to be discovered. Recent detections include $HOCO^+$, C_3O, C_3H, HCl, CH_3C_3N, CH_3C_4N, $HC_{11}N$, $HCNH^+$ and the first organic ring molecule C_3H_2. To the list of molecules observed in external galaxies, CS may be added. Some molecules have left the list of those detected, including CH_4, HNO and CO^+, but the heavy ion SO^+ is a tentative addition. If SO^+ is present, there should be other more abundant molecular ions. The isomer HOC^+ may be present though the possibility was raised that the line attributed to HOC^+ belongs to $Si^{33}S$. There are many unattributed lines and some

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challenging identifications have been advanced that laboratory studies should be able to confirm or reject. In many instances, astronomical observations have provided higher quality data on the molecular parameters than have laboratory experiments. Theoretical quantum chemical calculations are a valuable component of the identification of new species. The ring molecule, cyclopropenylidene or C_3H_2, appears to be ubiquitous in the galaxy. It exists in ortho and para forms. In certain density ranges, theoretical calculations suggest that one form may be seen in emission and the other in absorption so that C_3H_2 is a potentially powerful diagnostic probe of the molecular environment.

Other ring molecules await detection and it was suggested by Lorne Avery that we are leaving the decade of the chains and entering the decade of the rings. The possibility was advanced that polycyclic aromatic hydrocarbons (PAH) are widespread and perhaps responsible for the diffuse interstellar bands, although questions remain about their durability and their formation mechanisms in the interstellar gas.

The study of isotopic molecules provides unique information on interstellar chemistry and the physical conditions in which interstellar molecules exist and the deuterium-hydrogen abundance [D]/[H] ratio, which can be derived from the molecular data on deuterated species, is a crucial cosmological parameter. Future instrumental developments may see the detection of DCN and the determination of [D]/[H] in nearby galaxies. Vibrationally excited species have also been detected, raising new questions about their chemistry and the mode of excitation.

Observations at high spatial resolution have revealed large variations in the abundances seen in different regions which may be in part due to conditions of excitation but some of which may be ascribed to real changes in chemical composition. Different molecules serve as probes of the several dynamical structures that have been identified such as the ridge, plateau and expanding shells in the region of the Kleinman-Low nebula. Evidence has been found of molecules in jets, accreting disks, and bipolar outflows. Magnetic field effects have been explored utilising the Zeeman effect in molecules such as OH and fields between 20 and 30μG were derived for NGC 2024. Outflow from molecular clouds along the magnetic field direction has apparently been observed.

Far infrared and submillimeter observations provide data on shocked regions arising from the interactions of outflowing gas with the surrounding interstellar material, on warm dusty regions and on the inner regions of dense clouds. A rich harvest of results is anticipated. Infrared emission from shocked vibrationally excited molecular hydrogen and from rotationally excited carbon monoxide is a characteristic response of interstellar gas to a propagating shock wave. Infrared emission of H_2 that is attributable to pumping by ultraviolet photons has been observed in the ionization front in Orion, in a reflection nebula and in two planetary nebulae. With the advent of Space Telescope the ultraviolet lines emitted in the fluorescence process will become detectable.

In theoretical studies of interstellar chemistry, bold ambitious steps are being taken to develop dynamic models of considerable

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sophistication with the intent in part of finding evolutionary sequences into which different kinds of molecular clouds with different chemical compositions might be placed. The steps seem ambitious, even hazardous, because our knowledge of the chemistry is so incomplete. The much simpler steady state and time-dependent chemical models which assume a density and temperature distribution yield chemical abundances which differ in the various models often by orders of magnitude and which sometimes fail by orders of magnitude to reproduce observations despite the very considerable flexibility allowed by uncertainties in the basic chemical reaction rates. Even for what seems to be the relatively uncomplicated diffuse clouds where the physical constraints on density, temperature and radiation field can be well-defined, substantial and perplexing discrepancies still remain between the models and the measurements of chemical composition.

Despite heroic efforts by many laboratory investigators, experimenters and theorists, enormous gaps exist in our knowledge of the rate coefficients of the majority of the important processes. Almost nothing is known about the branching ratios of reactions with more than one possible end product. The determination of coefficients is complicated by the very different populations of internal rotational, vibrational and fine-structure modes that occur in the laboratory and in astronomical environments. It was encouraging to hear of measurements carried out at very low temperatures near to those obtaining in cold interstellar clouds. The measurements include the radiative association of CH_3^+ And H_2. Radiative association is a critical process in models which build complex organic species by gas phase reactions.

A crucial question remains unanswered as to the carbon/oxygen ratio in astronomical objects. Because carbon monoxide is readily formed, the chemical consequences of different ratios are large. The abundance of carbon atoms in dense regions may be related to the C/O ratio. Other explanations have been advanced. It was reported that in M17 the atomic carbon peaks inward of carbon monoxide so that less of the carbon is in molecular form in the inner shielded region. An interior dissociation source may be indicated. It would be a considerable assistance if the persistent uncertainties about the basic mechanisms in the photodissociation of carbon monoxide could be removed.

Shocks have a profound effect on the chemical composition because in the heated gas endothermic reactions with molecular hydrogen occur rapidly. A gas irradiated by X-rays has a warm region which behaves similarly. Magnetic fields exercise a profound influence and reactions involving ions may be driven by the streaming of the ions through the neutral gas. The molecular ion CH^+ seen in diffuse clouds may be produced in this way. Observations were reported that velocity differences between CH^+ and CH exist in half the cases in which both have been observed. It may be equally significant to note that in half the cases no velocity difference was found.

The important role of grains as a sink and as a source of molecules was emphasized and features appearing in astronomical spectra were attributed to molecules on grain surfaces. Mechanisms by which molecules are released from grains were analyzed and the initial composition of the molecules was examined. Transient heating by shock waves and by energetic particles and processing by ultraviolet radiation all modify the initial composition. Laboratory studies, which are crucial to efforts to unify gas phase and surface interstellar chemistry, were reported, but more research in conditions appropriate to the interstellar medium is needed.

Substantial progress has occurred in our understanding of circumstellar chemistry. The observations of molecules in circumstellar shells provide significant data on mass loss and stellar evolution and offer also a better characterized environment in which to test ideas about gas phase and grain chemistries, though ultraviolet emission from the chromosphere, excitation by infrared pumping and self-shielding may complicate the interpretations. Millimeter and infrared observations show that large differences in composition occur between oxygen-rich and carbon-rich objects and provide a data base for exploring the effects of differing C/O ratios. Though little is known of their characteristics or their modes of formation, it is clear that grains play a major role and together with photodissociation processes control the chemistry of the outer layers of the shells.

Reliable thermochemical data comprise an essential component of circumstellar chemistry and equally of the chemistry of stellar atmospheres. Complex polyatomic species may contribute to the stellar opacity. Valuable information about the elements and their isotopes can be obtained from molecular data. There occur real differences in $^{13}C/^{12}C$ ratio and ^{13}C-rich stars are rare. In some stars, the chemical composition may be changed by shock waves and conditions depart from local thermodynamic equilibrium

Because of their importance in star forming regions and stellar evolution, masers warrant special mention. Elaborate models have been constructed of mechanisms for achieving population inversion and gain though none is clearly established. Different molecular masers demand different interpretations and the excitation mechanisms and the molecular formation and destruction processes are intimately related.

The chemistry of cometary atmospheres bears some similarity to circumstellar chemistry with the advantage that the radiation field is known. Much of the chemistry is not. Highly sophisticated models have been constructed of the dynamics of the coma and tail but there are major uncertainties in the chemical rate coefficients, in the photodissociation rates and products and in the determination of the excitation mechanisms. We cannot yet infer reliably from the measured abundances the production rates of the possible parent molecules, other than H_2O, and we cannot yet draw any definite conclusions about the possible interstellar origin of cometary molecules. The quality and quantity of the observational data have grown markedly in recent years. They will be dramatically enhanced with the arrival of comet Halley and its observation with ground-based and space-born instrumentation.

The exciting possibility exists that comets carry remnants of pristine interstellar material which might be collected. However, we may already have some in hand. Anomalous isotope ratios and molecular abundances raise questions about chemical fractionation but also suggest that certain classes of meteorites contain unprocessed extrasolar material. Meteoritic chemistry is a rich field of investigation.

The unification of early Universe chemistry, interstellar chemistry, circumstellar and stellar chemistry, cometary and meteoritic chemistry (together with planetary atmosphere chemistry) is a challenging task which requires research in many different branches of physics, chemistry, geology and astronomy. Its successful completion will teach us much about the Universe and its evolution. The symposium brought together representatives of the different disciplines and their mutual interactions made apparent many promising areas of future research. We can be confident that the next several years will see substantial progress in our understanding of the chemistry of astronomical objects.

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