Astro2010 Science White Paper

The Molecular Universe:

From the Diffuse Interstellar Medium to Planetary Systems

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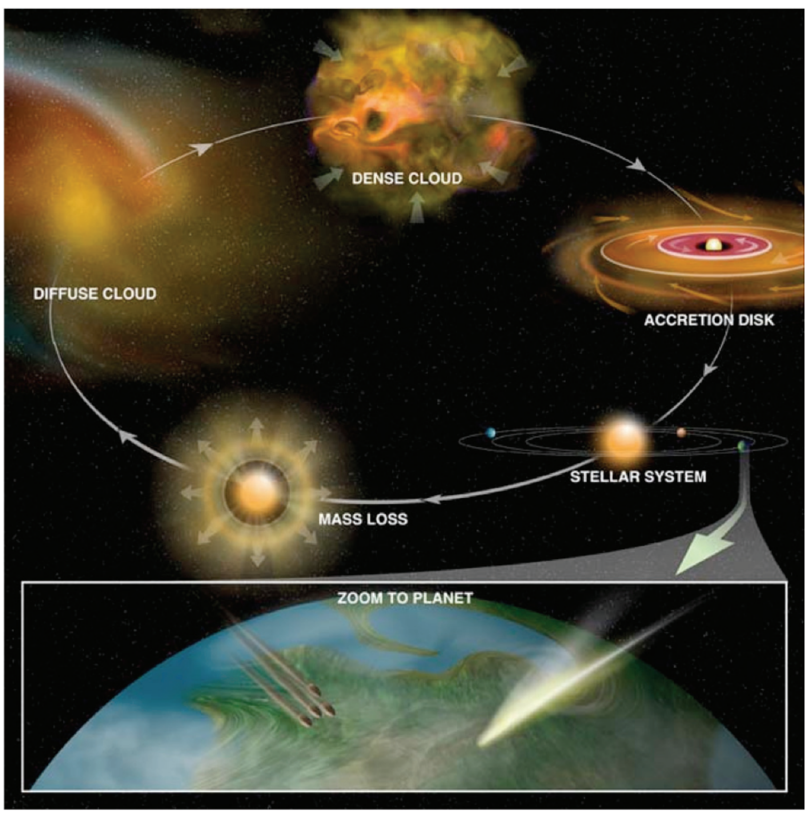

The life cycle of the Molecular Universe

Abstract

One of the central questions of our times concerns *the life cycle of molecules in the Universe—from the diffuse interstellar medium to planetary systems—and the chemical pathways leading from simple diatomic molecules to complex organic species*. In the past decade, new ground- and space-based facilities at millimeter and submillimeter wavelengths have provided exciting new discoveries on these topics. Ongoing and planned submillimeter wide-field continuum surveys will yield hundreds of potential galactic targets suitable for detailed spectroscopic follow-ups. Recent advances in detector and digital spectrometer technologies promise to truly revolutionize further the field of high-resolution submillimeter spectroscopy and its application to the study of the life cycle of molecules. Unbiased spectroscopic surveys of these sources, using a combination of ground-based and sub-orbital facilities that are expected to become operational within the next decade will greatly improve our understanding of *astrochemistry, astrobiology, the origin of life on Earth*, and allow assessing the possibilities of *life in other planetary systems*.

Chemical Evolution within the Molecular Universe

One of the fundamental questions in modern astronomy concerns the life cycle of molecular material in the universe. The study of the origin of the heavy elements in stars, their processing into molecular material in interstellar clouds, incorporation into planet-forming bodies, and eventually into life itself, has fascinated astronomers, planetary scientists, and biologists. A critical question in the quest to understand the origin of life on Earth and to assess the possibilities for life in other planetary environments, is the source of pre-biotic and, ultimately, proto-biotic molecules. Although synthesis on Earth from atmospheric chemistry or other sources may contribute, it is clear that extraterrestrial organic material is delivered to the Earth even today in the form of carbonaceous chondrite meteorites and interplanetary dust particles. An inventory of the molecular universe traces the path of elements throughout the Galaxy, from stars to the planetary bodies in our Solar System (Fig. 1, cover page; image: www.space.com). In the following sections we trace the chemical evolution in regions of increasing density, moving from diffuse clouds to dense cloud cores, and to protostellar disks.

Diffuse Clouds and Molecular Clouds

Diffuse molecular clouds constitute the first step in the evolutionary pathway from low-density atomic hydrogen (HI) clouds to the Molecular Universe. They are transition objects between the atomic and molecular phases of the interstellar medium, and provide a relatively simple laboratory for the study of fundamental chemical processes.

Such clouds are most easily studied through absorption line observations of bright, background continuum sources. Several foreground diffuse clouds can often be studied in parallel with single judiciously chosen hot cores. For the diffuse ISM, high sensitivity, exquisite spectral resolution, and immense spectral coverage are required to obtain a full chemical inventory. Absorption spectroscopy of diffuse molecular clouds can be carried out at all wavelengths between the radio and ultraviolet, providing that a suitable background source is present. Combination of multi-spectral absorption observations will be essential for unraveling the full chemistry of these regions.

Thus far, the known molecular content of diffuse molecular clouds consists primarily of diatomic molecules, only a few polyatomic species having been identified to date. However, spectroscopic surveys of these objects may lead to the discovery of new molecules, particularly simple hydrides. Furthermore, the calculation of molecular column densities from absorption line equivalent widths is usually very straightforward—unlike in the case of emission line observations, the column density determination does not depend upon such poorly-known quantities as the gas density and temperature (and distribution thereof) or upon the rate coefficient for collisional excitation.

A critical observation is the detection of deuterated hydrogen (HD) via its first rotational transition at 112 μm. Absorption spectroscopy will allow accurate determination of the column density of HD along lines of sight to background sources. HD itself is predicted to be the dominant reservoir of deuterium in molecular regions but its abundance relative to H_2 is an important starting point for determining the fractionation processes and modeling conditions in cold, dense pre-stellar regions. HD can also be detected in emission in shocked gas throughout the galaxy. When supplemented by observations of H_2 from Stratospheric Observatory for Infrared Astronomy (SOFIA), the Spitzer archive, or James Webb Space Telescope (JWST), HD can be used to probe the D/H ratio of molecular gas over a large fraction of the Galaxy.

Dense Cloud Cores

Insterstellar clouds are thought to evolve from diffuse to molecular phase as a result of processes that increase their column density and thus reduce photo-destruction rates. We find most of the over 140 molecules discovered to date in space in dense "molecular clouds", and analogous gas and grain chemistry can be expected to produce a wide range of complex organic species. The six biogenic elements required to build such structures on our planet include some of the most common elements: H, O, C, N, S, and P. Phosphorous, although some 1000 times less abundant than carbon, is critical in the transition from pre-biotic to biotic chemistry. Only the two most abundant elements (hydrogen and oxygen) are required to produce water. Four elements (H, O, C, and N) are sufficient to form all of the nucleic acids and, with phosphorous, eighteen of the twenty amino acids commonly found in biological structures. The remaining two amino acids, cystine and methionine, require the availability of sulfur. Thus, with five elements (H, O, C, N, and S) a pre-biotic system could form in an appropriate solvent (water), take on shape (structural proteins, lipoproteins, and polysaccharides), and facilitate chemical reactions (enzymatic proteins).

The dense condensations containing up to a few tens of solar masses of material at temperatures of ~10 K are referred to as "cloud cores" or "dense cores". Deuterium-bearing species have been shown to be excellent probes of these cold regions prior to star formation. The lowest-lying transitions of H_2D^+ and D_2H^+ are of great interest (in particular the completely unexplored transitions near 1.4 THz) and can be studied in absorption against strong continuum sources or in emission in dense regions where they are predicted and observed to be abundant. The two molecules are key for star formation studies because they do not deplete onto grains and are *the best* tracers of the dense gas in the center of star forming cores (as well as of the midplane of protoplanetary disks). Ammonia isotopologues, with their fundamental rotational transitions in the submillimeter, are also well suited for such studies.

Star formation occurs within cloud cores. The combination of high densities, heating by young embedded stars, and illumination by nearby sources of hard radiation drives the chemical evolution in these regions. Here, one can expect enhancement of both gas-phase chemical reactions and grain-surface chemistry. The higher temperatures open many chemical pathways, which are endothermic and therefore closed at lower temperatures. High densities (and to a lesser extent high temperatures) increase the rate of collisions of chemically interacting partners.

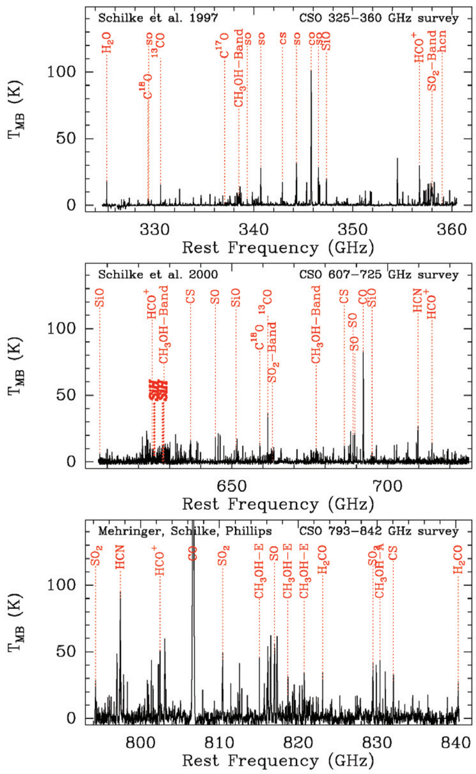

Figure 2—Ground-based spectroscopic surveys of Orion KL (data: Caltech Submillimeter Observatory, CSO).

Penetrating X-rays and UV radiation ionize atomic and molecular species, thereby greatly increasing their chemical interaction cross-sections. This radiation may also dissociate larger molecules and thus provide additional chemical pathways for producing smaller molecules.

Hard radiation also creates radicals on grain surfaces, which—combined with the mobility due to elevated grain temperatures—leads to enhanced chemical processing. If grain reactions are sufficiently exothermic, the resulting molecules will be directly released from the grain surface. If not released at their creation, they could leave the surface later when the grain temperature is sufficiently high. Or the molecules could become part of the grain's molecular coating, influencing its optical properties, its ability to coagulate with other grains and produce a larger particle (a necessary step towards planet formation), or simply be present and participate in the creation of more complex species.

These chemical complexities are revealed in "hot cores" when the massive star is born. Hot cores offer the best opportunity to explore and understand via theoretical models the limits of the creation of organics via interstellar chemistry. This is critical, as it is this stage that produces the ices and organics that are seeded to the planet-forming disk by infall.

Disk Chemistry and the Solar System Connection

The accretion disks around young stars form the pivotal link between star formation and (exo)planetary science. A detailed understanding of their chemical and physical properties is essential in providing constraints on dispersal mechanisms and timescales for nebular gas and dust. Furthermore, an understanding of how various volatile species (water, carbon monoxide, methane, ammonia, nitrogen, etc.) are distributed in the outer regions of circumstellar disks is particularly important to examining the connection between interstellar and nebular processes in the formation of icy planetesimals such as comets and Kuiper Belt objects.

Stars form within the density-peaked cloud cores discussed above via gravitational collapse. When a single star forms, most material will have too much angular momentum to fall directly onto the embryo "protostar", and the circumstellar disk that is formed plays an essential role in the further evolution of these systems. Finally, the relatively high densities and relative quiescence of young disks provide an ideal environment for the further growth and evolution of dust grains, affecting the disk's opacity and consequently its energetics and appearance. This evolving dust provides the seeds for the formation of meteorites, planetesimals, comets, Kuiper Belt objects, moons and ultimately planets around stars.

At disk surfaces, molecules can be dissociated by UV radiation, or ionized by UV photons, X-rays and cosmic rays, and so the resulting chemistry is a combination of "Photon

Dominated Region-like" and cosmic ray induced reaction networks at the distances where icy planetesimals are assembled. Due to the non-thermal excitation near disk surfaces, it is essential that wide spectral coverage be obtained in order for an accurate physical and chemical model of the disk to be obtained. In addition, important measurements such as the D/H ratio in water will be possible using water observations from space (Herschel/HIFI), combined with HDO measurements from the ground. Spectral line surveys of disks would be a major step forward in our understanding of the formation of planetary systems.

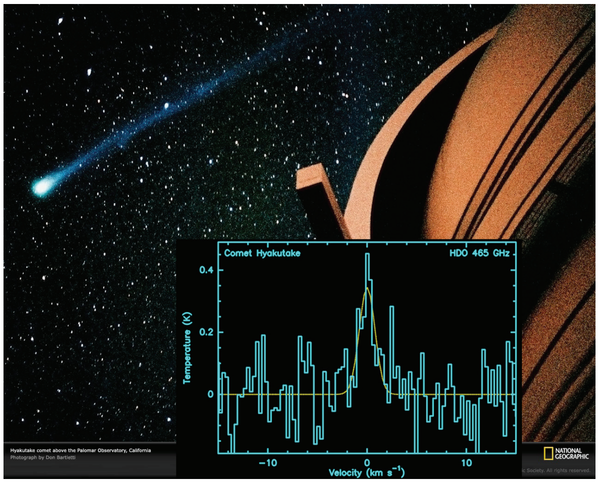

Figure 3—Comet Hyakutake as seen from Palomar, with overlaid spectrum of heavy water (data: CSO; image: National Geographic).

Over the past few years it has become apparent that the evolution of disks and the formation of the parent star is not a static process. Instead, the accretion is episodic in nature, which reveals itself in variable infrared excesses in the inner disk, as seen from ground-based programs and the c2d Spitzer results, as well as in the large scale outflows. Chemistry offers a tremendous opportunity to unlock some of the secrets of this process. When a burst of accretion energy is released, the chemical state of surrounding molecular material (in the disk or envelope) is altered. The primary effect is the release of molecules frozen on the grain surfaces, which then remain in the gas when it cools back down to pre-outburst levels. The timescales of the accretion event will therefore interact with the timescale for the chemistry to re-assert itself. Chemistry offers the *best* opportunity to understand this problem. Studies of these effects will require large telescopes with a sensitivity to arc-minute scales, as the chemistry of the inner envelope must be contrasted with the outermost layers.

Comets are among the most primitive bodies left over from the planetesimal building stage of the solar nebula, and so their physical and chemical composition provides an important link between nebular and "interstellar" (or outer disk) processes. Here, submillimeter observations are again extremely powerful, having provided the most accurate estimates of the composition of the nucleus of comets and the isotopic ratios in key species (water, HCN, etc.). The most complex molecules seen in comets (methyl cyanide, methyl formate, ethylene glycol) have also been detected at (sub)millimeter wavelengths. Only heterodyne spectroscopy can provide an unbiased view of the submillimeter wave spectra of comets, and therefore of the composition of the nucleus itself (particularly if the observations are combined with simultaneous IR spectra of species without permanent dipole moments, such as CO_2 and CH_4).

Deuterium fractionation in interstellar water, as compared to that measured in solar system objects, in particular in comets, is also of great interest (Fig. 3). A D/H ratio of 3×10^{-4}, measured in a handful of comets studied to date, corresponds to a factor of 12 enrichment with respect to the proto-solar value in H_2, but is significantly lower than the values measured in dense interstellar clouds. This suggests that comets incorporated material reprocessed in the inner solar nebula that was transported outward by turbulent diffusion. Measurements of the D/H ratio in a large sample of comets, including short-period comets, are needed to fully understand *the turbulent mixing in the Solar Nebula and the origin of terrestrial water*. SOFIA will provide the necessary measurements of the water production rate in relatively bright comets beyond the lifetime of Herschel, through observations of $H_2^{18}O$ and OH lines.

Finally, large, complex molecules (even on grain surfaces) have unique signatures in the far-infrared/submillimeter (via torsional and floppy modes) that allow their unambiguous identification. Finding and identifying these species in star-forming regions and in the disks surrounding young stars and protostars will help us understand the chemical pathway for pre-biotic material and the raw material for life.

Contrasts of cometary and meteoritic chemistry with that of the interstellar medium (via quiescent and hot cores) are crucial for understanding how primitive these materials are and how much processing they have undergone in the disk itself. This is a central aspect of this scientific endeavor, as an understanding of each phase is needed to set the initial conditions for the next.

Exploration of the Molecular Universe

Observational astrochemistry has proven to be a powerful tool for studying the life history of the interstellar gas and dust. To investigate the physical and chemical processes involved, it is necessary to study *all major components of the dust and gas environments from cloud collapse to planetesimal formation*. To trace the formation, evolution and destruction, freeze out, and coagulation processes of these molecules in the gas-grain environment, we must observe them in a variety of objects.

The submillimeter band, broadly defined as a decade of wavelengths between 1 mm and 100 μm, gives access to cold, dust enshrouded objects that are often hidden from view at shorter wavelengths. Dust continuum sources with temperatures of order 30 K peak near 100 μm. In colder sources, such as prestellar cores before the onset of star formation, the emission is shifted to even longer wavelengths. High-resolution heterodyne spectroscopic techniques ($R \sim 10^6$) provide velocity-resolved spectra of the rotational lines of abundant gas-phase molecules. Such observations provide invaluable information about the kinematics (infall, outflow, rotation) and physical conditions (temperature, density, UV field intensity, ionization fraction). The line forest of heavy organic species that dominates the line spectrum at longer millimeter wavelengths gradually gives way to fundamental rotational transitions of light hydrides and deuterides in the submillimeter. Fine structure atomic lines of abundant elements: C, O, and N are also present and are important coolants of the gas.

Infrared spectroscopy also offers a potential means for detecting complex molecules, which are difficult to detect by their rotational transitions at radio/mm wavelengths. Indeed, the far infrared is well suited for identification of large organic compounds, including amino acids, under the conditions present in the warm, dense interstellar gas and in the planet forming gas around protostars. Under these conditions, we should be able to detect the "puckering" or "flopping" modes of large organics. While the near- and mid-infrared wavelengths have proved very useful in confirming the presence of complex molecules in interstellar ices, they lack sufficient specificity to allow identification of individual species unless they are fairly simple (e.g., H_2O, C_2H_2).

The HIFI instrument on the Herschel Space Observatory will provide for the first time a complete view of the submillimeter band, unobscured by the Earth's atmosphere. Unbiased spectral line surveys will be carried out *in a few representative sources*, providing templates for future studies. However, observations of a statistically significant sample of ISM sources are needed to follow the chemical evolution of the universe's molecular gas component as it cycles from diffuse clouds, to material that forms solar systems, and finally to dying stars that enrich the

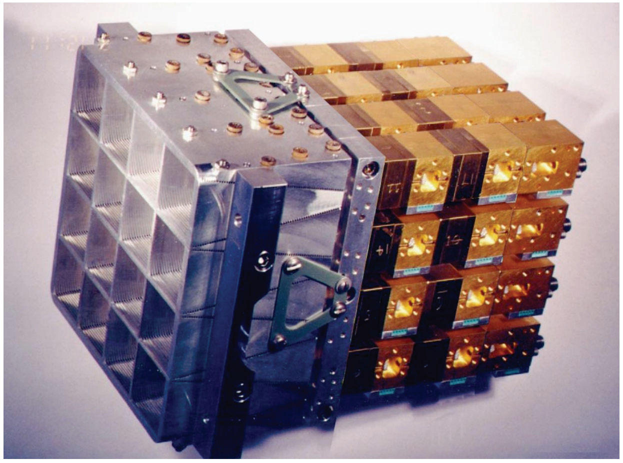

Figure 4—Picture of the SEQUOIA array at the Five College Radio Astronomy Observatory (FCRAO).

interstellar medium. Following this cycle with wideband spectral scans is the broad definition of the "Exploration of the Molecular Universe". These enormous line survey data sets will contain a complete chemical inventory, the chemical history and evolutionary state, the line to continuum ratio, the excitation and cooling conditions and a nearly complete dynamical picture of all objects surveyed. They will provide a foundation and an overall context for more detailed investigations of specific sources and processes with more limited spectral coverage. The fundamental questions to be addressed by these studies are: *What is the life cycle of molecules in the Universe—from the diffuse interstellar medium to planetary systems, what are the chemical pathways leading from simple diatomic molecules to complex organic species and what is the distribution and types of organics that seed the habitable zone around stars?*

Another important goal is relating the chemistry of molecular gas to that of star formation. For twenty years, since the inception of molecular astronomy, it was accepted that CO and its isotopologues are the best tracers of temperature and total column of molecular gas, while high-dipole moment molecules (e.g. H_2CO and CS) best traced the dense star-forming core. Today we know that prior to star formation the dense gas is cold and these species are frozen onto grains. This has led us to view star formation in the light of our growing understanding of the complex cloud core chemistry. Detailed chemo-dynamical models have been developed that can utilize the fact that the chemistry has a built in time dependence that can be used to determine collapse timescales. While Atacama Large Millimeter/Submillimeter Array (ALMA) will study the heart of star formation, the area where collapse likely begins, a complete picture will ultimately require looking beyond the central condensation to explore the initial collapse dynamics from cloud to envelope and the central core—this requires sensitivity to large scales that are accessible to large ground-based radio telescopes (e.g., Cornell Caltech Atacama Telescope, CCAT).

Facilities and Instrumentation

The research program outlined in this paper cannot be carried out using a single facility, existing or planned. Instead a coordinated effort using multiple facilities will be required. Some astrophysically important molecules, such as water or oxygen, can only be studied from space. Over the next few years, *Herschel* will be exploring the water universe and will leave a tremendous legacy for years to come. However, in order to fully understand the chemical evolution within the Molecular Universe, high volume of supporting ground-based and airborne data will be required. Observations to date have clearly demonstrated that a large fraction of the submillimeter band is accessible from high-altitude mountain sites, such as Mauna Kea or Chajnantor. Sub-orbital platforms (e.g., SOFIA and balloons) will provide additional opportunities to study key species that are not accessible from the ground (e.g., HD, CII, $H_2{}^{18}O$, OH), well beyond the lifetime of Herschel.

ALMA, when it becomes operational in the next decade, with its unparalleled sensitivity and angular resolution, will offer outstanding spectroscopic capabilities. This instrument will be perfectly suited for studies of the chemical composition of the compact hot core regions in the immediate vicinity of the newly formed stars, where the intense heating causes ice-mantle sublimation, driving rich, complex chemistry. Nevertheless, even with ALMA, complete spectroscopic surveys of hundreds of sources over the full wavelength range will be prohibitive. Moreover, the extended emission will be largely resolved out in the interferometric data. Since the roots of the chemical complexity of the hot core sources can be related to the initial conditions within the envelopes and their earlier history, observations of *all relevant spatial scales* are needed.

A new generation of wideband heterodyne array receivers, covering full atmospheric windows, or multiple windows simultaneously, will make this feasible in the next decade. More advanced calibration techniques, much improved sideband deconvolution, and the large numbers of lines from the same species, provide the opportunity to extract much more definitive results than previously obtained or even contemplated. The line shapes and intensities from the spectroscopic surveys will provide hundreds to thousands of constraints on physical and chemical models of sources and of the molecular astrophysics as well. For a relatively simple physical model of some component of a source, the physical parameters of the astronomical region can be determined using the multiple line spectra of simple, well-characterized molecules, but inevitably more complex models will be required to properly model the temporal and spatial variations of conditions within a source, and these models will rely on the spectral map data that this program will provide.

The observational data complementary to that provided by ALMA can be supplied by large single-dish telescope (e.g. Green Bank Telescope, GBT; Large Millimeter Telescope, LMT; and CCAT), equipped with large-format heterodyne arrays (Fig. 4), with bandwidths covering full atmospheric windows. Arrays with as many as 64 pixels are currently under construction and next generation instruments with hundreds of pixels can be envisioned. Recent progress in digital spectrometer technology has largely solved the problem of high-resolution spectroscopic analysis of multiple pixel systems. SOFIA will also be a platform for proving new spectroscopic imaging capabilities at wavelengths not accessible from the ground and in this respect, it complements future large ground based telescopes.

Analysis and interpretation of the vast quantities of data that will be collected within this program will require coordinated efforts in laboratory spectroscopy (line identification) and theoretical modeling (chemistry and radiative transfer, incorporated into dynamical cloud, core, and disk models). There is the critical need for collisional rate coefficients along with spectroscopic identifications, as well as laboratory and theoretical studies of fundamental chemical processes (e.g., to determine bimolecular reaction rates). This work is already partly under way in preparation for Herschel, SOFIA, and ALMA.