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WORKING GROUP ON ASTROCHEMISTRY
(GROUPE DE TRAVAIL POUR L'ASTROCHIMIE)

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1. INTRODUCTION

The field of Molecular Astrophysics or "Astrochemistry" has grown considerably since its inception in the late 1930's. Molecules have been observed in astronomical environments as diverse as comets in the solar system and galaxies at the highest redshifts. The common thread in these studies is that molecules are excellent probes of the physical structure and dynamics of such regions, owing to the complexity of their energy level structure and the resulting emission and absorption spectra. In addition, the chemical characteristics provide a powerful tool to study the evolution of astrophysical regions. Molecules also play an active role in the energy balance of clouds. Interstellar space is a unique laboratory in which chemical processes can occur that are not normally found on Earth. Indeed, astrochemistry is a highly interdisciplinary subject, linking the macrocosm (galaxies, stars, planets) with the microcosm (basic chemical processes and spectroscopy). The increased potential of ground- and space-based observational facilities over the full wavelength range provides a wealth of information about the physical environments in which molecules occur and makes it possible to study the development of molecular complexity throughout the Universe.

These developments have resulted in an active and growing community in astrochemistry, which is well spread across the nations of the IAU. This has led to the establishment of the IAU working group on "Astrochemistry" (under Division VI on Interstellar Matter) in the early 1980's. Its main activities are to ensure that scientific meetings are regularly held (e.g., van Dishoeck 1997). Over the last three years, the working group has concentrated on the organization of IAU Symposium 197 on "Astrochemistry: From Molecular Clouds to Planetary Systems". The following sections summarize the science discussed at that meeting, which reflects the progress in the field.

The working group maintains a web page at `http://www.strw.leidenuniv.nl/~iau34`, which contains links to astrochemistry groups world-wide, molecular data bases, reaction networks, as well as observational facilities.

2. IAU SYMPOSIUM 197

About 262 participants from at least 24 countries and nationalities gathered August 23–27 1999 in South Korea to participate in IAU Symposium 197. The meeting was held near Sogwipo, a small fishing port on the south coast of the beautiful Cheju Island, near the southern tip of the Korean peninsula. Thanks to the excellent and very efficient local organization, chaired by Young Chol Minh, the 5–day symposium proceeded very smoothly.

The scientific part of the program featured 48 oral review and invited papers, ~170 posters and 1 panel discussion (see `http://www.issa.re.kr/~iau197/` for abstracts). In contrast with previous IAU Symposia, the program did not cover all aspects of astrochemistry but centered around the specific theme of the chemical evolution during star formation,

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thereby complementing the many conferences which focus on the physical aspects of star- and planet formation. The oral papers will be published in Minh & van Dishoeck (2000).

2.1. Pre-stellar cores and low-mass star-forming regions

The program started with a discussion on the chemistry in dark clouds prior to (low-mass) star formation. There is now strong observational evidence for substantial depletions of heavy molecules (including CO) in the inner, coldest parts of clouds, in particular those which appear to be on the verge of collapse. The ionization fraction plays a crucial role in the collapse process, and observational and theoretical progress in constraining this important parameter was reported. Beautiful single-dish and interferometer data on the distribution of molecules in the earliest, deeply embedded stage of low-mass star-formation were shown, leading to a broad classification of the various chemical characteristics.

Throughout the conference, it was stressed that a more quantitative analysis of chemical abundances requires improved models of the physical components present in the beam, coupled with sophisticated radiative transfer in continuum and lines. An overview of radiative transfer methods currently used by astrochemists was presented, and a coordinated approach to compare and improve codes was called for (see `http://www.strw.leidenuniv.nl/~radtrans` for summary).

2.2. High-mass star-forming regions

Submillimeter telescopes equipped with sensitive high-frequency receivers continue to highlight the richness of molecular spectra found in high-mass star-forming regions. In addition, the ISO satellite has provided a wealth of new information on complementary features at infrared wavelengths, including atoms, ions and gas-phase molecules, PAHs, ices and silicates. Together, these data allow a nearly complete inventory of both the gas and the solid-state composition, and reveal the chemical and physical differentiation of the objects from the collapse phase to the UC H II region phase. The importance of various physical processes (dispersion of the envelope, shocks, UV radiation) can be studied. Clear evidence is found for heating and evaporation of ices, which drives a rich chemistry in the hot core phase. Progress has been made in the development of gas-grain models, although uncertainties in the precise nature of the chemical processes on a variety of surfaces remain. Pure gas-phase chemical models in steady-state appear to reproduce well the systematic data on various molecules in translucent clouds, but not the unexpectedly large abundances of polyatomic species (HCO^+, HCN, H_3^+, ...) in diffuse clouds.

The first results from the SWAS satellite formed a highlight of the meeting. The ground-state line of H_2O has been detected in many star-forming clouds, but the O_2 molecule is still elusive. In contrast with ISO, the SWAS data are sensitive to H_2O in cold gas, and the inferred abundances are surprisingly low, much lower than those predicted by quiescent gas-phase models.

2.3. Basic molecular processes

Accurate information on basic molecular data continues to be essential for progress in astrochemistry. Advances in instrumentation have provided new insight into many processes, ranging from the rates and/or products of gas-phase neutral-neutral reactions under ultracold conditions to the measurement of the microwave spectra of carbon-chain molecules. Heavy-ion storage rings are now used to study the dissociative recombination of polyatomic ions, and show a surprisingly large fraction of three-body fragmentation, preventing the build-up of large molecules. Compared with previous symposia, there was a substantial increase in the number of papers describing new experimental set-ups for studying PAHs and surface processes. In addition, theoretical simulations of realistic grain-surface processes can now be carried out. The molecular data needs were summarized toward the end of the conference in a panel discussion.

2.4. Grains and large molecules

The broad characteristics of existing grain models were reviewed, and tested against new observational constraints, in particular the revised interstellar abundances of oxygen and carbon. The nature of the carriers of the diffuse interstellar bands —a mystery for more than 70 years— is still not clear, but good progress is made in narrowing down the possible candidates by comparing laboratory spectra of gas-phase carbon-chains and PAHs with ultra-high resolution astronomical spectra. The wealth of UIR bands found in the ISO spectra leaves little doubt that the carriers of these features are PAHs. The high-quality of the data allows quantitative analyses of their abundances and reveals changes in the composition in different physical environments.

2.5. Envelopes of late-type stars

High resolution interferometer images of molecules in the shells around late-type stars offer a unique tool to test time-dependent gas-phase models. The close coincidence of the distribution of various carbon-bearing species is inconsistent with published models. ISO spectra of (post-)AGB stars reveal a wealth of carbon-chain molecules and highlight the importance of infrared pumping in analysis of the data.

2.6. Outflows, shocks, PDRs and masers

New diagnostic tools of PDRs and shocks in star-forming regions are provided by ISO observations of the pure rotational lines of H_2, even up to its dissociation limit. The excitation temperatures found in PDRs are higher than predicted by models, pointing to an incomplete understanding of the heating mechanisms and/or the H_2 formation on grains at high temperatures. Millimeter surveys of molecules in bipolar outflows, together with optical and near-infrared imaging of jets, illustrate the complex physical structure of these regions. Enhanced abundances are found due to sputtering of grains in bow-shocks and to desorption of grain mantles in entrained material. Surprisingly, the kinematics of CH_3OH masers in high-mass star-forming regions are more consistent with motions in circumstellar disks than in outflows, and provide the best evidence to date for the presence of disks around high-mass stars.

2.7. Circumstellar disks

The chemistry of circumstellar disks formed an entirely new topic at astrochemistry conferences. Surveys at infrared and millimeter wavelengths show that most young stars are surrounded by disks with sizes of a few hundred AU and masses of $\sim 0.01\ M_{\odot}$, comparable to that of our own primitive solar nebula. Observations of CO and its isotopes indicate that the molecular gas persists up to 10^7 yr, and that most of the matter enters the disk at distances greater than the orbits of the major planets in our own solar system, providing important constraints on the chemistry. Photoevaporation was shown to be a dominant mechanism for the truncation and removal of circumstellar disks, especially in regions of high UV radiation such as Orion. Observations of molecules other than CO are just becoming feasible and new single-dish and interferometer results were presented. The data indicate significant depletions in the outer regions of the disk (> 30 AU), but also show evidence for ion-molecule chemistry and photodissociation. Various theoretical models for the vertical and radial distribution of molecules were presented, and highlighted the importance of gas-grain interactions. Beautiful new ISO spectra of disks reveal solid-state features due to crystalline silicates and water ice for the first time, some of which are remarkably similar to those found in comets.

2.8. Outer solar system

Another new area of research in astrochemistry is the study of the surface composition of small bodies in the outer solar system, including Kuiper Belt objects, Centaurs and Pluto/Charon. Near-infrared spectroscopy of these very faint objects has become possible with the advent of 8–10m class optical telescopes. Large variations in the albedos and colors are found, and the spectra show evidence for abundant H_2O-ice, mixed with CH_3OH, CH_4 and/or NH_3. Closer in the solar system, new data on elemental abundances from the Galileo probe mass spectrometer provide important constraints on formation models of Jupiter, whereas infrared data from HST reveal the presence of water ice on Titan and a mixture of ice, amorphous carbon and organic material on the dark side of Iapetus. The D/H ratio in the giant planets measured by ISO indicates that their atmospheres originate from a mix of solar nebula gas, with enhancements due to evaporated gases from icy planetesimals. The distribution of NH_3 and hydrocarbons probe the meteorology of the atmospheres of Jovian planets. The detection of H_2O requires an external source of oxygen, most likely provided by interplanetary dust particles (IDPs).

2.9. Atmospheres of brown dwarfs and planets

A very exciting new area of research is formed by the recent discovery of extrasolar giant planets and brown dwarfs, i.e., objects with masses ranging from 35–80 M_J which bridge the gap between planets and stars. Much progress has been made in modeling the atmospheres of these systems. The spectra of a variety of L-dwarfs and brown dwarfs show a transition from metal-rich to metal-poor atmospheres due to the formation of clouds and rain-out, which can be traced by strong alkali-metal absorption in the visible.

2.10. Inner solar nebula, meteorites and IDPs

Information on the events and time-scales of the physical processes in the inner solar nebula comes from sophisticated studies of the composition and isotope ratios found in meteorites, in particular the least processed carbonaceous chondrites. IDPs collected in the Earth's stratosphere show exciting evidence for preservation of interstellar material, opening up a new avenue to probe nebular processes. Improved models highlight the importance of lightning events and Fischer-Tropsh catalysis. It is clear that the primitive solar nebula needs to be treated as a dynamical process, rather than a static object.

2.11. Comets

The wealth of observational data at all wavelengths on comets, especially Hyakutake and Hale-Bopp, have been discussed. The comparison with abundances found in interstellar ices and hot cores greatly strengthens the connection between interstellar and solar-system material.

The symposium concluded with a stimulating summary by D.A. Williams, who emphasized the thrills and fun of the recent discoveries. Although our understanding of many phenomena is still incomplete, Astrochemistry clearly has come of age in the last 20 years.

E.F. van Dishoeck
Secretary of the Working Group

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