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Conference Summary

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Abstract. By any measure, IAU Symposium 280 has been an outstanding success: more than 400 participants represented at least 30 countries with 74 presentations and more than 300 posters. Beyond these numbers, it is evident that the cross-disciplinary field of astrochemistry is flourishing with excellent prospects for growth in the future. We have enjoyed the excitement of new, unexpected results from the Herschel Space Observatory and eagerly await new opportunities and facilities that will arise in the coming months and years.

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The task of summarizing a very full week of almost 400 presentations – oral and posters – is, to quote Ian Smith, "...challenging, by which I mean impossible". In particular, I cannot give due credit to all authors and their work. Instead, I will try to identify a selection of important themes in astrochemistry with emphasis on areas that have progressed rapidly since the last symposium and areas that show special promise of development during the next few years.

Astrochemistry is concerned with all aspects of cosmic evolution. At the present time much effort and many resources are devoted to understanding how stars and planets form. This chemical and physical evolution takes place within the context of a universe that has been expanding for some 13.7 gigayears starting with an initial baryonic composition of hydrogen and helium nuclei. Our molecular universe is interesting because so much of it is out of equilibrium. This is precisely why astrochemistry is such a rich and essential research area: astronomical phenomena can be fully understood only with detailed knowledge of myriad atomic and molecular processes.

Let me offer a few general observations about what we have seen during this week.

• The large number of young scientists here suggests that astrochemistry is healthy. The new facilities and large projects related to astrochemistry offer hope that the new generation of researchers can remain employed and stimulated.

• Very interesting research is being carried out effectively through large, international collaborations.

• Databases and data archives are expanding. Free and effective access to data has long been one of the moral glories of astronomy. It is gratifying to see the growth of databases for molecular spectra and processes, as well as public-domain computer codes for modeling. However, databases make it easy for users to overlook the original sources of the data. We can continue feeding our inexhaustible appetite for molecular data only if we support the efforts of colleagues who measure, compute, and publish the data by giving proper credit to original sources and by stressing the importance of laboratory astrophysics to funding agencies. Fortunately, many of the things that are of interest in astrochemistry lie close enough to the state of the art in molecular physics and physical chemistry that there are strong and basic justifications for the work.

• Observations are rapidly outrunning theory and models, especially in three-dimensional detail at high resolution.

The thrill of discovery has been in the air around Toledo this week, especially with the flood of new results from Herschel Space Observatory during the last year, as the spectrum at submillimeter and far-infrared wavelengths has been opened to extremely sensitive observation. Commissioning data from the Atacama Large Millimeter/submillimeter Array (ALMA) have just been released. The looming deadline for ALMA early-science proposals will surely make it difficult for authors and editors to meet the publication deadline of this book! What is new?

• Fullerenes C_{60} and C_{70} have been unambiguously identified in space.

• New and important interstellar molecules have been reported, in some cases with surprisingly high abundances: OH^+, H_2O^+, SH^+, H_2Cl^+.

• The large bandwidths of heterodyne receivers are revolutionizing spectroscopy in radio and submm-wave astronomy. This will increase the demands on molecular data and on our ability to analyze spectra.

• Molecular anions have been added to the inventory of interstellar and circumstellar molecules since the last IAU symposium on astrochemistry. This has stimulated new laboratory experiments and efforts to include more anions in chemical models.

Themes

Panchromatic astronomy. Although the submillimeter and infrared parts of the electromagnetic spectrum have predominated here, other regions are important. X-ray absorption spectroscopy makes it possible to measure total abundances of elements in both gaseous and solid forms. In the ultraviolet, there is a new capability with the sensitive Cosmic Origins Spectrograph on Hubble Space Telescope. This has already revealed interesting CO fluorescence in disks of young stellar objects. Those who construct models of such disks should keep in mind that some T Tau stars are directly observed in the ultraviolet; therefore, it is possible to use empirical UV spectra as input to photochemistry, rather than to depend on inappropriate model atmospheres of more evolved stars. In the future, we will certainly see more interplay between molecular astrophysics and high-energy astrophysics as molecular tracers of cosmic-ray and X-ray ionization (e.g. H_3^+, OH^+, H_2O^+) lead us to a better understanding of buried sources of energetic particles and photons. We will also see more cases where electronic and vibrational transitions in molecules affect their rotational excitation.

Models. The Herschel/HEXOS project has provided a dramatic illustration of the problems involved in doing a spectroscopic analysis of some 10^5 lines in the submm-wave spectrum of Orion. Models of photon-dominated regions (PDR) are now able to include hydrodynamics, ice processing, grain growth, stochastic surface chemistry, and even fractal structures. Model-makers of exoplanet atmospheres should be reminded to benchmark their models against a one Jupiter-mass planet at 5 astronomical units from a G2 V star – remember that the UV/EUV spectrum of the sun is well observed and its intensity varies.

"Water, water everywhere, nor any drop to drink". The plain of La Mancha can be rather arid, but apparently nothing like low-mass young stellar objects, whose cores are quite devoid of H_2O. The question – why is there so little water? – will probably still be with us for a few years to come. Likewise the origin of the water on Earth is still an unsolved problem. The Cassini space mission has revealed remarkable transport of water between Saturn's atmosphere and its system of satellites and rings. The ortho and para

nuclear-spin symmetry species of the water molecule seem to reflect a characteristically low spin temperature in comets. More data on water and its singly deuterated isotopologue HDO in protoplanetary disks suggest long-term mixing of warm and cold regions. Water exists in both gaseous and solid form in space and its phase changes are an important part of the chemical evolution of planet-forming disks.

New insight from our own solar system. Fascinating new results have come both from traditional meteoritics and from space probes that capture solid particles in interplanetary space and return them to terrestrial laboratories. For example, the Japanese HAYABUSA mission that returned samples from an asteroid after a seven-year journey is a thrilling story of space travel, aside from the chemical insights that will soon emerge from detailed analysis of the samples. The Stardust spacecraft that sampled Comet 81P/Wild 2 has revealed heterogeneous distributions of both minerals and organic materials that are mostly protosolar rather than pre-solar. There is evidence of extensive mixing between the inner and outer parts of the protosolar nebula, without significant processing within the comet.

Exoplanets and their atmospheres. At the time of the symposium more than 500 planets had been discovered around other stars, with a rapidly growing list of new identifications and candidates from the CoRoT and Kepler space missions, which search for photometric evidence of transiting planets. Spectroscopic signatures of atmospheres have been reported for a few exoplanets. The structure and atmospheric chemistry of a gas-giant planet located very close (less than 0.1 astronomical unit) to its parent star pose interesting problems for theory and models. Although such hydrogenic atmospheres may seem similar to photon-dominated regions of interstellar clouds at first glance, they are likely to have dynamical outer boundaries and to suffer large effects of transport and mixing that static PDR lack. The search for habitable, Earth-like planets has intensified, and along with it the need for a better understanding of remotely detectable signatures of life.

Evolved stars. Both carbon-rich and oxygen rich circumstellar envelopes show extremely rich spectra at submm and infrared wavelengths. Red giant stars in the asymptotic giant branch (AGB) phase of evolution tend to show the largest rates of mass loss in winds, which produce extended molecular envelopes. Some of them process gas into very large molecules and solid dust particles. Aromatic infrared bands are not seen in AGB stars, but do appear in a later evolutionary stage of young planetary nebulae after the envelope has detached from the central core of the star and stands exposed to intense ultraviolet radiation of the hot core. Whether the appearance of aromatic bands in the proto-planetary nebulae is mainly a chemical effect or a result of UV excitation is not certain yet. Spatially resolved circumstellar envelopes show stratified molecular distributions. The extreme supergiant star VY CMa is not even spherically symmetric. A recent interferometric spectrum survey (270-355 GHz) has been carried out in close cooperation with laboratory spectroscopy, both to identify possible new molecules and to determine abundances. This is one of the few cases where H_2O is found to be the second most abundant molecular after H_2, rather than CO. Herschel observations of CW Leo (IRC $+10^o216$) reveal that H_2O molecules arise deep inside despite the predominance of carbon in its outer envelope. Arcs of dust are detected out to 300 arcseconds around CW Leo and thus represent a record of mass-losing events over thousands of years. The most extreme forms of mass loss occur in supernova explosions. Molecules like CO and SiO have been detected in the spectra of supernovae. Chemistry and dust processing evidently continue in the expanding remnants of these explosions, although it is still difficult to distinguish molecules and dust particles formed in supernovae remnants from those that have been swept up from the surrounding interstellar medium.

PDR, XDR, and TDR. Photon-dominated regions (PDR) of molecular clouds attract attention because they tend to be the brightest thermal sources in galaxies at submm and far-infrared wavelengths. An important variation on this theme is the X-ray-dominated region (XDR). Renewed interest in both PDR and XDR has come from Herschel observations of star-forming galaxies and gas surrounding active galactic nuclei: although it is difficult to distinguish between PDR and XDR at mm wavelengths, models show that the spectroscopic diagnostics become more distinct in molecular transitions in the submm and far-infrared parts of the spectrum. Turbulence is an important property of the interstellar medium on all scales from the dimensions of giant molecular clouds down to the microscopic scale (dissipation length). In recent years the statistical properties of turbulence in the diffuse interstellar medium have become better characterized by observation. In parallel, magnetohydrodynamical simulations gas clouds and theoretical models of small vortices have helped to elucidate the many physical and chemical implications of interstellar turbulence. Turbulent dissipation regions (TDR) associated with small-scale structures of high vorticity appear able to explain the observed products of high-temperature chemistry (e.g. interstellar CH^+ and SH^+) as well as excess emission in pure rotational lines of H_2.

Chemistry of the early universe and the first stars. We can be impressed that cosmology is now claimed to be a precise science, with well constrained values for the most important cosmological parameters. However, we should be alarmed to be informed that the rates of fundamental chemical reactions, like three-body association of hydrogen

$$H + H + H \rightarrow H_2 + H,$$

are sufficiently uncertain to limit theoretical simulations of accretion and fragmentation in primordial protostars. At the same time, it is gratifying that cosmologists take such a keen interest in the details of atomic and molecular processes that affect the evolution of structure in the Universe. The chemistry of star-forming clouds at early epochs may differ significantly from that at the present time, with hydrides like OH predominating over heavier molecules like CO.

Molecules in galaxies at low and high redshift. Even though molecular clouds remain spatially unresolved in all but nearby galaxies, it is now becoming possible to do more quantitative chemistry. The broad bandwidths now available for mm/submm-wave spectroscopy of emission lines in galaxies make it possible to estimate both molecular abundances and average physical conditions in line-forming regions. A recent, unbiased absorption line survey at 7 mm wavelength of the interstellar gas in a galaxy at redshift $z = 0.89$ identified 34 different molecules plus isotopic variants. Although the number of suitable mm-wave background sources is very limited, such measurements are an important complement to high-resolution optical absorption spectroscopy of distant quasi-stellar objects, which can be used to measure redshifted ultraviolet lines of H, H_2, HD, and CO at high redshift. We can expect to see more and more sensitive cosmological tests of rolling fundamental constants and of the z-dependence of the cosmic background radiation temperature. Out of more than 35000 catalogued quasars, there are now approximately 30 with detected CO emission lines.

Laboratory astrochemistry. After twenty-five years, the PAH hypothesis (polycyclic aromatic hydrocarbons as the carriers of strong, broad emission bands in the mid-infrared) is alive and well. This hypothesis has stimulated a wide range of experimental work ranging from spectroscopy of gas-phase PAH molecules to investigation of their chemical interactions and behavior in both anionic and cationic charge states. Many groups are struggling valiantly to meet the increasing demands for spectroscopic data of molecules, for reaction rates at low temperatures, and for inelastic collision cross sections and rates.

There is a parallel development of databases, which are gradually being incorporated into the international virtual observatory and into the pipelines for proposals and data at real observatories. Among the many interesting posters were several quantum chemical studies relating to reaction dynamics and experimental studies of neutral atom-molecule reactions at temperatures as low as 10 K. Ion traps are being used in various ways to investigate processes of astrophysical interest. It is especially gratifying to see results of projects that combine such disparate techniques as molecular dynamics computations, phase-space theory, and astrochemical modeling in order to investigate problems like the survival of PAH clusters in PDR.

The promise and peril of ALMA. The Atacama Large Millimeter/submillimeter Array (ALMA) will go into partial operation this year. ALMA will surely stimulate even more activity in astrochemistry. At the same time, ALMA may overwhelm our capacity to interpret observations. Owing to the large bandwidths of the receivers, every spectroscopic observation will represent a line survey, with a terrific demand on analysis tools to identify, measure, and model line intensities. The high angular resolution (of the order of arcsec or better) over a relatively small instantaneous field of view (of the order of arcmin) will make it difficult to see the details in relation to their larger-scale environments. Fortunately, this symposium has demonstrated that all aspects of astrochemistry are thriving and maturing, so I am hopeful that we will cope with the next wave of discovery. In particular, informal and formal networks of collaboration growing and becoming more effective, I think.

Thanks to the Local Organizing Committee and all the sponsors for a wonderful meeting in a lovely environment. Thanks to all the participants for a splendid symposium!