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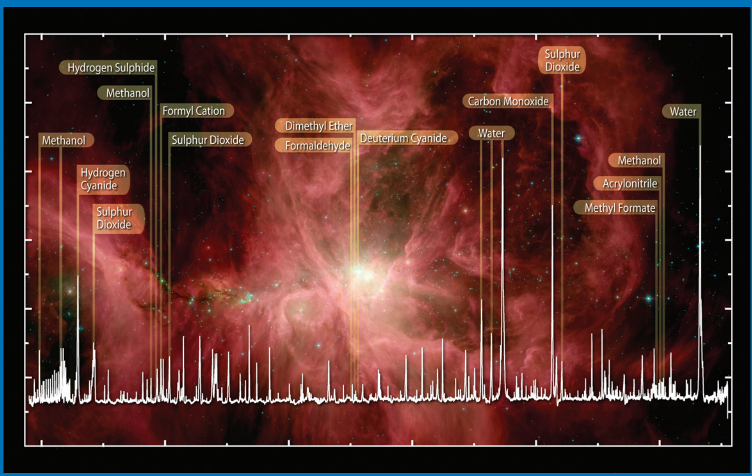
280

30 May - 3 June 2011
Toledo, Spain

The Molecular Universe

Edited by

José Cernicharo
Rafael Bachiller



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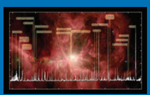

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COVER ILLUSTRATION:

The far infrared spectrum of the Orion Nebula, observed by the Herschel Space Observatory, superimposed on an image obtained by the Spitzer telescope.

The Orion Nebula is known to be one of the most prolific chemical factories in space, although the full extent of its chemistry and the pathways for molecule formation are not well understood. This extremely rich spectrum, obtained with the HIFI spectrometer in January 2010, covers the range 1.059 to 1.115 THz. Among the molecules that can be identified in this spectrum (marked on the corresponding lines) are water, carbon monoxide, formaldehyde, methanol, dimethyl ether, hydrogen cyanide, sulphur oxide, sulphur dioxide and their isotope analogues. It is expected that many new organic molecules will also be identified. Identification of the many spectral features visible in the Orion spectrum with transitions of particular molecular species requires sophisticated molecular spectroscopy databases, which collect the results from many years of theoretical and laboratory spectroscopy work.

HERSCHEL is an ESA space observatory with science instruments provided by European-led Principal Investigator consortia, with important participation from NASA. The high resolution spectrometer HIFI was designed and built by a nationally-funded consortium led by SRON Netherlands Institute for Space Research. The consortium includes institutes from France, Germany, USA, Canada, Ireland, Italy, Poland, Russia, Spain, Sweden, Switzerland, and Taiwan.

Credit of the image: ESA, NASA, Spitzer, HIFI consortium, E. Bergin and the HEXOS team.

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PROCEEDINGS OF THE 280th SYMPOSIUM OF THE INTERNATIONAL ASTRONOMICAL UNION HELD IN TOLEDO, SPAIN MAY 30 - JUNE 3, 2011

Edited by

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Preface

Astrochemistry is experiencing a true golden age. The role of molecules in astronomy is becoming so important that it is no longer an exaggeration to refer to a sizeable portion of the universe as "The Molecular Universe", the title that has been adopted for this symposium.

Recent successes in the field result from advances in observational, laboratory, theoretical, and modeling work.

To illustrate the recent observational advances, it can be mentioned that molecules other than CO have now been detected up to redshifts of more than 6. On the scale of entire galaxies, molecular maps are revealing striking spatial differences reflecting different physical processes (photodissociation, shocks, high temperature chemistry, etc.). On a local scale, hot cores, regions of complex molecular growth in the vicinity of high- and low-mass young stellar objects, have been observed to be far more complex and heterogeneous than previously thought. Negatively charged molecular anions have been found for the first time in a variety of sources, including the cold core TMC-1 and the envelopes of evolved stars. Millimeter-wave interferometers and infrared telescopes (both ground-based and in space) are revealing a surprisingly rich chemistry in the planet-forming zones of circumstellar disks and, at the same time, are providing a complete inventory of ices in star- and planet-forming regions. The study of exoplanetary atmospheres has begun, and evidence exists for methane, carbon dioxide, and water. The inventory of molecules in cometary atmospheres continues to grow, with interesting variations found among comets of different origin.

The laboratory studies, which were traditionally focused on gas-phase processes, are now significantly shifting emphasis toward gas-grain interactions. Surface science experiments are being applied to chemical and physical processes on analogs of interstellar dust particles. For example, the efficiency of photodesorption has been measured for the first time for simple ices, and the photodissociation of methanol ice along with impurities supports new models of complex molecule formation on ices. The complicated formation of water ice on surfaces at low temperature, relevant to the interpretation of Herschel data, has been studied, as has the thermal evaporation of mixed ices. The formation of molecular hydrogen on high-temperature grains, a complex process, has been thoroughly investigated. Cometary samples returned from the Stardust mission as well as meteoritic and IDP samples are studied in the laboratory with increasingly sophisticated instruments. Much effort has gone into the study of gas-phase rotational spectra at frequencies as high as 2 THz; an indispensable work for the identification of spectral lines to be detected with Herschel, SOFIA and ALMA. Laboratory studies of PAHs continue to be essential to interpret the wealth and variety of infrared features detected in the interstellar medium.

From the theoretical point of view, the chemical processes that occur on dust grains are normally treated in models by so-called rate equations. In some instances, these equations are inaccurate, and more computationally intensive methods, known as stochastic approaches, must be used. Much progress has been made in creating models that combine gas-phase chemistry, which is treated by rate equations, and surface chemistry, which is treated stochastically with new methods. Quantum chemical potentials, used sometimes with classical dynamics and sometimes with quantum mechanical dynamics, have been employed to determine accurate inelastic scattering cross sections, needed in the analysis of molecular spectral intensities.

Chemical simulations are improving in a number of ways. The major networks of gas-phase reactions now include processes involving anions, which act as catalysts for the production of larger neutral species. The formation of complex molecules in hot cores is being studied with a new approach: complex gas-phase species are produced on granular surfaces as they are heating up in the presence of a young stellar object; the rising temperature allows molecules and radicals produced by photodissociation to diffuse more readily around grains and eventually evaporate. Models of protoplanetary disks are being challenged to reproduce the mid-infrared detection of water, acetylene (HCCH), HCN, and other species. The inner disk regions require that chemical networks be able to operate at temperatures as high as 1000 K. Models of photon-dominated regions (PDRs) have reached new levels of sophistication and are now available for general distribution. Hydrodynamics is being applied to more chemical models in an attempt to merge realistic dynamics and chemistry.

We finally note that molecular databases, coupled with radiative transfer programs, continue to be developed for general distribution and provide astronomers with a variety of tools to make line intensity predictions. These tools can either be combined with the output of chemo-dynamical models or used in a stand-alone mode to analyze molecular observations in terms of physical conditions and molecular abundances. Such tools are indeed becoming increasingly important in the preparation of observations for ALMA, JWST and ELTs, whether applied to the smallest scales in nearby protoplanetary disks or to the most distant galaxies.

The above examples illustrate the broad variety and high interest of hot topics in current Astrochemistry. The symposium was so intense, and the number of oral and poster contributions so high, that only the review and invited talks have found place in this volume. The abstracts of all contributions were published in a booklet produced by the Local Organizing Committee and were posted at the SAO/NASA Astrophysics Data System (ADS). The nearly 400 contributions (including oral presentations and posters) which are not present in this volume are listed here as an Appendix, and have been made public in the Internet web site of the conference *(http://cab.inta-csic.es/molecular_universe/)* forming an excellent and indispensable complement to this book.

We very much hope that this book will make investigators aware of the many and exciting new progresses achieved by Astrochemistry on the last 6 years. and we also hope to acquaint them about the explosive growth in the subject to be coming in the next few years, when ALMA, JWST and the ELTs will come along, opening a fully new era both in Astrophysics and Astrochemistry.

José Cernicharo and Rafael Bachiller
Editors
Madrid, July 31, 2011

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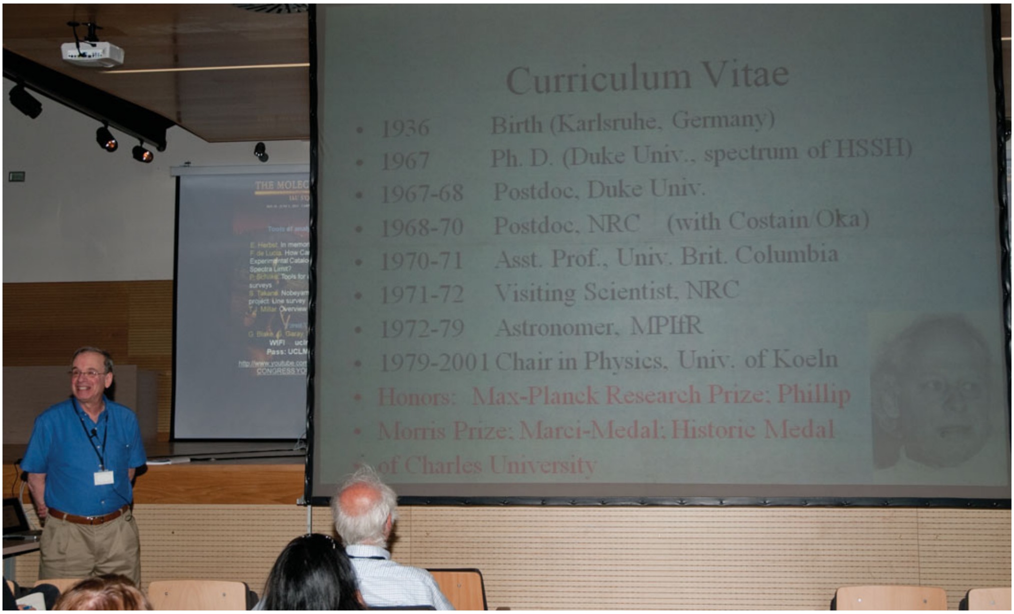

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Address by the Scientific Organizing Committee

Over 435 participants from 31 countries gathered in Toledo, Spain to attend IAU Symposium 280, entitled The Molecular Universe, which took place from 30 May to 3 June 2011 at the Technological Campus of the University of Castilla-La Mancha in Toledo, Spain. This is the main worldwide conference in the field of astrochemistry, held every ∼5 years, and covering all areas in which molecules are found, from Solar system to the highest redshift galaxies. This breadth of topics sets the IAU symposia series apart from other meetings in the field.

The Local Organizing Committee, chaired by J. Cernicharo and R. Bachiller, organized both the scientific and structural aspects of the meeting very well. Almost all possible logistic problems were handled amicably by M. Castellanos together with the other members of the LOC. The cultural mecca that is Toledo added a sense of awe and excitement to the symposium. The large size of the meeting did not interfere with the proceedings in any way. A large number of questions were asked of speakers, who, given their relative youth and diversity, brought many different viewpoints to the discussions. The three dedicated 2.5-hr. poster sessions were very well attended and enriched the experience of the participants. Informal conversations, held at intermissions from the speaking program, and during the poster sessions, were many and spirited. The large number of younger scientists at the meeting was quite impressive, and confirmed that the field of astrochemistry is entering a period of rapid growth led by new and exceedingly powerful telescopes.

The scientific organization of the symposium was undertaken by a very active IAU Working Group on Astrochemistry, under the sponsorship of IAU Commission 34 (Division VI), with co-sponsorship provided by Division VI (Interstellar Matter), Division VIII (Galaxies and the Universe), Division X (Radio Astronomy) as well as Commissions 51 (Bio-astronomy), 36 (Theory of Stellar Atmospheres), and 14 (Atomic and Molecular Data). There have now been six IAU symposia on astrochemistry, starting with the one held in India (1985; IAU Symposium 120). Later meetings in the series were held in Brazil (1991; IAU Symposium 150), the Netherlands (1996; IAU Symposium 178); South Korea (1999; IAU Symposium 197), and California, USA (2005; IAU Symposium 231). Each symposium has been larger than its predecessor, showing that astrochemistry is becoming a larger and more diverse community.

The scientific program of the symposium was divided into three parts: invited and review talks, contributed talks, and poster presentations. The Scientific Organizing Committee, which was the Working Group on Astrochemistry, democratically elected the speakers who gave contributed talks among the many applicants. Overall, there were 42 invited and review talks, 32 contributed talks, and nearly 360 posters. In the oral program were three sessions on new results from the Herschel Space Observatory labeled Herschel hot results, as well as a panel discussion entitled On to ALMA. The panel members adjudicated a contest in which young investigators competed to win a prize for the best and next best projects for ALMA with the constraint of at most 10 hours observing time. There were three large poster sessions, and awards were given to the best posters in each of the three from personal funds by E. van Dishoeck. During the third poster session, there were also computer demonstrations of databases.

After brief words of welcome by E. van Dishoeck, chair of the SOC, and J. Cernicharo, chair of the LOC, the 4.5-day oral program started with a general introduction on the molecular universe by A. Tielens, which was followed by a session on star formation. This field has become broader since the last astrochemistry symposium, and observational

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talks concerning stages of both low-mass and high-mass star formation were given, as was a theoretical talk on a new class of models that combine hydrodynamics with chemical simulations in the formation of protostellar cores. This session was followed by the first session of hot results from Herschel, which emphasized observations of water vapor, molecules in protostellar shocks, and a wide spectral survey toward Orion KL.

Astrochemistry certainly extends to planetary studies, including solar system objects. A session on these objects was held on the first day of the meeting, starting with a review talk on the chemistry of the solar system, including the origin of water on Earth, which was followed by talks on comets, meteorites, and the atmospheres of Titan and Saturn. The power of sample return missions to solar system bodies was emphasized. The second day of the meeting started with a session on evolved stars, in which supernova chemistry was also discussed. Talks on the molecular evolution from AGB stars to planetary nebulae, the role of time-dependent anionic chemistry (involving negatively-charge molecules) in IRC+10216, and the detection of fullerenes in assorted environments rounded out the session. Complex molecules are well known in IRC+10216 and other selected circumstellar sources, so this session merged well with the next one on star formation and complex molecules. Here observations of complex molecules were discussed in a variety of objects, along with current gas-grain simulations as well as possible future simulations involving the use of stochastic methods to improve the surface chemistry occurring in granular icy mantles.

Astrochemistry is based on the laboratory and theoretical study of basic atomic and molecular processes, and two sessions were held on this subject. The first concerned gas-phase processes, where a review talk was given on gas-phase reactions as a function of temperature, followed by a talk concerning the theory of low-temperature reactions, and one on experimental studies on the rates of reactions involving anions and how they relate to the observations of such species in various sources. The second day of the meeting ended with another Herschel hot topic session, highlighted by the report of an unambiguous detection of molecular oxygen in the interstellar medium.

The topic of protoplanetary disks occupied the first group of speakers on Wednesday, with talks on the phenomenal developments in observations at a variety of wavelengths ranging from the millimeter to the far-UV and an emphasis on interferometry. Modeling was also discussed, as was the chemical history of molecules from the hot core to the disk stage. Another session on basic molecular processes followed, this one emphasizing surface processes in the laboratory and in space. Much progress has been made during the last decade in this field, but there is still a great need for further laboratory studies before robust interstellar chemical simulations including surface processes can be constructed.

Although most of astrochemistry still revolves around galactic sources, the field of extragalactic astrochemistry will receive a big boost with the onset of ALMA observations. So, it was quite appropriate to have a session on extragalactic astrochemistry, which was held on Thursday morning. This field was understood to include the early universe, so talks on early chemistry were included along with a talk on extragalactic line surveys. It is impressive to see spectra of extragalactic sources with similar complexity to those found in galactic star-forming regions three decades ago! Next in line was the explosive topic of exoplanets and their atmospheres, which will occupy more and more astrochemists as more is learned about planetary atmospheres. Talks on observations, atmospheric models and their chemistry, as well as biomarkers of habitable worlds were included. The inclusion of astrobiology is a sign that this field is gaining importance and certainly overlaps with areas of astrochemistry such as the formation of complex molecules. The final session on Thursday concerned the tools of analysis and databases. Starting with a brief memorial to the late astronomer and astrochemist Gisbert Winnewisser, this session included talks on how to reduce the problem of unidentified lines in hot cores, on various tools for analysis of spectral surveys, on a legacy line survey from the Nobeyama telescope, and on databases and their uses. The session ended with the panel discussion discussed previously.

The last day of the symposium started with a session nominally on diffuse clouds and photon-dominated regions (PDRs). The role of turbulence in diffuse clouds was discussed, as was a controversial candidate for a carrier of several diffuse interstellar bands (H_2C_3). A talk on both PDRs and XDRs (X-ray dominated regions) was given as was a more general talk on diffuse interstellar bands. A number of aspects of the PAH hypothesis were touched upon. Finally, the complex nature of the central molecular zone of our galaxy, as seen through the infra-red spectrum of H_3^+, was explored. Next came the third of the Herschel hot topic sessions, which included talks on observations of diffuse clouds in the spiral arms of the Milky Way, carbon chemistry in translucent clouds, and the detection of C_3 in envelopes of star-forming regions. The detection of the reactive ions OH^+ and H_2O^+ in a variety of sources was an exceptionally interesting topic. The oral program was concluded with an exceedingly thoughtful summary of the field, past, present, and future, by J. Black.

The reader of this volume will find a cornucopia of riches concerning the state of astrochemistry before the fundamental changes that will occur when observations using the ALMA interferometer add greatly to our knowledge of sources throughout the universe. By the time of the next astrochemical symposium, much progress will have been made and the field will have grown both in size and, we trust, in understanding.

Eric Herbst
Secretary, Scientific Organizing Committee
Toledo, June 2011

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