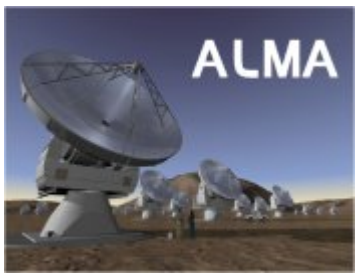

Complex Molecules in Space
Present status and prospects with ALMA

8th-11th May 2006

Fuglsøcentret, Denmark

Including a one day meeting of the EU Network "The Molecular Universe"

Sponsored by the EU, the Danish National Research Council, the Instrument Centre for Danish Astrophysics and the Department of Physics and Astronomy, University of Aarhus.

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ALMA and chemistry surveys

Ewine van Dishoeck

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ALMA will revolutionize the field of astrochemistry due to its exceptional sensitivity and angular resolution down to 10 milliarcsec scales (1 AU in the nearest star- and planet-forming regions). In this talk, the prospects for ALMA will be placed in the context of recent unbiased and selected line surveys of a variety of astronomical sources, including low- and high-mass protostars, outflows, disks and envelopes around evolved stars. Special attention will be paid to those scientific questions which ALMA will be particularly well placed to address, including the origin of complex organic molecules. The need for powerful analysis tools and molecular databases to address the huge ALMA data sets will be emphasized.

The Impact of Interferometry on the Detection of Large Molecules

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Up to the present, measurements with interferometers have not led to the detection of large molecules (with the notable exception of acetic acid, which was detected with the BIMA and OVRO arrays). These instruments have however contributed to our understanding of the physical conditions in which large molecules are found. The reasons for this state of affairs are investigated. We discuss new and future instruments such as the CARMA array and ALMA. We estimate how these would have contributed to the discoveries of large molecules made in the last few years.

Line Surveys in Orion and SgrB2

Claudia Comito[1], Arnaud Belloche[1], Carolin Hieret[1], Karl M. Menten[1], Holger S.P. Müller[1,2], Peter Schilke[1]

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[2] I. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, Köln, 50937, Germany

I will present an overview of the current knowledge arising from millimeter and submillimeter line surveys of the two best studied regions of massive star formation, Orion and SgrB2. Issues such as the analysis of datasets containing thousands of lines, and the detection and identification of previously undetected, complex species will also be addressed. Finally, I will provide a preview on the HEXOS Key Project for Herschel/HIFI.

Molecules in Orion

Peter Schilke

Max Planck Institute for Radioastronomie, Auf dem Högel 69, Bonn, 53121, Germany

The Spectral Legacy Survey: a spectral imaging survey with JCMT

G. Fuller [1], F. Helmich [2], R. Plume [3] and the SLS collaboration

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[2] SRON, Groningen, Netherlands
[3] Department of Physics & Astronomy, University of Calgary, Canada

Molecules provide the only probes which can reveal the dynamics, physics, chemistry and evolution of the cold dense regions of molecular clouds in which stars form. The Spectral Legacy Survey (SLS) is being undertaken to study the molecular inventory of a sample of molecular cloud sources. The observations will be used to investigate how the molecular properties of a source are related to the physical conditions in the gas and the source's evolutionary status.

Using the new 16 pixel 345 GHz array receiver HARP-B on the James Clerk Maxwell Telescope (JCMT), the SLS will produce spectral scans of five sources over the frequency range 330 GHz to 360 GHz. For every spectral channel throughout this frequency range of the survey will produce a fully sampled image. The five target sources to be observed have been selected to span a range of different evolutionary stages and different physical environments in molecular clouds. In this presentation I will discuss the strategy and goals of the SLS.

An Orion KL line survey with the Odin submm satellite

A.O.H. Olofsson [1], C. Persson [1], Å. Hjalmarson [1], P. Bergman, P. Bernath, J. Black, U. Frisk, W. Geppert, T. Hasegawa, N. Koning, B. Larsson, A. Lecacheux, S. Kwok, A. Nummelin, M. Olberg, Aa. Sandqvist, K. Volk and E.S. Wirström

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We have performed a satellite based 40 GHz submm spectral survey of Orion KL in wavelength regions inaccessible from the ground due to atmospheric opacity. The frequency ranges covered are 486.4-492.1 and 541.4-577.6 GHz, and the spectral resolution is 1 MHz.

Examples of lines/molecules in the survey are 4 water isotopologues (ortho- and para-$H_2{}^{16}O$, $H_2{}^{17}O$, $H_2{}^{18}O$, HDO), the J=5-4 lines from 4 carbon monoxide isotopologues (^{12}CO, ^{13}CO, $C^{18}O$, $C^{17}O$), ammonia ($^{14}NH_3$ and $^{15}NH_3$), and possible designations of line features from ND, SO^+, SH^-. The latter ones are not to be considered identifications since the features are very weak and it would require a number of coincidences in order to claim detections.

In total, we have identified about 300 lines from 38 molecules. An additional ~60 line features remain unidentified.

Our result also indicate that line crowding may become a problem in similar observations using future instruments such as Herschel and ALMA with higher beam filling factors and sensitivities. In particular, high-velocity line wings in the strong emission lines - often present in observations towards high-mass star forming cores - will have significant contributions from other species with high line densities such as SO_2. In order to correctly reconstruct such line wings, the strength and shape of the 'polluting' line must be accurately predicted and subtracted.

Odin is an astronomy/aeronomy satellite launched in February 2001 as a result of a collaboration between the space agencies in Sweden, France, Canada and Finland. It remains in good health and will continue operation for at least another year.

References to this work:

Olofsson, A.O.H., Persson, C., et al. 2006,
"A spectral survey of Orion KL from 487-492 and 542-577 GHz with
the Odin satellite. I. The observational data." To be submitted to A&A

Persson, C., Olofsson, A.O.H. et al. 2006,
"A spectral survey of Orion KL from 487-492 and 542-577 GHz with
the Odin satellite. II. Analysis and interpretation." To be submitted to A&A

Exterminating the weeds in the astronomical garden

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The existence of unidentified features in interstellar spectra has persisted almost from the beginning of the field. In recent years the number of such lines has rapidly increased in parallel with the sensitivity and frequency range of new observational systems. Estimates of the numbers vary with source, but are typically tens of percent of all of the observed lines. Initially, they often were from 'exotic' species, such as HCO^+, but now the origins of these lines are overwhelmingly from large molecules with dense spectra. It is expected that most of these 'weeds' are associated with previously identified interstellar species. The origin of the identification problem lies in the nature of the spectroscopic approach that has typically been used in the millimeter and submillimeter spectral region: the bootstrap observation, assignment, and theoretical prediction cycle. While this cycle is dear to the hearts of many of us, these 'weeds' arise from complex spectra involving many low lying and often interacting vibrational states. The resulting spectroscopic complexity makes the calculation of 'complete' astronomical spectra a very long-term project. In fact, the observational efforts are accelerating away from their supporting data base at a rapid pace. In this talk we will describe a purely experimental approach to this problem with does not require spectra assignment but rather relies on the observation of 'complete' spectra over a range of temperatures. This approach is enabled by the FASSST spectroscopic system and the use of Collisional Cooling cells to provide reference spectra at low temperature. Experimental and theoretical results will be presented.

Tools for ALMA: data, databases, analysis software and the Virtual Observatory

M.L. Dubernet[1] and A. Walters[2]

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Observatories such as ALMA or Herschel will provide much larger quantities of data than current instruments. Extraction of the information useful for scientific interpretation will require the use of complex numerical models including the dynamics, radiative transfer and chemistry of sources. While much effort is invested in the development of data reduction software (calibration), the tools available for high level scientific analysis of observations are poorly adapted to these new instruments and significant progress is required in this field. This is essential to maximize the scientific return from the investments made in instrumentation.

We present here the status of ongoing work on the provision of atomic and molecular reference data and on the development of automated analysis software systems.
Virtual Observatories provide a framework for gathering and providing standardized access to spectroscopic and collisional data. Recently, a data model for accessing atomic and molecular linelists has been developped and proposed as a VO standard. Another data model providing access to other types of atomic and molecular data is currently under way.

In parallel, work on databases is progressing. The current BASECOL database (http://www.obspm.fr/basecol) provides classical web interfaces and standardized automatic access to collisional rate coefficients for the ro-vibrational excitation of molecules by H, He, H_2 and customized spectroscopic data from JPL/CDMS. The data sets are fully documented and referenced. Visualisation tools are also provided.

CASSIS (http://pc-126.cesr.fr/ Centre d'Analyse Scientifique de Spectres Infrarouges et Sub-millimétriques) provides interactive software allowing the user to visualize and analyse spectra taken with radiotelescopes. It accepts data files generated by CLASS software (post summer 2005) or ASCII tables (CASSIS Format), is coupled with databases and basic models, and is particularly useful for identifying lines and deducing physical parameters. The CASSIS interactive spectrum analyser is available in two modes: a dual (server + applet) standalone Java application and a web Java applet interface.

MAGIX is a collaborative project headed by the MPIfR in collaboration with several teams. This software will be a generic interface to numerical codes and will allow the user to easily fit the output of numerical models (galaxy, protostellar object, etc...) to observed data (spectrum, image, datacube, ...) in order to extract physical information. Program execution will be controlled through a user friendly graphical user interface and will not require any specific programming skills. The interface will provide the user with all the information required to understand the physics of the numerical codes and will allow the user to focus exclusively on the adjustment of the model parameters and the scientific interpretation of the data. A variety of analysis tools will also be provided to allow a critical interpretation of the modelling. As such, this interface will offer a new way to analyse data adapted to all wavelengths.

Radiative transfer tools and molecular databases for ALMA

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In order to fully utilize future (sub)millimetre and infrared telescopes, such as ALMA, it is important that detailed tools are available to the general astronomical community that can match the quality of the data. Presented here is a summary of current publically available radiative transfer codes and molecular data bases. A new project named *Exciter,* aimed at providing the user with a set of advanced tools for performing both line and continuum radiative transfer calculations, will also be presented.

Observations of Circumstellar Disks using the Submillimeter Array

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Circumstellar disks around T Tauri and Herbig Ae stars are considered to be most probable sites for planet formation, and detailed studies on them at higher angular resolutions are crucial for us to understand the mechanism of planet formation. The Submillimeter Array (SMA), recently constructed at the top of Mauna Kea, Hawaii, as a collaborative project of the Smithsonian Astronomical Observatory (SAO) and the Academia Sinica Institute of Astronomy & Astrophysics (ASIAA), is a powerful tool to observe circumstellar disks. We have been observing circumstellar disks at 230 GHz, 345 GHz, and 690 GHz bands using the SMA, revealing new aspects of circumstellar disks. In my talk, I will review observations of circumstellar disks conducted using the SMA.

Molecules in protostellar outflows: prospects with ALMA

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The propagation of a supersonic protostellar outflow through its surrounding medium happens via shock waves. The rapid heating and compression of the gas trigger different microscopic processes – such as molecular dissociation, endothermic reactions, ice sublimation, and dust grain disruption –, which do not operate in the unperturbed gas, generating peculiar chemical anomalies.

We review, from an observational point of view, the influence of shocks on chemistry emphasizing recent observations of outflows from Class 0 sources with favorable orientation in the sky (i.e. high inclination with respect to the line of sight). With less confusion than that found around massive outflows, the shocked regions of low-mass high-collimation outflows, often adopt the form of well-defined bows which are well separated spatially with respect to the quiescent gas. The behaviour of key molecules such as SiO, CH_3OH, H_2CO, HCO^+, CN, etc, is summarized. Particular attention is paid to the chemistry of sulfur bearing molecules (H_2S, OCS, CS, SO, SO_2) since it has been recently proposed to be a potential tool to construct chemical clocks to date outflows (and hence their protostellar driving sources). We also present recent results of a comprehensive chemical survey aimed to study the evolution of young protostellar outflows (Ph. D. work of J. Santiago). It appears that the peculiarities of the chemical behaviour together with other structural parameters such as the presence of extremely high velocity features ("molecular bullets"), the collimation factors, and the mechanical power efficiencies, can be used to produce a rough classification of the observed outflows and to suggest a time evolutionary sequence.

We finally provide some prospects with the future ALMA observations. The superb sub-arcsecond angular resolution together with the high sensitivity in a variety of molecular lines will be particularly useful to study the outflow launching regions, the details of the entrainment mechanisms, and the abundance of very rare molecules which are expected to be created by the shocks.

The complex organic molecules in the hot corinos of Sun-like protostars

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Sun-like stars form from cold and dense condensations inside molecular clouds. During the first phases, heavy element bearing molecules freeze-out onto the dust grains forming mantle of water ices with traces of other molecules. When the collapse finally starts, the object at the center of the condensation increases in mass and in luminosity. The central regions are consequently heated up, and can reach the temperature at which the icy grain mantles sublimate, injecting back the molecules accreted during the pre-collapse phase, along with those created on the grain surfaces. These central regions have been observed in a few low mass protostars, and have been named "hot corinos" to distinguish them from the massive cousins "hot cores". The radii of the hot corinos are less than about 150 AU and the densities are larger than about 10^7 cm^{-3}. Although very few cases have been studied in detail, there is a strong evidence that hot corinos are a common phase in the life of a Sun-like protostar. The observations also suggest that complex organic molecules are very abundant in hot corinos, equating the abundance of formaldehyde and/or methanol. Remarkably, complex organic molecules seem to be more abundant in hot corinos than in massive hot cores, when compared to methanol and formaldehyde in both classes of objects. It is unclear yet whether this is due to a different temperature in the hot cores and corinos, or rather totally to a substantial difference in the composition of the grain mantles. Based on the observations so far available, it seems likely that the observed complex organic molecules are mostly formed on the grain surfaces. In this contribution I will review this topics and discuss how ALMA will represent a revolutionary instrument for these studies, allowing to detect and image the hot corinos, whose predicted typical sizes are out of reach of the current interferometers.

How Are Complex Molecules Produced In Hot Cores And Corinos?

Eric Herbst

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Hot cores and corinos are warm (100-300 K) regions in the vicinity of protostars where a large variety of hydrogen-rich organic molecules are found. Until recently, it had been thought that the molecules were produced in the gas mainly from the precursor molecule methanol, which had been synthesized on the surfaces of dust particles in a previous colder eon before the onset of star formation. Once evaporated into the gas as temperatures increase, the methanol is protonated, leading to a rich ion-molecule chemistry. Unfortunately, some of the reactions thought to form more complex molecules have now been measured not to occur. We suggest another method in which larger molecules can be produced – in this scenario the molecules are produced as the temperatures increase during star formation and not only afterwards. The basic idea is that a distinct chemistry can occur on the surfaces of dust particles warmed to higher temperatures than 20 K, where H atoms are not as important in the chemistry as at lower temperatures and heavy radicals are able to diffuse and react with one another. As the surface temperatures increase to 100 K, the newly formed species are evaporated and change the nature of the gas-phase chemistry.. The specific case of methyl formate, a common and abundant species in hot cores, is looked at in some detail.

Testing grain-surface chemistry in massive hot-core regions

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Many complex organic molecules, such as CH_3OH, CH_3OCH_3 and CH_3CH_2CN, have been detected in star-forming regions. Studying their chemistry is important, since these species may eventually be incorporated into circum-stellar disks and thus become part of the material from which future planetary systems are made. Two scenarios for their formation have been proposed: grain-surface chemistry and high-temperature gas-phase reactions (see e.g., van Dishoeck & Hogerheijde, 1999 for a review). In the former case, grain-surface reactions during the cold pre-stellar and proto-stellar phases are thought to lead to the formation of hydrogenated molecules, which subsequently evaporate into the gas when the young star heats its surroundings. In the latter case, high-temperature gas-phase reactions involving evaporated molecules produce complex organic species like CH_3OCH_3 (Charnley et al., 1992). The resulting molecules from these two schemes are also known as ``first generation'' and ``second generation'' species. Currently, it is very difficult to distinguish between these two scenarios since the rates of even some of the most basic surface reactions are not known.

Deep searches for a set of molecules, that are thought to have formed on grain surfaces, have been performed for 7 high mass Young Stellar Objects with the James Clerk Maxwell Telescope (JCMT). We detect emission from H_2CO, CH_3OH, CH_2CO, CH_3CHO, C_2H_5OH, HCOOH, HNCO and NH_2CHO. Additionally, molecules that are thought to form from gas phase reactions with CH_3OH, such as CH_3OCH_3, and CH_3OCHO, have been detected. CH_3CHO is not detected with the JCMT for any source; it was previously detected by Ikeda et al. (2002) with rotational temperatures of only 20-30 K, which is much lower than the lowest rotational transition that can be probed with the JCMT at 71 K. This is also confirmed by our detections of CH_3CHO transitions with energy levels below 45 K in N7538 IRS1, and W3(H_2O) with IRAM, two of the sources from our JCMT sample. The resulting rotational temperatures, derived from rotation diagrams, are about 100 K or higher for most target molecules, but are significantly lower for CH_2CO, and CH_3CHO, implying that these are not present in the same region.

The derived column densities vary by more than an order of magnitude between the different sources. The relative column densities are however very similar for some molecular species, e.g., H_2CO, CH_3OH, C_2H_5OH, CH_3OCHO, CH_3OCH_3. Surprisingly, this includes both molecules that are thought to form due to grain-surface reactions and gas phase chemistry. The column densities of the nitrogen-bearing species HNCO and NH_2CHO behave very similar as well, but peak for other sources compared to the oxygen-bearing species. Abundances are derived by comparing to H_2 column densities estimated from dust radiative transfer models. Strong correlations are found between those species that show very similar column density variations suggesting that they are chemically related through their formation mechanisms.

Probing the Inner 200 AU of Low-Mass Protostars with the Submillimeter Array and Spitzer Space Telescope

Jes K. Jørgensen[1], and the PROSAC[2] and c2d[3] teams

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[2] Protostellar Submillimeter Array Campaign
[2] "Cores to Disks" Spitzer Space Telescope Legacy program

One of the more exciting recent developments in astrochemistry is the detection of complex organic molecules in the envelopes around low-mass protostars. Studies of this chemistry are important because part of this material may eventually be incorporated in circumstellar disks and new planetary systems. Low-mass protostars are now known to contain "hot corinos" similar to the hot cores observed for high-mass protostars, i.e., warm (T ~ 100 K), dense ($n_{H2} \sim 10^7$ cm^{-3}) regions where icy grain mantles evaporate, injecting organic molecules into the gas-phase where they can further react to form more complex species (e.g., Ceccarelli et al. 2000, Schöier et al. 2002, Cazaux et al. 2003).

The origin of this warm gas with complex molecules is strongly debated, however. In addition to evaporation of ices following passive heating of the inner envelope by the protostar, also interactions of the outflow with the inner envelope can be important. For example, H_2CO and CH_3OH - often taken as signposts for hot corinos - have been shown to be affected by shocks in a number of protostellar outflows on both large scales and in the immediate vicinity of low-mass protostars (e.g., Bachiller et al. 1995, Jørgensen et al. 2005). Also, estimates of molecular abundance variations rely on a good understanding on the envelope physical structure, in particular its density and temperature, down to smallest scales. Estimates of these parameters often rely on extrapolations of the structure from the outermost regions and may break down on small scales where also the protoplanetary disks are formed.

In this talk I will discuss some of the observational constraints on the structure of the inner envelope and the chemistry in the immediate environments of low-mass protostars. In particular, I will focus on a survey of a large sample of low-mass protostars using the Submillimeter Array (SMA). Those observations directly image high excitation transitions probing the warm and dense gas in the protostellar envelopes and make it possible to trace the physical and chemical structure down to scales of a few hundred AU. In particular, the importance of shocks on those scales is apparent in the data. The SMA observations also place strong constraints on the existence and sizes of circumstellar disks on small scales.

I will also discuss recent Spitzer Space Telescope observations from the c2d legacy team that provide further clues to the structure of the innermost regions of protostellar envelopes. In particular, the mid-IR detections of the heavily obscured protostars suggest the existence of inner cavities within which material is falling toward the central circumstellar disks. The Spitzer observations also provide direct images of the warm gas in the shocks through imaging H_2 rotational emission – and show clear correlations with the strong CH_3OH emission on scales from a few hundred to thousand AU scales.

New SMA and JCMT results on the remarkable class 0 source Barnard 1c

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We report recent results from molecular line studies on the Smithsonian Submillimeter Array and the James Clerk Maxwell Telescope toward the recently identified class 0 object, Barnard 1c. This source, first identified in polarimetry mapping with SCUBA (Matthews & Wilson 2002), was primarily of interest due to its unique polarization properties compared to all other low mass cores. In B1c, there is evidence that grains are well aligned by the magnetic field all the way to the core centre. Followup studies of the core interior were undertaken to understand why the polarization properties of this core are so unique. B1c is now known to drive a spectacular precessing outflow as imaged by Spitzer (Jørgensen et al. 2006) associated with a CO outflow as detected with the SMA (see Figure 1) and exhibits a rotating molecular torus on the order of 1000 AU encompassing a central heated cavity as detected with the BIMA array (Figure 1, Matthews et al. 2006). We will present our most recent results from the SMA and JCMT which reveal the flattening of the central heated core and the evidence for strong deuteration in this object, which can be linked to strong coupling of the gas to the magnetic field.

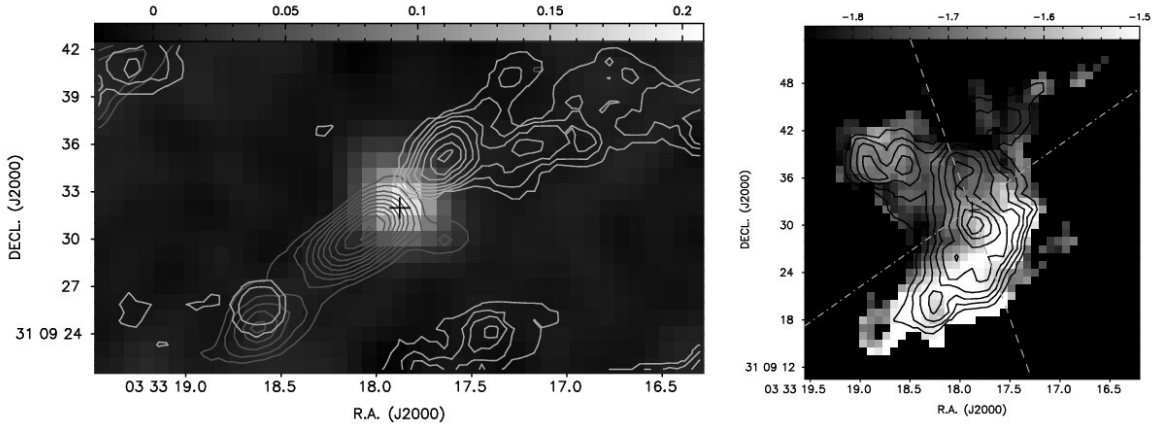

Figure 1: *Left*: The CO outflow is strongly detected in CO 2-1 emission from the SMA. The greyscale shows the 1.3 mm emission. As detected in the CO 1-0 emission, we see evidence of a shift from blue (dark grey contours) to red-shifted (light grey contours) emission where the Spitzer data reveal a change in the direction of the outflow. *Right*: The greyscale shows the first moment of a single hyperfine component of N_2H^+ 1-0 emission from B1c; the rotation from roughly north to south is evident. The contours show the zeroth moment; two peaks of N_2H^+ 1-0 emission are roughly symmetric about the continuum peak, indicated by the cross. The outflow axis and alignment of the peaks are indicated by the dash-dot and dashed grey lines, respectively.

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Molecules in massive star formation observed with high angular resolution

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One of the open promises in (high-mass) star formation research is to develop chemical clocks allowing to better determine ages and evolutionary sequences. While some theoretical models exist, the observational database to calibrate the models against is still poor. This is specifically the case for high-angular-resolution observations resolving the various sub-sources within the evolving massive proto-clusters. I will present recent spectral line observations from (sub)mm wavelength Interferometers toward massive star-forming regions of various evolutionary stages, outlining the present state of research and the current observational possibilities. A short outlook on the progress expected by ALMA will be given as well.

Probing high-mass star formation through different molecules

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Star formation proceeds through inside-out collapse of molecular cores, with accretion onto a compact kernel, the protostar. While this certainly holds for low-mass stars, the same mechanism cannot be trivially applied to high-mass ones (i.e. stars in excess of about 8 M_{sun}), as their powerful radiation pressure could halt and even reverse the infall. Observations can shed light on this issue by analysing the structure and kinematics of the gas from the scale of the molecular cores hosting OB star formation (0.1 pc) to the regions where accretion is expected to dominate (<1000 AU). After briefly reviewing the characteristics of OB star forming regions, I will show how different molecular transitions can be used to probe different parts of the star forming environment. In particular I will focus on the detection of rotation and infall towards high-mass young stellar objects, which will be illustrated in detail by means of detailed studies of selected objects. Application of the most powerful observational techniques available to date suggests that only the combination of sub-arcsec angular resolution, high sensitivity, and - last but not least - wide spectral coverage provided by ALMA will make it possible to establish the mechanism by which massive stars form.

Chemical complexity with ALMA: looking for new molecular species near the line confusion limit

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From Molecules to Dust

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The dust injection from Asymptotic Giant Branch (AGB) stars into the interstellar medium very likely plays a key role for the dust formation in a galaxy. Determining the amount of dust injected by AGB stars into the interstellar medium as well as the composition of the dust is a pre-requisite for any attempt to model the evolution of interstellar matter. The dust in the interstellar medium is assumed to play a significant role for the formation of molecules, in particular for H_2, whose abundance relative to H atoms in the ISM cannot be accounted for by gas-phase reactions and methanol which involve heterogenenous reactions on grain surfaces or in the icy mantles.

In most dusty objects the grain component is intimately interwoven with the gas component and the radiation field and therefore strongly affects the thermodynamical, the hydro-dynamical and the chemical structure of the object.

Dust is formed by a series of chemical reactions in which atoms or molecules from the gas phase combine to clusters of increasing size. The molecular composition of the gas phase determines which atoms and molecules are available for the cluster formation and grain growth. This can lead to a layered structure in a circumstellar envelope. Dust formation alters the atmospheric structure which significant influence the local and global circumstellar envelope dynamics and the detailed time-dependent spectral appearance.

In the pulsating atmospheres of AGB stars the condensation of dust grains is strongly connected with the shock wave structure of the circumstellar envelope, usually triggered by a two step mechanism. First there is nucleation of critical clusters from molecules and this is followed by growth to macroscopic dust grains. Grain growth will usually proceed far from equilibrium and it is necessary to use a time-dependent description of grain growth to determine the degree of condensation and other relevant properties of the dust.

We are currently investigating how the predicted wind properties of AGB stars are influenced by the choice of micro-physical dust parameters and the stellar metallicity.

The Cologne database for molecular spectroscopy and requirements of laboratory spectroscopy for ALMA

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The internet browser-accessible Cologne Database for Molecular Spectroscopy, CDMS, contains as one main part a catalogue of rotational and, to a lesser extent, rovibrational transition frequencies of molecular species that have been or may be identified in the interstellar medium, circumstellar envelopes, or planetary atmospheres. The entries have been created by fitting critically evaluated experimental data, mostly from laboratory experiments, to suitable Hamiltonian models to ensure entries as reliable as possible. Particular emphasis has been put on supplying data in the (sub-) millimeter and terahertz ranges for telescopes such as APEX and the SMA as well as for the upcoming Herschel mission and ALMA. Furthermore, the CDMS provides data with increased accuracy for many species. Separate entries are provided for minor isotopic species or for molecules in excited vibrational states as far as appropriate. The database is available online free of charge through a link on the KOSMA web-site **http://www.ph1.uni-koeln.de/** or via the short-cut **http://www.cdms.de/**.

The catalogue is updated continuously. As of April 2006, the catalogue contains more than 360 species of astro-physical, astrochemical, and planetary interest. The basic features of the CDMS as well as recent and future activities in the field of complex molecules will be discussed.

A second part of the talk will be devoted to some issues concerning the detectability of complex molecules in the interstellar medium. In this context, a few selected examples of often not so complex molecules will be given that need further laboratory spectroscopic investigations.

The Cologne THz Spectrometers: Recent Advances and Perspectives

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Technical developments of recent years have lead to an extension of the accessible spectral range towards shorter wavelengths and into the so called Terahertz region. Many molecules, especially those of astrophysical importance, have characteristic spectral features at Terahertz frequencies, e. g., the pure rotational transitions of light hydrides, XH and XH_2 (X=C, O, N, S) or the low lying bending modes of carbon containing chain and ring molecules.

The Cologne group uses backward wave oscillators (BWOs) and a far-infrared laser sideband system to cover the spectral range up to 2 THz at very high resolution. New superlattice frequency multipliers have extended the accessible spectral range up to 2.7 THz. The spectrometers are combined with supersonic jet and trap apparatuses where unstable and highly reactive molecules are produced in a cold jet expansion or storage device. We report on our latest results and new technical developments on Terahertz radiation sources as well as laser induced reactions, a novel method for spectroscopy with ultimate sensitivity.

All molecular parameters and line catalogues are made available via the Cologne Database for Molecular Spectroscopy (CDMS) for future observations.

Molecular spectroscopy and the search for (large) molecules with ALMA

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The Atacama Large Millimeter Array, ALMA, will enable the investigation of astronomical molecules at high sensitivity and unique spatial resolution. It will also be a prime facility to search for new molecules in space. The analysis of these observational data – in particular from line rich sources - will be tedious and largely dependent on the availability and accuracy of corresponding laboratory data. Selected examples of plausible candidates for astronomical detection will be given.

The Rotational Spectra of Nucleobases

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The nucleic acids bases (nucleobases) are one of the major constituents of DNA and RNA, and they represent next to amino acids and sugars another class of prebiotic molecules of potential astrophysical interest. Nucleobases are nitrogen containing heterocyclic compounds and can be divided into two groups according to their molecular structure: uracil, cytosine and thymine consist of a single six-membered ring and belong to the pyrimidine derivatives, whereas adenine and guanine are purine derivatives, consisting of a six-membered ring fused to a five-membered ring. They exhibit a dense rotational spectrum and are fairly polar with dipole moments ranging from 2-5 Debye.

In this talk I am going to give a summary of the available experimental data on the rotational spectra of the five nucleobases [1] and present recent results on uracil, the smallest member of the class. The existing dataset on this molecule has been extended both to the astrophysical important frequency range between 70-100 GHz, where the strongest lines are expected for interstellar sources with excitation temperatures around 10 K, and towards the microwave region, which allowed for the analysis of its complex nuclear hyperfine structure.

Additionally, possible sources for its astrophysical detection will be discussed.

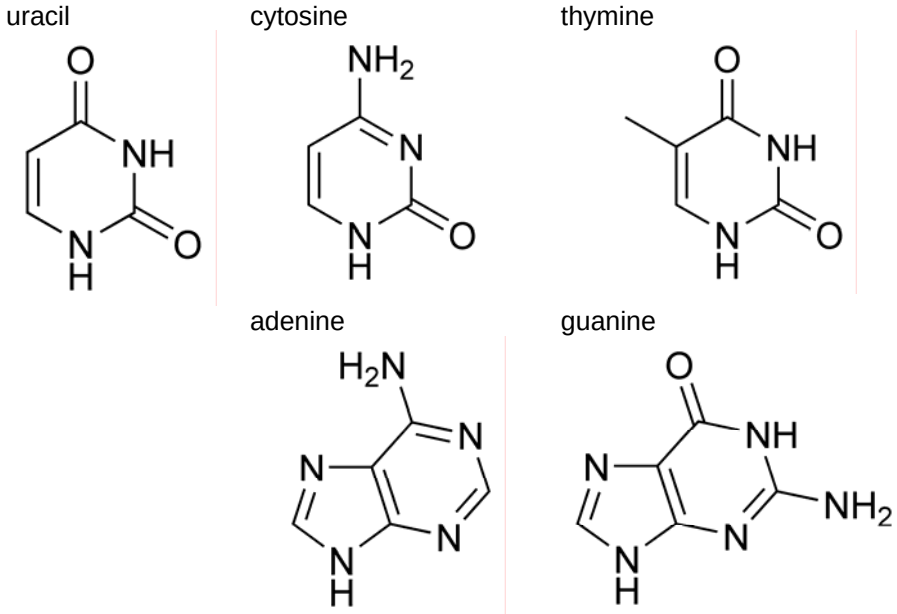

Figure 1: Chemical structure of the five nucleobases.

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Exploring an Early Stage of Protostellar Evolution with Complex Organic Molecules

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Complex organic molecules such as $HCOOCH_3$, CH_3OCH_3, and C_2H_5CN are known to exist in hot cores of massive star forming regions, and are key molecules to diagnose in the densest part of star forming regions. However, recently these complex organic molecules have also been detected toward a few low mass star forming regions, IRAS16293-2422, NGC1333IRS4A, NGC1333IRAS2A and NGC1333IRAS4B (Cazaux. et al. 2003, Bottinelli et al. 2004, Jørgensen et al. 2005, Sakai et al. 2006). Figure 1 shows our detection of $HCOOCH_3$ toward NGC1333IRAS4B at 89.3 GHz with Nobeyama 45 m telescope. These results clearly established the existence of "hot cores" even in a low mass star forming region. Complex organic molecules are produced by grain mantle evaporation and subsequent gas phase reactions just after the onset of star formation. Furthermore these sources are all the class 0 protostars, indicating that the complex organic molecules can exist in the early stage of protostellar evolution. Particularly NGC1333IRAS4B is reported to be extremely young (~a few 100 yr) according to the dynamical age of the molecular outflow (Choi 2001). Since large organic molecules are generally absent in starless cores (Kaifu et al. 2004), their spectral lines could be used as a novel tracer for detecting an onset of star formation.

Very recently we have found a similar trend in a massive star forming region, NGC2264, located 800 pc from the Sun. Figure 2 shows integrated intensity map of CS(7-6) (Shreyer et al.1997). In this region, IRS1 is a young stellar object with the brightest IR source. But we were not able to detect the complex organic molecules there. In contrast, we have detected the lines of $HCOOCH_3$ in this southern region including MMS3, which is reported to be younger than IRS1 (Ward-Thompson et al. 2000).

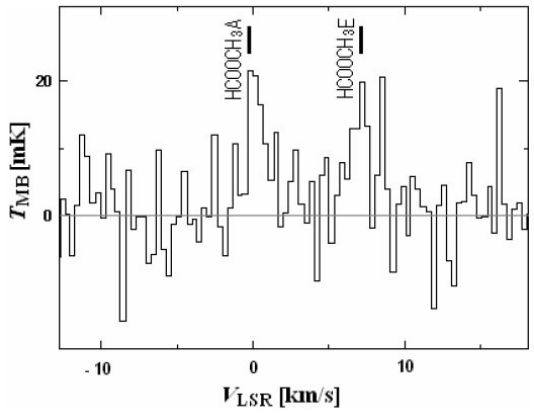

Fig. 1 Spectral line profile of $HCOOCH_3$ toward NGC1333 IRAS 4B (81, 8 - 71, 7 E and A).

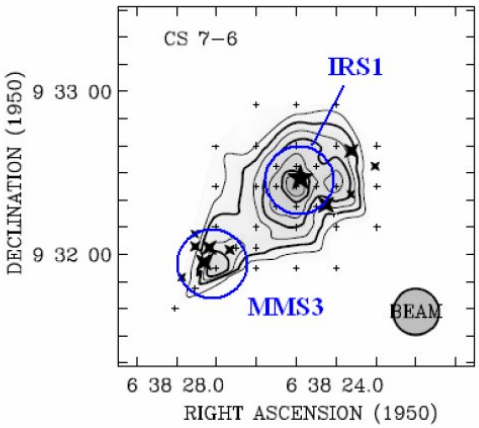

Fig. 2 Integrated intensity map of CS(7-6) in NGC2264 IRS1 region.
(Shreyer et al.1997 JCMT)

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ALMA's Window on Molecular Emission: Small Ions to Complex Prebiotics

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The Atacama Large Millimeter Array (ALMA[11]) is a large international telescope project under construction in northern Chile on a site at Chajnantor of 5 km elevation. The excellent atmospheric transmission at that site in the millimeter and sub-millimeter wavelength ranges will allow ALMA to provide detailed images of the sources of the the Cosmic Microwave Background and the Cosmic Far-Infrared Background radiation, near the wavelengths of the two strongest peaks in the spectral energy distribution of the Universe. ALMA's images will contain all of the flux in the imaged field through the use of two parts: (1) the "12m Array", composed of up to sixty-four 12-meter antennas that can be placed on 186 different stations for baselines up to 18 km (see Table 1) and (2) the "Atacama Compact Array", or ACA, that consists of twelve 7 meter telescopes placed in compact configurations and four 12 meter telescopes for measuring source total power. At the shortest planned wavelength, λ=0.3 mm, and longest baseline, the angular resolution will be 0.004". The receivers use superconducting (SIS) mixers which, in combination with the excellent site transparency (median τ_{225} =0.061) and the large array collecting area (8152 m^2), will provide a sensitivity at 1mm wavelength of 1 mJy in a few seconds for average atmospheric conditions; this is more than two orders of magnitude better than any array operating today. Complete frequency coverage from 10mm to 0.3mm will offer unprecedented access to the spectrum of interstellar molecules at this high sensitivity. At first light for the ALMA project the 6 highest priority receiver bands will be installed (see Table), each observing both polarizations with a bandwidth of 8 GHz; construction of the additional four bands will be accomplished during the Operations phase of ALMA. The ability to map the spatial distribution of large molecules at high sensitivity and resolution and in many transitions will revolutionize our understanding of the mechanisms of formation of these species in the interstellar medium.

ALMA Front End Key Specifications (and Preliminary Results)
All Bands Offer Dual Linear Polarization; 8GHz Output per Polarization
Each 12m Antenna will also be equipped with a 183 GHz Water Vapor Radiometer

ALMA BAND	FREQUENCY (GHZ)	T_{RX} 80% OF BAND	MIXING SCHEME	RECEIVER TECHNOLOGY
1	31.3-45.	17	USB	HEMT
2	67-90	30	LSB	HEMT
3	84-116	37 (35)	2SB	SIS
4	125-169	51	2SB	SIS
5[a]	163-211	65	2SB	SIS
6	211-270	83 (40)	2SB	SIS
7	270-373*	147 (80)	2SB	SIS
8	385-500	98	DSB	SIS
9	602-720	175 (120)	DSB	SIS
10[b]	787-950	230	DSB	SIS

**between 370 – 373 GHz Trx is less than 300 K*
a Six receivers in construction phase.
b Full complement to be finished after construction phase.

[1] ALMA is an equal partnership between Europe and North America, in cooperation with the Republic of Chile, and is funded in North America by the U.S. National Science Foundation (NSF) in cooperation with the National Research Council of Canada (NRC), and in Europe by the European Southern Observatory (ESO) and Spain. In the bilateral project, ALMA construction and operations are led on behalf of North America by the National Radio Astronomy Observatory (NRAO), which is managed by Associated Universities, Inc. (AUI), and on behalf of Europe by ESO. In addition, Japan has also entered the ALMA project.

Bridging the molecular divide between molecular clouds and biology, a spectroscopist's view of detectability

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More than 130 molecules have been identified in the interstellar medium and numerous unidentified features widely believed to molecules transcend the spectrum from radio through the near ultraviolet. The identified molecules include examples of all the functional groups of organic chemistry suggesting that interstellar processing is partly if not completely responsible for the chemistry leading to life. Constraining the interstellar role in the evolution of biology is a central question in understanding the likelihood of life elsewhere. ALMA, Herschel and other large telescope facilities have a scientific mandate to bridge the gap between the relatively simple molecules already identified and the macromolecules of biology. The three micron bands provide a compelling case that more complex molecules do exist in the ISM, but there is no identification of any specific carriers. The physics and chemistry of large molecules make detection and identification difficult due to large partition functions, low volatility, and large rotational constants. However, there are many large molecules that have favorable ro-vibrational characteristics for detection. Identifying the more likely candidate molecules and eliminating the contamination lines from known molecules is required for convincing detections. Both cases will require a focused investment in laboratory work that transcends telescope facilities and wavelengths.

Spectroscopy of PAHs at IR/submm wavelengths

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In the last few years, we have developed an experimental set-up in order to record gas phase emission and absorption spectra of small PAHs in the far-infrared region. Their spectra have been obtained by means of a high resolution Fourier transform spectrometer. Thermal emission of PAH vapour at about 450 °K was emitted from an electric furnace loaded with solid PAH sample following the method described in ref. (1) and (2). Emission vibrational bands of naphthalene, anthracene, phenanthrene, chrysene and pyrene have been recorded in the spectral range 50-700 cm^{-1}. A Tight-Binding Molecular Dynamics approach allows the prediction of their spectral positions (3). Absorption spectroscopy was carried out on naphthalene at 300 °K, in the same spectral range, at higher resolution, by using a multiple reflection cell. The resulting spectrum can be straightforwardly compared with its 300 ° K emission spectrum recorded by using an appropriate set-up. Thanks to the high resolution, some features observed in the absorption spectrum of naphthalene can be tentatively assigned.

These far-infrared measurements provide information on the entire molecular skeleton of each PAH and characterise each species. It is hoped that they will help in the identification of some spectral astrophysical structures.

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High-resolution spectroscopy of large molecules

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Recent results on the recombination of PAH cations with electrons

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Mid-infrared astronomical observations suggest that Polycyclic Aromatic Hydrocarbons (PAHs) are ubiquitous in the Universe. However, various aspects of the chemistry of PAHs remain not well understood. This is partly due to the scarcity of laboratory data, especially in the gas phase, as it is challenging to investigate the spectroscopy and kinetics of free molecular species of such low vapour pressure.

As PAHs molecules have low ionization potential they can easily be ionized in space, either by charge exchange or by photoionization. The cations can then react with neutral atoms or molecules or recombine with electrons. Among all the processes that take place in the interstellar medium, recombination may play an important role in the destruction of PAH ions.

In our laboratory, we have recently developed a new method dubbed F*l*API (Flowing Afterglow with PhotoIons) for measuring the recombination rate of large ionized species such as PAHs with electrons in a flowing afterglow at room temperature. A very small amount of neutral PAH molecules is injected into the afterglow plasma by evaporation from a plate coated with the PAH solid sample. PAH ions are then produced by photoionization of the parent molecule using a pulsed VUV laser (157nm). The laser beam is oriented along the flow-tube and so a constant spatial concentration of photoions is obtained. The electron concentration along the flow-tube is measured by means of a movable Langmuir probe. Ion concentration decay in time is measured at a fixed position using a quadrupole mass spectrometer which is triggered by the laser pulse. The recombination rate is then obtained from the time profile of the photoions which depend on the electron number density present in excess. The F*l*API method has been successfully applied to the measurement of the recombination rate of anthracene, pyrene, azulene and acenaphthene cations[1,2]. Our measurements reveal a definite trend of increasing rate with the size of the PAH (number of carbon atoms).

However, the F*l*API method is limited by the vapour pressure of PAHs which strongly decrease with size. To overcome this limitation, we are currently working on a new implementation to produce the PAH ions and extend our investigations to larger species. Feasibility studies suggest that large PAHs may be efficiently photo-desorbed in situ from a pellet positioned in the flow by a first laser (λ=266 nm) and then ionized by a second high energy laser (λ=157 nm). From the history of the packet of PAH ions and photoelectrons, reconstructed by time resolved Langmuir probe and mass spectrometry measurements, and guided by numerical simulations, we can access the recombination coefficient. Preliminary results suggest that the method may hold a great potential for the measurement of the recombination rate coefficient of large condensable species such as PAHs.

This work is supported by the Programme de Physique et Chimie du Milieu Interstellaire.

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Chemistry of interstellar PAH candidates : from space to the laboratory

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Polycyclic Aromatic Hydrocarbons (PAHs) are the best candidates to account for the Aromatic Infrared Bands (AIBs) observed in emission between 3.3 and 12.7 μm in many astronomical environments irradiated by UV photons. Despite a wealth of observational data, no individual molecule could be identified so far. The true nature of interstellar PAHs has therefore to be questioned, considering the formation mechanism of these species, the processing by UV photons and the reactivity with gas-phase species. These studies require a multidisciplinary approach combining observations, fundamental data from theory or experiment, and astrophysical models.

One of the challenges for laboratory experiments is to approach the physical conditions that prevail in interstellar space: cold environment (10-50 K), absence of collisions on long timescales and presence of stellar UV photons ($h\nu<13.6$ eV) at the surface of clouds. PIRENEA, *"Piège à Ions pour la Recherche et l'Etude de Nouvelles Espèces Astrochimiques"*, is an experimental set-up which has been developed according to these specifications. Using the trapping, and the mass spectrometry analysis of an ion cyclotron resonance (ICR) cell that is connected to cryogenic shields, novel studies can be performed on processes which occur on long timescales and which are of interstellar relevance: IR radiative cooling, photodissociation in low energy channels, radiative association.

Results will be presented on the photodissociation of PAH species and their reactivity with small molecules. These studies extend now to nano-grains such as PAH clusters and PAH-iron complexes.

Carbon chain spectroscopy

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Carbon chains represent the dominant structural theme of the more than 130 known interstellar and circumstellar molecules, and many more chains are likely to be detected in space once their laboratory spectra have been found and measured. New, highly precise measurements in the infrared and far-infrared region are very timely for the upcoming new generation of astrophysical instrumentation such as the Herschel satellite and the airborne observatory SOFIA (Stratospheric Observatory For Infrared Astronomy), covering the frequency domain in which many of the carbon chain spectra are presumably located.

The application of Terahertz- and infrared-spectroscopy to supersonic molecular beams has overcome the production difficulty, yielding the detection of various reactive and highly unsaturated carbon molecules. Recent results on pure carbon chain molecules and carbon hydrids will be presented and compared to high level *ab initio* calculations.

Molecular beam studies on reactions of C atoms and C_2 radicals with unsaturated hydrocarbons: a possible synthetic route to interstellar carbon chains

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The reactions of ground-state carbon atoms, C(^{3}P) and dicarbon molecules, C2($X^1\Sigma_g^+$), with unsaturated hydrocarbons are of basic chemical interest and of great importance for understanding combustion processes and the chemical evolution of extraterrestrial environments such as molecular clouds and circumstellar envelopes of dying carbon starts, as for instance, IRC + 10216. Kinetic studies found these neutral-neutral reactions very fast down to very low temperature (15 K for C [1] and 24 K for C_2 [2]) and suggested that these are barrierless reactions that may have a critical role in the chemistry of the interstellar medium (ISM). An issue of key importance is how larger molecules are assembled and, in particular, how molecules containing chains of several carbon atoms are synthesized.

Here we report on the investigation of the dynamics of the prototypical and perhaps most important reaction of C and C_2, that with the acetylene molecule, by using the crossed molecular beam (CMB) scattering technique with mass-spectrometric detection [3]. Primary products and branching ratios were determined as a function of collision energy (i.e., relative translational energy). We exploit the capability (a) of generating *continuous* supersonic beams of C and C_2, (b) of crossing the reactant beams at variable angles (45°-90°-135º) to widen the range of collision energies, and (c) of detecting the products by "soft" electron-ionization [4,5].

Angular distributions and time-of-flight (TOF) spectra at *m/z* = 37 (C_3H) and 36 (C_3) were recorded in a wide range of collision energies (E_c~3.5-50 kJ/mol) for the reaction C(^{3}P)+C_2H_2. We have identified the primary products of the competing pathways leading to *linear (l)/cyclic* (c)-C_3H + H and C_3 + H_2, derived their center-of-mass (CM) angular and translational energy distributions, determined the branching ratios, and characterized the reaction micro-mechanism [5]. Information on the *c*-C_3H/*l*-C_3H branching ratio and respective exoergicities are also obtained. The spin-forbidden pathway leading to $C_3(X^1\Sigma_g^+)$+$H_2(X^1\Sigma_g^+)$ is rationalized in terms of intersystem crossing between triplet and singlet potential energy surfaces. Since our C beams contain, in addition to C(^{3}P), also a significant concentration of excited C(^{1}D) atoms, we have characterized the dynamics of C_3H and C_3 formation from also the C(^{1}D)+C_2H_2 reaction (of relevance in comets). These studies extend significantly our previous investigation at E_c=29.3 kJ/mol [6] and earlier CMB studies with pulsed beams [7]. Notably, from measurements of electron-ionization efficiency curves of the reaction products down to very low electron energies, the first experimental estimate of the ionization energy (IE) of *l*-,*c*-C_3H radicals is also obtained (the experimental IE compare well with theoretical predictions [8]). Angular distributions and TOF spectra at *m/z*=49 (C_4H) from the reactions $C_2(X^1\Sigma_g^+/a^3\Pi_u)$ + C_2H_2 were recorded at E_c=13.1 and 36.8 kJ/mol. The product CM angular and translational energy distributions are determined. The dynamics of the buta-1,3-diynyl [$C_4H(X^2\Sigma^+)$, HCCCC] radical product as a function of E_c is determined and compared with the results of recent CMB experiments carried out using pulsed beams [9].

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Intra- and intermolecular dynamics of cyanoacetylene and its complexes with helium

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Accurate potential energy surfaces and nearly exact methods describing the nuclear motions are of primary importance to understand spectroscopic and collisional properties of molecules. In my talk I will show on the example of cyanoacetylene how modern quantum chemical methods can be applied with trust to describe state resolved spectroscopic and collisional experiments. Special attention will be paid to the state-of-the-art *ab initio* techniques for the calculation of the intramolecular potential energy surface of cyanoacetylene and to methods needed on the route from the potential energy surface to the rovibrational spectra. The exact Hamiltonian describing the nuclear motions will be introduced, and a hierarchy of possible decoupling schemes for an approximate calculation of the rovibrational energy levels will be discussed. Nearly exact energy levels from variational 10D calculations, as well as some approximate values obtained by using some decoupling procedures, will be reported and compared with high-resolution experimental data from microwave and infrared spectroscopy.

Polyynes And Cyanopolyynes: From Astrochemistry To Their Easy Synthesis In A Carbon Arc

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A parallelism has been discovered between the polyynes formed by laser ablation experiments of graphite targets and those produced from the submerged electric arc between graphite electrodes. In both cases the same products are obtained.

Hydrogen-terminated polyynes are obtained when the carbon arc is struck under water; monocyanopolyynes (mixed with hydrogen-terminated polyynes) are the products if the carbon arc is sparked in acetonitrile or ammonia; dicyanopolyynes if the arc is struck in liquid nitrogen. The mechanism of formation of polyynes in the submerged carbon arc involves essentially neutral species as it happens around the circumstellar environment.

It is shown that the relative abundances of the polyynes formed in the submerged carbon arc or in a carbon arc in vacuum decreases by a factor between 3 to 5 as the chain length increases by a C_2 unit. Exactly the same trend has been observed both for polyynes and cyanopolyynes in the circumstellar environment around carbon-rich stars. This fact suggests that the mechanism of formation of the polyynes in the carbon arc is the same occurring in the surroundings of the carbon-rich stars.

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Formation of interstellar methanol and other oxygen containing compounds: Non-feasibility of gas-phase mechanisms

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For astronomical observers, methanol is one of the most interesting molecules. Multi-line observation on methanol can be used to determine temperature and spacial density of in an interstellar cloud with *one* molecule only, thereby avoiding the problem of different spatial distributions of different tracers.[2] Masers of methanol are seen as excellent tracers of star formation.[3] Furthermore, the compound can be used as an evolution indicator during the embedded phase of massive star formation.[4] Contrary to its importance for astronomical observations, comparatively little information is available on the formation of interstellar methanol. A two-step mechanism including radiative association of CH_3^+ and H_2O and dissociative recombination of the produced ion has hitherto been held responsible:

$$CH_3^+ + H_2O \rightarrow CH_3OH_2^+ \quad (1)$$
$$CH_3OH_2^+ + e^- \rightarrow CH_3OH + H \quad (2)$$

To assess the feasibility of this process in the gas-phase the efficiency of reactions 1 and 2 has to be assessed. Therefore, branching ratios of the different reaction pathways and the overall rate coefficients of the dissociative recombination of $CH_3OH_2^+$ (Reaction 2) has been measured at the CRYRING storage ring located in Stockholm, Sweden. Analysis of the data yielded that formation of methanol accounted for only 3 % of the total rate in $CH_3OH_2^+$ (6 % in the isotopomer $CD_3OD_2^+$). Largely, dissociative recombination of $CH_3OH_2^+$ involves fragmentation of the C-O bond, the major process being the three-body break-up forming CH_3, OH and. The overall cross section is best fitted by. $\sigma = 1.2 \pm 0.1 \times 10^{-15}\ E^{-1.15 \pm 0.02}$ cm^2. From these value the thermal reaction rate coefficients of $k(T) = 8.9 \pm 0.9 \times 10^{-7}\ (T/300)^{-0.59\pm0.02}$ cm^3 s^{-1} can be calculated.

These values, along with a recently measured upper limit for the rate coefficient of reaction (1)[5] have been used as input for a model calculation of a dark interstellar cloud resembling TMC-1 using the UMIST code.[6] This calculation yields a peak methanol abundance of 7×10^{-13} (H_2) which is definitely below the observed values in dark clouds and probably below the detection limits for existing telescopes. A non-negligible formation of interstellar methanol by the previously proposed mechanism is therefore very unlikely and a grain surface process for methanol production *via* repetitive hydrogenation of CO is invoked. Very recently, it has been established by Hidaka *et al.*[7] in a surface reaction experiment that the formation of methanol by hydrogenation of CO with H on pure CO and mixed CO/H_2O ices proceeds efficiently at 10 K. Moreover, once produced, CH_3OH is not degraded by irradiation.

Very recently, the dissociative recombination of protonated dimethylether $(CH_3)_2OH^+$ has also been investigated, which has been regarded as the final step in formation of interstellar dimethyl ether.[8] Preliminary analysis shows that the branching ratio for dimethyl ether formation in this reaction amounts to only 6 %, which, in analogy to the findings on methanol, renders the previously assumed formation pathway very improbable.

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Experimental studies of H_2 formation on grains: overview and recent results

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Irradiation and thermal processing of silicates in the laboratory: Insights in extraterrestrial grain properties

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Before the results from the Short Wavelength Spectrometer instrument (SWS) on board the Infrared Space Observatory (ISO), it was largely thought that all silicate dust in space was totally amorphous. The extensive results provided by ISO have shown the existence of different forms of dust (crystalline, amorphous and/or both of them), depending essentially on the astrophysical environment where they are detected. Many studies have been devoted to understand the primary modifications (structure and chemical composition) due to ionic irradiations [1-3] or thermal processing [4-5], but very little has been done regarding further evolution of irradiated silicates. In order to evaluate the dust ability to crystallize in cold environments, we have studied thermal processing of silicates after a further irradiation stage [6]. For this, we have developed an experimental protocol simulating different stages of the life-cycle of the dust. Thin silicate films (typically 50 to 100 nm in thickness) are synthesized by electron-beam evaporation of San-Carlos olivine ($Mg_{1.8}Fe_{0.19}Ni_{0.01}SiO_4$) onto 3 mm diameter diamond discs. He^+ irradiations, under vacuum at room temperature at low energies (5 keV and 10 keV) and at fluences similar to those of interstellar shock waves (10^{16} and 10^{17} cm^{-2}) were used in order to completely amorphize the samples. Thermal processing was performed in a tubular furnace under vacuum at different temperatures. The evolution of the silicate structure was monitored by infrared spectroscopy. Using the 10 μm band evolution with annealing time we have determined the activation energy of crystallization after an irradiation stage [6]. Our result clearly suggests that the presence of crystalline silicates in cold environments can not be explained by a local thermal diffusion process. One can thus invoke the radial mixing between the inner regions of the nebula and the outer cooler and comet-forming regions [7].

The smooth surface of the diamond allows an easy extraction of the film for TEM characterization. Micro-structural analyses are obtained with a Philips CM30 TEM operating at 300 kV and the crystallographic characterization is achieved using selected area electron diffraction (SAED). The microscope is also equipped with an X-ray energy dispersive spectrometer (EDS) for microanalysis. We show the possibility to form spheroid metallic (iron and nickel) nano-particles (2-50 nm) randomly distributed within the silicate films, which are still amorphous after annealing at 870 K even for long time duration (up to 780 hours). The iron initially present in form of FeO has thus segregated from the amorphous phase in the form of metallic globules (Figure1). This clearly suggests that a reduction has occurred according to the reaction $FeO \rightarrow Fe + ½\ O_2$. The obtained microstructures closely resemble those of the GEMS (Glass Embedded with Metal and Sulfides) found in chondritic IDPs (Interplanetary Dust Particles) [8]. Locking iron as metallic particles within the silicates explains first why astronomical silicates always appear observationally Fe-poor. Secondly, these metallic inclusions could explain the dust alignment in the galactic magnetic field. Measurements to determine the magnetic susceptibility of our minute samples are under progress with the goal of understanding the magnetic properties of such small metallic iron inclusions in interstellar grains.

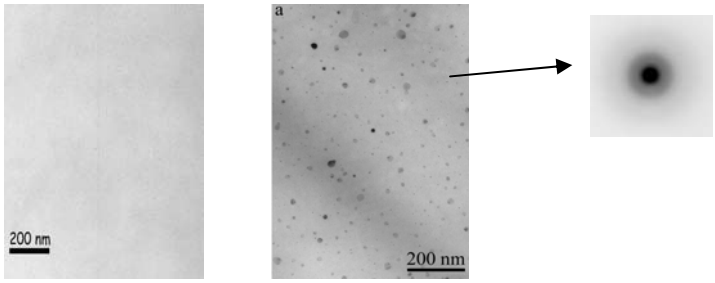

Figure1: TEM micrograph of the sample before (on the left) and after (on the right) annealing at 600°C during ~ 800 hours. Note the presence of inclusions in the heated sample which is still amorphous as showed by the diffraction pattern given on the top right.

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Photo- And Radioracemization Of Chiral Molecules And The Radiation-Induced Amplification Of Chirality

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The biochemistry of the biological world is based on molecules and macromolecules having one or more centers of asymmetry, these molecules are called chiral molecules. Thus, life is strictly linked to the chirality of the molecules and macromolecules. No life can be conceived without chirality because all the complex chemistry and biochemistry, i.e. high selectivity in chemical reactions in living organism, which are the basis of life would be impossible.

A central problem of the research of the origin of life is the origin of chirality. Phenomena like the action of circularly polarized light on racemic mixture of certain molecules have been pointed out as the spontaneous source of chiral excess in an abiotic world. Thus, it is thought that the chiral molecules are formed already in the interstellar medium, in the molecular clouds and then they are incorporated into primitive bodies like comets and meteorites. Experimental evidences are of support to these hypotheses.

However, there are two phenomena which play against the preservation of chirality of asymmetric molecules in space: the photoracemization and the radioracemization. In fact the photolysis and the radiolysis of chiral molecules caused by high energy radiation and by cosmic rays in general cause a reduction in the optical activity. Apparent and true photo- and radioracemization must be distinguished.

An additional problem must be discussed, the fact that the chiral excess produced by spontaneous phenomena like the action of circularly polarized light on racemic mixtures yields only scalemic mixtures with a small enantiomeric excess which is further penalized by the natural photo- and radioracemization phenomena. Therefore, natural amplification mechanisms of chirality should exist in order to be able to increase the enantiomeric excess of scalemic mixtures and make them useful for the emergence of the primordial life.

Very recently we have demonstrated that such mechanism of chiral amplification is offered for examples by the radiopolymerization of chiral monomers which are able to yield products with higher optical activity than the starting monomer.

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Spectroscopy of complex and organic chemistry in Titan.

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Can amino acids be formed during the evolution of molecular cloud?

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Using a reasonably large gas phase chemical reaction network consisting of 421 species and H_2 formation on grain we investigate the formation of simple amino acids like, glycine and alanine. We studied the chemical evolution of molecular clouds during the static and the collapse phase of star formation. These findings may shed light on the present debate on glycine detection in molecular clouds. We found glycine could form in detectable amount in both static and collapsing phase of the molecular cloud. However, we find that β-alanine and propionic acid is not produced in detectable amount in both types of clouds.

Keywords: ISM: molecules, Molecular clouds, Star formation, Chemical evolution, Bio-molecules

Detection of the gaseous disk around the B0 star R Mon

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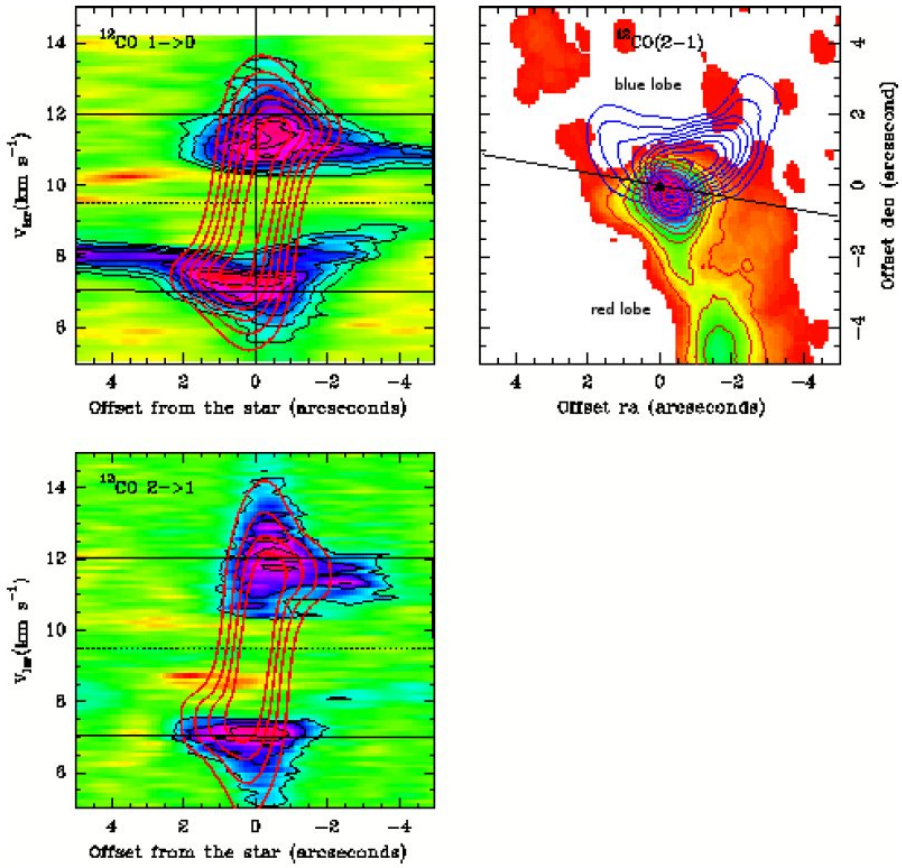
We present high angular resolution observations of the ^{12}CO 1→0 (beam = 2.3" x 1.3") and 2→1 (beam = 1.5" x 0.9") rotational lines. At this scale (1" = 800 AU at the distance of R Mon) the high velocity CO emission has two components: the high velocity gas flowing outwards the star along twisted filaments located in the walls of the nebula cavity, and the circumstellar disk. We have used a plane disk model to fit the ^{12}CO 1→0 and 2→1 emission in a strip perpendicular to the outflow axis and to determine the kinematics of the gaseous disk. The model assumes standard ^{12}CO abundance (X(CO) = $8{\cdot}10^{5}$), radial dependent temperature and density laws (T (K) = $T_o\ r^{-\alpha}$, ρ (cm^{-3})= $\rho_o\ r^{-\beta}$), and Local Thermodinamic Equilibrium. The CO emission is consistent with a plane disk at the inclination angle of 20º in keplerian rotation around the star. The disk is fitted with a mass of 0.01 M_u, an outer radius of 1500 AU, a temperature of 4000 K at the inner radius of 1 UA, and values of α = 0.65 and β = 1.3 for the indexes of the temperature and density laws.

In addition, we present new continuum observations of the region with a beam ~0.72" x 0.33". These observations provide more accurate estimates of the position and size of the dusty disk, which are now settled to RA (2000): 06:39:09.96, DEC(2000): 08:44:09.55, and rout # 150 UA.



Right: Interferometric map in the ^{12}CO 2-1 line of the red (v < 7 km/s) and blue (v > 12 km/s) lobes of the outflow associated with the B0 star R Mon. A strip perpendicular to the outflow is drawn in this panel. Left: PositionVelocity (P-V) diagrams of the emission of the ^{12}CO 1-0 and 2-1 lines along the strip drawn in the top panel. These P-V diagrams are consistent with the existence of a disk in keplerian rotation around the star. We have overlaid in red contours the results obtained with our disk model. Note that the emission at the velocities of the molecular cloud (9.5 ± 2.5 km/s) has been filtered out by the interferometric observations.

The Far-Infrared Fourier Transform Emission Spectrum of HCN

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The rotational emission spectrum of hydrogen cyanide has been recorded by means of a high resolution Fourier transform spectrometer. Excited HCN was created in a low pressure N_2/C_2H_4 mixture flowing through a radio-frequency discharge. The spectrum covers the far-infrared spectral range 26-180 cm^{-1} (0.8-5.4 THz). No lines of HNC have been clearly identified. All the rotational lines of HCN assigned in the spectrum belong to its 15 lowest vibrational states. The highest observed state, namely (050), has been studied for the first time by rotational spectroscopy. It is perturbed by (021) through Coriolis interaction. Three vibration-rotation lines of the band (050) – (021) are identified in the spectrum in the range 76-80 cm^{-1} where the Coriolis interaction reach a maximum for J = 26. These lines have been found to produce laser emissions from electric discharges in compounds of hydrogen, carbon and nitrogen (1). A similar situation occurs at lower frequency (at about 30 cm^{-1}) between (040) and (011) and has been studied in a previous submillimeter-wave spectroscopy work (2). Strong maser emission have been detected between (040) and (011) at 805 and 891 GHz by Schilke et al. (3) and Schilke and Menten (4) respectively.

We have deduced molecular constants for the 15 lowest vibrational levels of HCN by combining our measurements with those reported in (2). They show a very good agreement with the results obtained from high resolution infrared emission spectroscopy (5). We hope they will help in the identification of highly excited HCN in the far infrared region.

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Complex reaction networks on dust grains in dense molecular clouds

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There are strong indications that networks of chemical reactions on dust grains play an important role in the production of molecules such as methanol and its deuterated versions in molecular clouds [1]. Due to the small size of the grains and the low flux, the populations of adsorbed atomic and molecular species are small and exhibit large fluctuations. As a result, rate equations are not suitable for the simulation of reaction networks on grains, which requires stochastic methods such as Monte Carlo simulations or direct integration of the master equation. An important advantage of the master equation is that it consists of differential equations which can be easily coupled to the rate equations of interstellar gas-phase chemistry. However, the number of equations proliferates making the master equation infeasible for complex reaction networks. Here we present two methods which provide a dramatic reduction in the number of equations. The multi-plane method maintains the structure of the master equation, but dramatically reduces the number of equations [2]. In the second method, based on moment equations, the number of equations if further reduced making it feasible to incorporate stochastic modelling of grain-surface reaction networks into models of interstellar chemistry.

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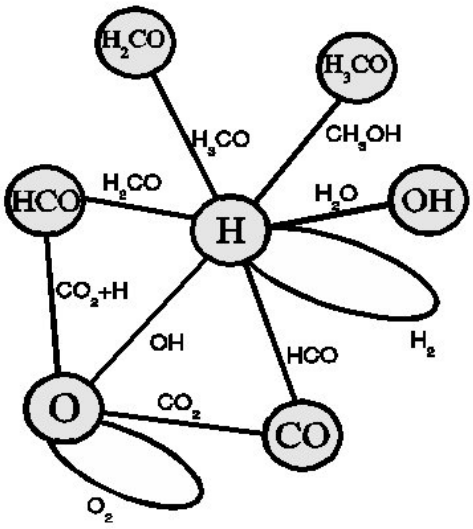
A graph describing the surface reaction network that produces methanol. The reactive species are shown in the nodes. Species that react with each other are connected by an edge. The reaction products are specified near the edges.



A 80 - 370 GHz Unbiased Spectral Survey of the Solar-Type protostar IRAS 16293-2422

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Unbiased line surveys are a unique way to determine the molecular content of astrophysical objects. They allow a complete study of the physics and chemistry in and around molecular sources. Among all class "0" solar-type protostars observed to date, IRAS16293-2422 has the richest line spectrum. It is the first one where several complex molecules have been observed (Cazaux et al. 2003) a well as many deuterated molecules (D2CO, Ceccarelli et al. 1998 and doubly and triply deuterated methanol, Parise et al. 2002, 2004). Ceccarelli et al. 1998 and Shoier et al. 2002 have shown that the structure of the IRAS16293 collapsing envelope has a inner hot corino ($r < 150$ AU) where the temperature exceeds 100 K and a colder outer envelope. This spatial structure is responsible for the abundance jumps for several molecules.

Due to its high temperature and density, this hot corino is responsible for the richness of the IRAS16293 spectrum. This richness comes also from the molecular content of the source itself, due both to the release of molecules trapped in icy mantles by the elevated temperatures, and to gas phase chemical reactions which can proceed faster at high density. High temperatures open many chemical pathways which, because they are endothermic, are closed at lower temperatures. We present here preliminary results of this 80 - 370 GHz unbiased spectral line survey.

IRAS16293 has a very rich molecular spectrum (~20 lines / GHz), regardless of the frequency. The total number of lines expected is a few thousand that constrained us to develop a specific software to handle these data (CASSIS, see the poster from A. Walters et al., this conference), One can note the presence of many lines originating from various molecules including complex and deuterated molecules. The line identification of the whole survey is in progress, and we plan to make public the line database by April 2007.

This kind of broad and unbiased survey is mandatory to obtain acceptable accuracy on the physical parameters. For most species, we will first derive the physical parameters (Tex and column density) from rotational diagrams. Species for which collisionnal coefficients are known will be analysed using more sophisticated models (LVG…), as done for the emission of HDO in IRAS16293 from this survey (Parise et al. 2005). A complete census of the molecular content of IRAS16293 will be built, and the detailed modelling of the chemistry governing its hot core and envelope will allow the comparison with massive hot core regions and will put stringent constraints on chemical models.

Monte Carlo Simulation of the Production of Hydrogen Molecules on Grain Surfaces

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Majority of the observed hydrogen molecules in the interstellar medium are formed on the grain surfaces. Dust grains are essential for the formation of the hydrogen molecule. On the grain surfaces, two H atoms combine to form a single hydrogen molecule. So far, the average recombination time to produce a hydrogen molecule used to be computed by a crude assumption about the diffusion of the H atom on a grain surface. Here, we perform a Monte-Carlo simulation to exactly quantify how the diffusion actually takes place. This enables us to calculate the average recombination time for the formation of hydrogen molecules. We find that the production rate of the hydrogen molecules on the grain surfaces is highly dependent on the grain size and the accretion rate. This is a very important conclusion in the context of the grain chemistry and it will affect the molecular abundances of hydrogen, and many complex molecules in the evolving cloud. We perform our calculations on two types of grain surfaces namely, on the amorphous carbon and the Olivine grain surfaces for a wide variety of grain parameters.

Time evolution of the Complex molecule formation in collapsing interstellar cloud

Sandip K. Chakrabarti, A. Das, K. Acharyya and S. Chakrabarti

S.N. Bose National Centre for Basic Sciences (AA) Centre for Space Physics (AA,AB, AC, AD)

We study the time evolution of the interstellar cloud and find how the density and velocity profiles evolve. With this hydrodynamics, we couple chemical evolution consisting of a large network of species and reaction cross-sections. For molecular hydrogen formation we utilise the grain chemistry by master equation or rate equation depending on the accretion rates. We also present Monte-Carlo simulation to show that the way the H2 molecular hydrogen formation is handled in the literature is seriously flawed. This is because we find that the effective recombination time of atomic hydrogens depend on the relative size of the grain and the accretion rate of the atomic hydrogen. We show how the chemical composition of the cloud evolves with time for various cloud and grain parameters.

Time dependent chemical evolution of molecular cloud

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More than 125 species of molecules have been observed in the interstellar clouds and star forming regions. Among them over half are organic. In the present work, we try to explain the observational abundances. We develop a time-dependent hydro-dynamic code which determines the hydrodynamic evolution of the molecular cloud. Using the output of this code, we study the chemical evolution of this molecular cloud with time. In the chemical evolution, we incorporate the grain chemistry to accurately determine the abundance of H_2. We compare our results with observations.

Disentangling the structure of intermediate mass hot cores at scales of ~200 AU

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[2]LAOG, BP 53, F38041 Grenoble Cedex 9, France
[3]IRAM, 300 Rue de la Piscine, Domaine Universitaire, F38406 St. Martin d'Hères, France
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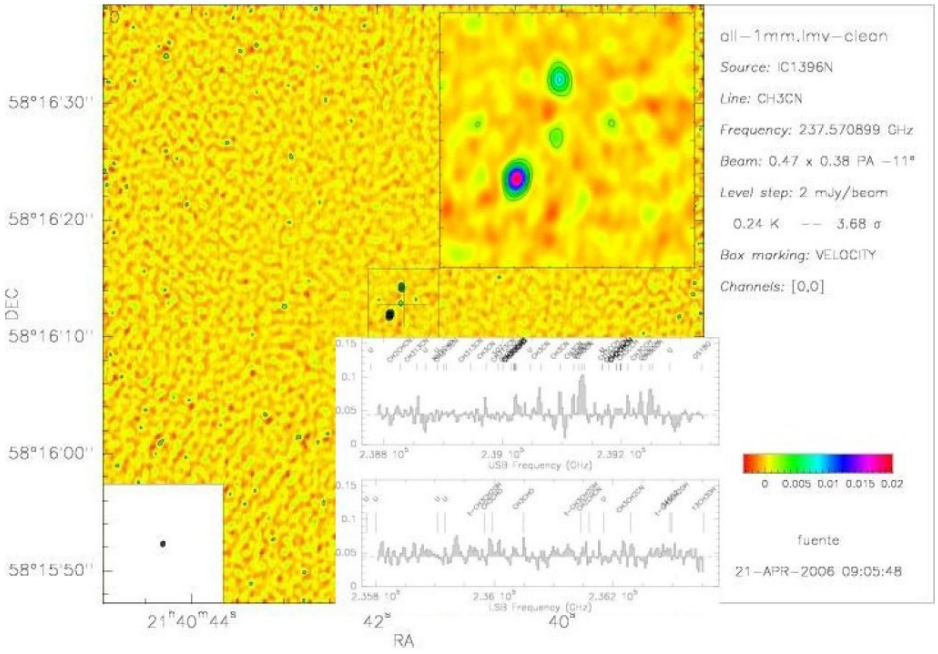
Hot cores are objects characterized by warm temperatures (T > 100 K), high density (n > 106 cm^3), and a very rich chemistry in complex molecules (CH_3OH, CH_3CN, CH_3CHOOH, CH_3OCH_3 ...). Hot cores have been thought to be associated with highmass protostars (M > 10 M_u) and represent an important phase in their evolution towards ultracompact and compact HII regions. Only recently, regions similar to hot cores have been detected in lowmass protostars. However, the amount of warm material involved, as well as the chemistry, are different in the two classes of objects and rise questions on the mechanisms that lead to the observed chemical complexity (Cazaux et al. 2003, ApJL 593, L51; Fuente et al., 2005, A&A 444, 481). The study of hot cores in intermediate mass protostars (M_* ~ 2-10 M_u) will provide an important clue to solve this problem. We have successfully searched for intermediate mass (IM) hot cores using the IRAM 30m telescope. In addition we have mapped four of these objects, IC1396 N, OMC2FIR4, CB 3, and Serpens-FIRS 1, using the new A+ configuration of the Plateau de Bure Interferometer. This configuration provides an angular resolution of ~ 0.2" which implies a spatial resolution of < 200 AU at the distance of these IM hot cores. This high angular resolution allows us to measure with unprecedented accuracy the position, sizes and spectral indexes of these hot cores. Furthermore, these observations reveal the existence of a "cluster" of hot cores in the interior of IC 1396 N and CB 3. Simultaneously with the continuum observations we have mapped the region in the CH_3CN 13k→12k line and some complex Obearing molecules. Since the interferometric observations resolve for the first time the different components of the cluster, we are able to have a first glance at the chemical differentiation between them.



Continuum image at 1 mm of the Class 0 protostar IC 1396 N. A zoom in the central region is shown in the inset. Note that there is a cluster of 3 hot cores in the interior of this protostar. The spectrum towards the most massive component of the cluster is also shown.

Turbulence, star formation and the need for high spatial resolution

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[2] NORDITA, Blegdamsvej 17, 2100 Copenhagen Ø, Denmark
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Theories about the influence of turbulence on star formation need to be constrained by observations. Important issues such as the driving mechanism, the effect of re-injection of energy by protostellar outflows, the effect of self-gravity and the dissipation mechanism can only be settled by observations and simulations ability to reproduce the observations.

In order to assess the dissipation scale, conventionally the scale at which bulk energy is converted into heat, as well as the scales of low mass star formation it is essential to obtain maps with as high spatial resolution as possible.

We use infrared observations of shock-excited H_2 at 2.12 micron to characterise the velocity field in the star-forming region OMC1 at scales from 70 AU to 30000 AU. The results generally follow the trends observed at larger scales from radio observations tracing the cold, bulk gas. Hereby the validity of the "Larson Law" is extended by two orders of magnitude in scale. However the structure functions show the presence of preferred scales in the medium. These scales can possibly be associated with outflows from low mass protostars and are also the correct scale for disks around protostars. We compare the observations with subsets of simulations of (non-magnetic) hydrodynamical turbulence, which are forced at large scales and without self-gravity. To represent best the observations the selected subsets include only the shocked part of the simulations. The simulations are unable to reproduce the preferred scales found in the observations.

Performing structure analysis using data of warm H_2 has the intrinsic caveat that only shocked gas is observed. With ALMA it will be possible to map for example CO and trace the cold gas with as high or higher spatial resolution as in the exciting infrared data, thus making it possible to reach the dissipation scale of turbulence.

Modelling water in the envelopes of low-mass protostars

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Water is one of the key molecules in the early stages of star formation, especially in the warm inner region of newly formed protostars, where ice mantles are evaporated from grains. In addition water is the basis of oxygen driven chemistry and essential for the creation of more complex molecules. The launch of the Herschel Space Observatory and the coming of ALMA will provide the opportunity to study gas-phase water in detail in YSOs at high sensitivity and resolution. The HIFI spectrometer on-board Herschel with a spectral resolution of $\lambda/\Delta\lambda = 10^7$ is especially suited to observe gas-phase rotational lines over a wide range of excitation conditions. ALMA provides the single most powerful probe into the warm inner region of circumstellar envelopes, which span ~tens of AU. Many isotopologues of water such as HDO and many complex molecules associated with water are also confined to these warm regions of the envelopes characteristic of Class 0 and Class I sources.

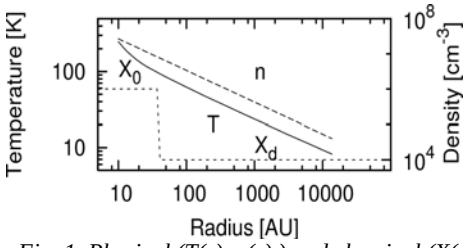

Fig. 1. Physical (T(r), n(r)) and chemical (X(r)) structure of a typical protostellar

We present here the first results of a parameter study on the role of water in YSOs, focussing on low-mass Class 0 and Class I protostars (Lada 1987, André et al, 1993) using the radiative transfer code RATRAN (Hogerheijde & van der Tak, 2002). The study was done in collaboration with a similar study on high-mass stars (Doty et al, 2006 in prep). Several parameters were investigated that influence the behaviour of water. The luminosity, *L*, of a protostar, which depends on both age and initial mass, determines the local temperatures throughout the envelope and is thus responsible for the spatial extend of the warm inner core, where water is abundant due to evaporation of the grain mantles. Second, the density of the envelope varies between different young protostars (Jørgensen et al, 2002), both in the density at a set radius, *n*, as well as the radial density gradient, α. In general it is seen that older protostars, such as Class I have steeper density (~2) gradients, then Class 0 (~ 1.5) and larger warm inner regions. Third, not much is known about the abundance of water relative to H_2, both in regions where water is abundant (T>100 K) and where it is frozen out onto the grains (T<100K). See Fig. 1 for an overview of the structure of circumstellar envelopes.

The goal is to constrain H_2O abundances for different models and provide accurate models that ALMA can probe. Our first result show that many lines for water are observable for typical low-mass protostars, but that a thorough understanding of the physical characteristics of each individual protostar is essential in understanding any modelled or observed flux of a given water line. Figures 2 and 3 show the ground state (557 GHz) and the 2_{21}-2_{12} excited state (1661 GHz) lines of ortho-water. One can clearly see that for a given luminosity (L = 2 L) and density distribution, the abundance of gaseous water influences the two lines differently. The ground state line traces the amount of gaseous cold water, that is not frozen out onto grains in the outer regions due to cosmic rays and interstellar radiation heating. Previous observations (Boonman et al., 2002) estimate this abundance at 10^{-6} - 10^{-8} with respect to . H_2. The excited state traces the inner warm region, but is still influenced by the cold water. Typical temperatures are 0.5-2 K km s^{-1} for the ground state and 0.1-3 K km s^{-1}, which shows the large dependency of water on the abundance.

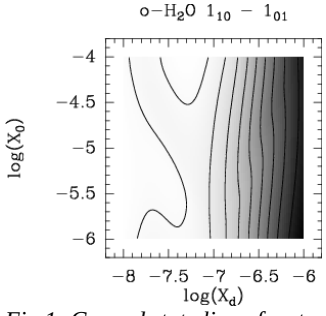

Fig.1: Ground state line of water for different abundances in warm region (X_0) and cold region (X_d) in integrated line fluxes (K)

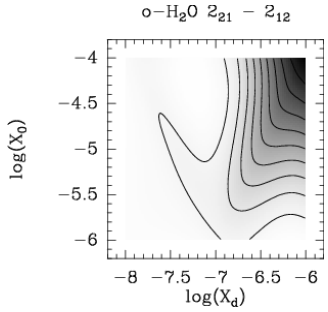

Fig. 2:Excited line of water for different abundances. Note the dependence on both cold and warm gaseous water

In a future publication (van Kempen et al., 2006, in prep) we present the results of a large parameter study on the emission of gas-phase rotational water lines, including the dependency of water on the luminosity of the protostar as well as the density distribution of the envelope. We conclude that an extensive knowledge about the local conditions of YSOs as well as a detailed modelling approach like we used, is essential in interpreting the future Herschel observations of water. ALMA will play an essential role in such observations if one wants to understand the role of water in the warm inner region. The resolution and wavelength coverage of ALMA will provide an excellent probe into these region with high-excited CO and water, providing strict constraints on the oxygen content and x-ray luminosity inside the high temperature regions of these protostellar systems.

Deuterared chemistry on amorphous water ice surfaces in the ISM

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We have shown (F. Dulieu et al talk and additional "Interaction of molecular hydrogen with Amorphous Water Ice Surfaces (ASW)" poster) that when both H_2 and D_2 are deposited at 10K on a 10ML amorphous water ice film, D_2 is occupying the more bound sites. When the temperature of the film increases, during a TPD (thermally programmed desorption) experiment, H_2 desorbs first leading then to a subsequent enrichment of the ice film in D_2. Such a situation may occur in some cold dense regions of the ISM at the surface of water ice covered interstellar grains, during the long pre-collapse stage of the star formation process, then favouring a deuterated chemistry to take place. At a later stage, when the temperature increases again, the resulting deuterated molecules are then released in the gas phase and become observable. IRAS16293-2422 (ρ Ophiucus star forming region) is an example of such regions where deuterated species appear to be 10^3 to 10^4 times more abundant than the average galactic ratio.

Evaluation of spectral data for radioastronomy, Herschel and ALMA. Contribution to the improvement of this data.

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Two spectroscopic databases are freely available through Internet and commonly used for radioastronomy, that of Cologne University (CDMS) and that of JPL. For CASSIS software (http://www.cesr.fr/~walters/web_cassis/) (which can be freely downloaded at http://pc-126.cesr.fr/ for prediction and analysis of astrophysical spectra from radiotelescopes) both of theses databases are combined for user-friendliness. In certain cases the same species may be found in both of these databases. We have hence carried out a rapid evaluation of these two databases (http://www.cesr.fr/~walters/web_cassis/Divers/Molec_tab.pdf) for astrophysical species and suggest a preference when necessary. This evaluation is gradually being improved and refined for priority species for which alternative data sources may be suggested. It will be used to provide templates with suggested database entries for CASSIS.

We have also started to contribute to the improvement in data available, especially in the new spectral region above 1 THz to be opened by Herschel and partially by terrestrial instruments in very good weather conditions. Measurements have recently been taken at JPL of the following species: HCO^+, DCO^+, $H^{13}CO^+$, $D^{13}CO^+$, CH_3D, CH_3CN, propane, HCCD and rovibrational transitions of DCCD.

Some examples of ongoing analysis will be given. In certain cases of species already measured at lower frequency, the data can be shifted by up to 100 MHz compared to earlier predictions. This shift is obviously very important for correctly identifying lines. Even small shifts of the order of a MHz can be important when accurate velocity information is to be obtained from the lineshape and Doppler shift.

Velocities of gas in star-forming regions: 70AU resolution and 1km/s results for OMC1.

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The Orion Molecular Cloud (OMC1) (D = 460 pc) is the closest highly active massive star-forming region. It has accordingly been studied over a large range of wavelengths from the X-ray to the radio (e.g. [1-6]) and has become a type-site for studies of star formation. We report IR H_2 v=1- 0 S(1) data for this region.

The data were obtained with the GriF instrument on the CHFT (see [7,8]). The novelty of these data is in the association of a high spatial resolution of 0.15" (70 AU) with velocity discrimination as good as 1 kms^{-1} (3♦). Results show striking evidence for the presence of shocks within OMC1 through the clear association of gas motions of tens of kms^{-1} with bright IR emission of H_2.

The study of 193 bright regions affords a detailed view of shocks within OMC1. Many new features are revealed, providing a new perspective on the nature of OMC1. Data are visualized in Fig. 3 in the poster.
The major conclusions of this study may be summarised as follows:
(i) 193 distinct bright H_2 emission features have been identified. 2/3 of these show clear radial velocity structure with well defined features of greater than 5 kms^{-1}, indicating that the emission is generated by shocks.
(ii) There are equal numbers of shocks in Peaks 1 and 2, implying a greater concentration of activity in Peak 2 which is less than half the size of Peak 1. Flows are found to be grouped more tightly in Peak 2. Blue-shifted flows are somewhat favoured over red-shifted, presumably due to dust obscuration. No velocities exceed 35-40 kms^{-1}, consistent with upper limits for C-type shocks in dense media.
(iii) In a distinct zone, lying south of Peak 1 and west of Peak 2, all flows are blue-shifted, with an average velocity of -18 ± 8 kms^{-1}, suggesting a collective outflow motion in this area.
(iv) Spatial correlation between maximum brightness of H_2 emission and maximum velocity reveals deviations typically of ≤ 0.5". These deviations are used to estimate the orientation angle of shocks, in the plane of the sky - but not their absolute direction. Orientations are found to be random in Peak 2 and with some preference for a NW direction in Peak 1, but show a strong preference for a NE-SW orientation in the outflow region (iii).
(v) In [8] it was noted that potential low mass star forming zones, identified through the presence of energetic flows in OMC1, showed higher densities and correspondingly higher energy flux, and are altogether less simply structured than more conventional Class 0 or 1 low mass isolated star formation regions. Here we identify a number of zones which show similar characteristics to those discussed in [8]. Data point in particular to the close physical association of numerous H_2 emission features. These associations may represent sites of multiple star formation characterised by episodic outbursts of activity.
(vi) The most striking feature is the blue-shifted outflow (iii). This is the IR counterpart to an outflow observed previously only in the radio [1,9]. The radio data show the presence of a flow, part of a general expansion, with a velocity of 18 ± 6 kms^{-1} in agreement with our value of 18 ± 8 kms^{-1}. The origin of this outflow is uncertain; candidates are the massive radio sources I and n [10]. Both are situated near the origin of the blue-shifted outflow, and both have shown evidence of outflow along a NE-SW axis in radio observations [11,12].
(vii) There is a remarkable feature in the H_2 emission data with strong velocity components, which, on the basis of a VLT image, is strongly suggestive of a region in which a blue-shifted flow has burst from behind, from source I, through the material of OMC1 sending shock waves through the medium. The axis of the outflow passes right through this object.

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Alcohol Chemistry In The Galactic Center. Hot Core Chemistry Without Hot Cores.

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We have carried out a systematic study of CH_3OH, C_2H_5OH, $(CH_3)_2O$, $HCOOCH_3$, HCOOH, CH_3COOH, H_2CO and CS in different Galactic center (GC) clouds. The abundance of CH_3OH ranges from few 10^{-8} to 10^{-6} (see fig. 1). While the abundance ratio of the molecules relative to CH_3OH is basically independent of the CH_3OH abundance and only varies in a factor of ~4-8, the abundance ratio of CS to CH_3OH, not affected by grain chemistry, varies by a factor of 60. Our data are compared with observations of the same molecules in short-lived objects like the hot cores. The abundance and the abundance ratios of the complex molecules relative to CH_3OH in massive hot cores are similar to that found in the GC clouds. Alcohol chemistry is believed to be driven by gas phase reactions after evaporation of alcohols from grain mantles. Gas phase chemistry after ejection of alcohol from grains cannot explain the observed abundances and relative abundances of some molecules. Our data suggest that basically all the molecules related to alcohol chemistry could be produced on grain mantles and/or depleted from gas phase after their formation. This interpretation requires frequent shocks in the GC region to keep the high abundances of these molecules in gas phase and a rather uniform average composition of the icy grain mantles. The molecular clouds associated with the Sickle and the Thermal Radio Archers, which seem to be affected by UV radiation show lower abundances of C_2H_5OH relative to CH_3OH which could be explained by the combination shock ejection and photo dissociation.

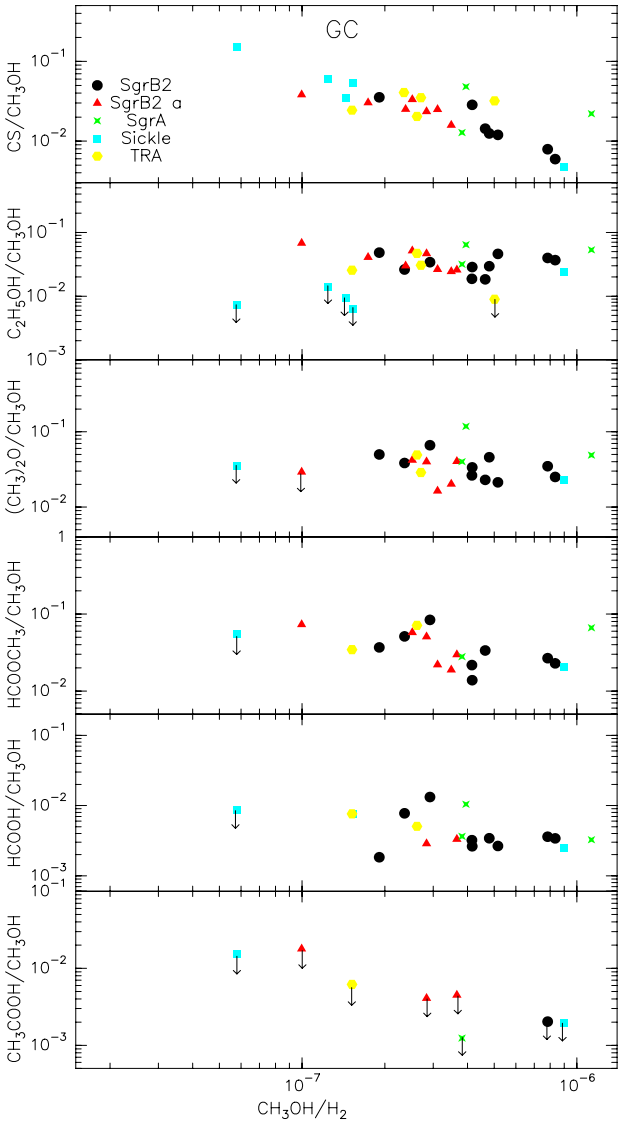

Figure 1: Relative abundances of the observed molecules respect to that of CH_3OH as a function of the CH_3OH abundances.

Radiative lifetimes and association cross-sections of CO^{2+}

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Despite the fact, all vibronic states of a dication are only metastable because of electrostatic repulsion, there are a couple of experimental measurements and also possibilities that these species could exist for a long time in the interstellar matter. As for CO^{2+} most of the lower electronic states have minima which are capable of supporting vibrational levels. Moreover, the levels that are trapped behind the barrier would classically be considered stable, but at the same time they lie in a continuum and so can lead to formation of the dication by radiative association.

This study is aimed to determinate the radiative lifetimes of vibrational levels in three lowest electronic states $^3\Pi$, $^1\Sigma^+$ and $^1\Pi$ and energy-dependent radiative association cross-section for the reaction $C^+(^2\Pi_u) + O^+(^4\Sigma_u)$. The calculations are preformed on the highly correlated icMRCI wavefunctions. These function have been used to calculate the potential energy (PE), spin-orbit coupling (SOC), dipole moment and transition moment functions for the lowest electronic states of CO^{2+} dication. Using PE and SOC functions, the positions and lifetimes of the corresponding vibronic states are evaluated by means of the complex coordinate method. Although, there are not many experimental results with which a comparison is possible, the calculated predissociating lifetimes are in qualitative accord with them.

Radiative lifetimes to v = 0 in terms of each one electronic state are shorter then predissociating lifetimes. So that the formation through radiative association is possible. As for radiative association cross-section, in spite of the transition dipole moment between singlet-triplet is spin-forbidden, singlet and triplet states in the {*ab initio*} calculations are not eigenstates of this CO^{2+} Hamiltonian. Transitions from $^1\Sigma^+$ and $^1\Pi$ to $X^3\Pi$ state occur because of mixing of states due to the spin-orbit of electronic states.

Reliability of the disk chemical modeling

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We study how uncertainties of the rate coefficients of chemical reactions in the UMIST\,95 database affect the modelled molecular abundances in a protoplanetary disk around a low-mass star. For that, we randomly varied the gas-phase reaction rates within their uncertainty limits and calculated sets of time-dependent abundances in several representative disk locations, using a gas-grain chemical model supplied with a set of surface reactions. All species are separated in different groups according to the sensitivity of their final abundances to the rate uncertainties. We found that such division depends on the disk location, since distinct processes control the chemical evolution of various disk regions. Typically, the modelled abundances of simple species are imprecise up to a half order of magnitude, and in general increase with the number of atoms in the molecule. We apply a straightforward sensitivity method introduced in [1] to analyze the correlations between the time-dependent abundances and varied rate values in order to identify those reactions whose rate uncertainties affect the resulting concentrations of the pre-selected, observationally important species to the largest extent. It is demonstrated that the rate coefficients of only a handful of chemical reactions need to be determined more accurately in order to improve significantly the reliability of disk astrochemical models, which might be a task for future laboratory studies and theoretical investigations.

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Rotational excitation of interstellar cyanoacetylene

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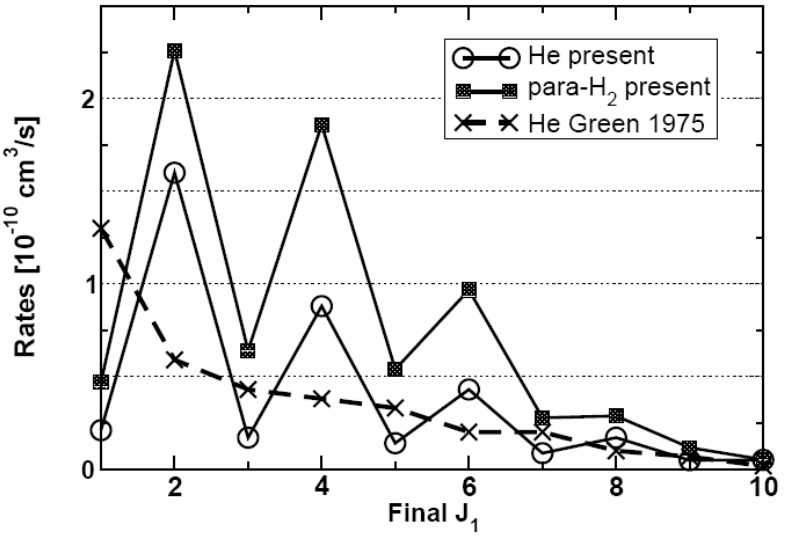
Cyanoacetylene (HC_3N), the simplest cyanopolyyne, is ubiquitous in space and is generally considered as an ideal probe of physical conditions in a variety of astronomical environments. We have computed rate coefficients for rotational excitation of HC_3N (J=0-50) by He and H_2 for kinetic temperatures lower than 100K. These rates have been obtained from extensive quantum and quasi-classical calculations using new high accuracy potential energy surfaces (PES). The symmetry of the PES is shown to induce strong collisional selection rules. As a first application, we present a simple steady-state population model that shows population inversions for the lowest HC_3N rotational sub-levels at H_2 densities in the range ~10^3–10^5 cm^{-3}.



Rate coefficients for rotational excitation of HC_3N (initial J_1=0) by H_2 and He as a function of the final J_1 for a kinetic temperature of 20K. The quasi-classical results of Green & Chapman (1978) are compared to the present quantum calculations. The strong quantum interferences reflect the quasi-symmetry of the potential energy surfaces.

Planet Formation - Traced with ALMA

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Planets are expected to form in circumstellar disks, which are considered as the natural outcome of the protostellar evolution, at least in the case of low and medium mass stars. While a detailed picture of the evolution of the circumstellar environment, in particular of protoplanetary disks, has been developed, the planet formation process is still under discussion. Adequate constraints from observations are required in order to either verify or rule out existing hypotheses about proposed planet formation scenarios.

Numerical simulations convincingly demonstrate that high-resolution imaging performed with observational facilities that are already available or will become available in the near future will allow to trace the formation and early evolution of planets in circumstellar disks. Theoretical investigations show that the signatures of planet formation are usually much larger in size than the planet itself and thus more easily detectable. The specific result of the planet-disk interaction depends on the evolutionary stage of the disk. Primary signatures of planets embedded in disks are gaps in the case of young disks and characteristic asymmetric density patterns in more evolved debris disks.

Based on the example of the Butterfly star in the star-forming Taurus region, it will be discussed how observations with the Submillimeter Array (SMA) now or with the Atacama Large Millimeter Array (ALMA) in the near future can be used not only to constrain the global disk structure but also to characterize the process of the grain growth, which is indicative for the earliest stage of planet formation. Furthermore, simulations concerning the observation of disk structures tracing the formation of planets, such as large-scale vortices, spiral density waves, gaps, and inner holes, will be outlined. For the late stages of giant planet formation, we will discuss the numerical simulations which demonstrate that ALMA will even allow to trace young giant planets in nearby protoplanetary disks (see Fig. 1). Furthermore, we will show that molecular line observations of planet formation signatures with ALMA will allow us to study in detail the kinematics of gas and gas-to-dust ratio across the discussed features.

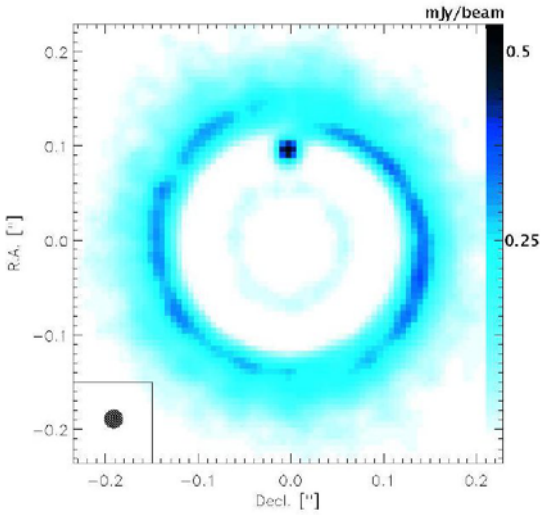

Figure 1: Simulation of ALMA observations of a disk with an embedded giant planet around a 0:5M_{sun} star (orbital radius: 5AU; assumed distance: 50 pc). The hot local environment of the 1M_{jup} planet is clearly seen as a bright region in the upper part of the low-density gap caused by the planet-disk-interaction. The disk mass amounts to M_{disk} = 1.0 H 10^{-2} $M_{sun.}$ The size of the combined beam is symbolized in the lower left corner. *[based on Wolf & D'Angelo (2005) ApJ, 619, 1114]*

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