Astrochemistry
and its uses in astronomy

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Extraterrestrische Physik

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ISSI workshop
Introduction

• Is interstellar chemistry useful? (Dalgarno 1986)
• Purpose of this talk: show that answer to this question is indeed YES!
• Molecular astrophysics forms an integral part in understanding formation of galaxies, stars, planets and perhaps even prebiotic material
• Illustrate here with a few examples
Where do we find molecules?

Orion
HST image
Horsehead nebula
Dark clouds: sites of star formation

Mass of cloud can be as large as $10^4 - 10^6 \, M_\odot$

1 l yr
Dark clouds: ‘coal sacks’

- 99% gas (H₂)
  1% dust (0.1 μm silicates+carbonaceous)
- Temperature: ~10 K
- Density: ~10⁴ particles per cubic cm

Unique chemical laboratory!
How do we study what is happening inside clouds?

Optical

Infrared

Long wavelengths!

Alves et al. 2001
From visible to infrared light

HH 46 star-forming region
Types of clouds

- **Diffuse and translucent clouds**
  - Observed primarily by absorption lines at visible (since 1900’s) and UV wavelengths (since 1970’s)

- **PDRs**
  - Dense clouds exposed to intense UV radiation, typically at least 100x average interstellar radiation field
  - Observed by far-infrared and submm emission lines

- **Cold dark clouds**
  - Observed by mm emission lines

- **Warm star-forming regions/hot cores**
  - Observed by submm/mm emission lines
  - IR absorption for ices

- **Shocks**
  - Observed by IR and submm/mm emission

- **Circumstellar shells evolved stars**
- **Protoplanetary disks**
- **Comets, planetary atmospheres**
  \[ T \sim 8-2000 \text{ K}, \ n(\text{H}_2) \sim 10^2-10^{13} \text{ cm}^{-3} \]
  \[ I_{\text{UV}} \sim 0.2-10^7 \]
NGC 1333 outflows

Q: effects of outflows, jets, shocks on chemistry?

Ha, [SII]
Walawender, Bally, Reipurth 2006
Spitzer/IRAC
Jørgensen et al. 2006
## Ingredients of clouds

<table>
<thead>
<tr>
<th>Element</th>
<th>Abundance</th>
<th>Element</th>
<th>Abundance</th>
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</thead>
<tbody>
<tr>
<td>H</td>
<td>1.00</td>
<td>Mg</td>
<td>4.2×10⁻⁵</td>
</tr>
<tr>
<td>He</td>
<td>0.075</td>
<td>Al</td>
<td>3.1×10⁻⁶</td>
</tr>
<tr>
<td>C</td>
<td>2.5×10⁻⁴</td>
<td>Si</td>
<td>4.3×10⁻⁵</td>
</tr>
<tr>
<td>N</td>
<td>6.3×10⁻⁵</td>
<td>S</td>
<td>1.7×10⁻⁵</td>
</tr>
<tr>
<td>O</td>
<td>4.5×10⁻⁴</td>
<td>Ca</td>
<td>2.2×10⁻⁶</td>
</tr>
<tr>
<td>Na</td>
<td>2.1×10⁻⁶</td>
<td>Fe</td>
<td>4.3×10⁻⁵</td>
</tr>
</tbody>
</table>

Note: abundances of C,N,O recently revised downward by almost factor of 2; other elements TBD
Approach

Observations + Instrumentation ↔ Laboratory

Models

\[ C^+ \rightarrow C \rightarrow CO \]
Submillimeter telescopes

JCMT 15m, Mauna Kea, Hawaii

CSO 10m

APEX, Chajnantor

IRAM 30m, Nobeyama

Pico Valeta, Spain
Infrared telescopes

Very Large Telescope, ESO, Paranal
Space observatories

ISO

Large part of infrared and submm blocked by atmosphere (i.p. H$_2$O, O$_2$ and CO$_2$)

Spitzer

SWAS/ODIN
Orion line surveys

Tercero & Cernicharo 2007
Blake, Sutton et al. 1985
Schilke, Comito et al. 1993, 1997
....
Orion line surveys

1 mm
1980’s

1990’s

Frequency (MHz)
Orion line surveys
Q: how far does chemical complexity go? Prebiotic molecules?
**Inventory of gas-phase molecules**

<table>
<thead>
<tr>
<th>Number of Atoms</th>
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<tbody>
<tr>
<td>2</td>
</tr>
<tr>
<td>-----</td>
</tr>
<tr>
<td>H2</td>
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<tr>
<td>AIF</td>
</tr>
<tr>
<td>AICI</td>
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<tr>
<td>C2</td>
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<td>CH</td>
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<td>CH+</td>
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<td>CN</td>
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<td>SO+</td>
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<tr>
<td>SiN</td>
</tr>
<tr>
<td>SiO</td>
</tr>
<tr>
<td>SiS</td>
</tr>
<tr>
<td>CS</td>
</tr>
</tbody>
</table>

- Abundances vary from $10^{-4}$ to $10^{-11}$ w.r.t. $H_2$
- Abundances vary from region to region
Some recent detections

Negative ions

Propene in TMC-1

McCarthy et al. 2006

Marcelino et al. 2007
Importance of molecules

- Molecules as physical diagnostics of temperature, density, mass, velocity, redshift, star-formation activity, ...
- Molecules as chemical diagnostics of ionization rate, temperature (history), evolutionary state protostars, ...
- Astrochemical evolution clouds => planets
- Molecules as coolants
- Basic chemistry under exotic conditions

\[
\text{CO (J=0)} \xrightarrow{\text{Collisions}} \text{CO (J=1)} \xrightarrow{\text{Radiation}} \text{CO (J=0)}
\]
Molecules as physical diagnostics

Pure rotational transitions

Higher transitions probe higher temperatures and densities
Derivation of abundances

Abundance can vary with position in cloud
Molecules as probe of star- and galaxy formation at high redshifts

From $z \sim 0$ to $z \sim 5$

in just 5 years

CO at $z = 2$

FIR background

SCUBA sources

(Eisenhardt et al. 1996)

(Guiderdoni et al. 1999)

(Hughes et al. 1998)

P. Shaver
Molecular astrophysics started shortly after Big Bang
- Dust and molecules are tracers of mass, dynamics, T, star formation activity of earliest galaxies
[C II] detection at $z=6.4$!

- [C II] will be primary probe of $z>7$ galaxies, when bright CO lines have shifted out of ALMA frequency range
- Luminosity 0.1-1% of $L_{\text{FIR}}$

Maiolino et al. 2005

Rest wavelength 157 $\mu$m
Ubiquitous PAH emission

- PAH’s dominate mid-IR spectra => redshift indicators
- PAH emission requires UV for excitation => diagnostic starburst vs. AGN

Allamandola, Tielens et al.
Léger, Puget
Role of molecular clouds in galaxy

Winnewisser et al. 1984
Detection of exoplanets: renewed interest in lifecycle of gas and dust

Based on Ehrenfreund & Charnley 2000

R.Ruiterkamp 2001
Cold cores: heavy freeze-out

Optical

Submm continuum => cold dust

More than 90% of all molecules except most volatile species frozen out on T~10 K grains

CO avoids densest, coldest part of core

Bergin et al. 2002
Caselli et al. 2002
Direct detection ices at infrared

From $10^5$ to <0.1 $L_{\odot}$ objects!

- Overall ice composition remarkably similar toward high- and low-mass YSOs
- Large abundance variations in minor species NH$_3$, OCN$^-$, CH$_3$OH on 1000 AU scales

**Q:** Origin large abundance variations?  
*Formation complex organics on grains? Is UV needed?*

Gibb et al. 2000  
Boogert et al. 2004, 2007  
Young et al. 2004
Infrared absorption

- Background star
- Embedded young star

**Flux**
- Continuum due to hot dust
- Absorption by cold dust

**Wavelength**

Infrared: vibrational transition of gases and solids

- Hot dust: 300–1000 K
- Gas-phase molecules: 20–200 K
- Cold dust (ice mantles): 10–100 K
Ices toward low-mass protostars

Boogert, Pontoppidan, Oberg, Bottinelli et al. 2007
Silicate subtracted spectra: NH$_3$ and CH$_3$OH!

Inversion/umbrella

Ingredients for complex organics!
Processing of ices produces complex molecules?

- Grain provides a ‘catalytic’ surface with a weak H-bonded network
- Cosmic Rays
- Photon Dominated Regions
  - Surface regions of dusty disks
  - Cometary Ices
- UV light
- Heating effects
  - Shocked regions (HH objects)
  - Collapsing Dense Clouds
  - Turbulent disks
- Surface diffusion brings adsorbed molecular species into close contact

Fraser, Collings & McCoustra
Cold cores: extreme deuteration: tracer of temperature and freeze-out

Strong $\text{H}_2\text{D}^+$ and $\text{D}_2\text{H}^+$ in cores

Triply deuterated ammonia: $\text{ND}_3$

- Caselli et al. 2003
- Vastel et al. 2006
- Stark et al. 1999
- $\text{H}_3^+, \text{D}_3^+: \text{IR}$

- Lis et al. 2002
- van der Tak et al. 2002
Interstellar $\text{H}_3^+$ as tracer of ionization

- Cosmic ray ionization rate varies from cloud to cloud?
- Strong $\text{H}_3^+$ absorption in diffuse clouds implies high cosmic ray ionization rate $\sim$few $\times 10^{-16}$ s$^{-1}$

Geballe & Oka 1996
McCall et al. 2003
vdTak & vD 2000
Pety et al. 2004
Pre-stellar core:
• Low temperature
• Depletion toward center
• ...but not edge

Protostellar core:
• Central heating ~ temperature gradient
• Thermal desorption toward center
• ...outside (low T): depletion/no depletion regions as in pre-stellar stages

Q: Is this an evolutionary sequence?  
Can chemistry constrain timescales?  
Current data suggest phase of heavy depletions (pre-+protostellar) lasts only ~10^5 yr  

Jørgensen et al. 2005
Hot cores/corinos: Inner envelope chemistry
Evaporated ices and complex organics around solar-mass star
IRAS 16293-2422

Abundance profiles

Doty et al. 2004
Molecules as chemical clocks

Charnley et al. 1992, 1997
Wakelam et al. 2004, 2006
Importance of water

- Dominant form of oxygen => affects all species
- Important role in energy balance as coolant
- Diagnostic for ‘hot spots’
- Origin of water on Earth (through HDO/H₂O)
  - Chemistry of life occurs in water
Gas phase water

- SWAS and ODIN (~3’): Water emission is weak => most water frozen out on grains in cold clouds

Herschel (10-40’’) =>
- zoom in on protostars
- many more lines
- isotopes H$_2^{18}$O, H$_2^{17}$O, HDO!

Q: what is water cycle from clouds => cores => protostars => disks?

Melnick et al. 2000
Water and organics in planet-forming zones of disks

-Probe chemistry in inner 10 AU => planet-forming zones
- Gas is hot: 400-700 K
- Abundances factor 1000 larger than in cold clouds
Hot water emission in disk atmospheres!

T~1000 K
=> 0.1-1 AU

Also hot HCN, C$_2$H$_2$
seen in emission

AS 205 disk in Oph
Spitzer observations

Carr & Najita 2008
Salyk, Pontoppidan et al. 2008
Near-IR OH/H$_2$O from ground

Disk in Tau

Disk in Oph

Keck
R=25000
Fully resolved with CRIRES

Note similarity in CO and H$_2$O line widths!  Salyk et al. 2008
Where is water in protoplanetary disks?

Q: use water as tracer of radial and vertical mixing; ‘snow’ line?
Future facilities: the best is still to come

Infrared

SIRTF 2003

Far-infrared/THz

SOFIA 2011

ASTRO-F 2005

Herschel 2008

JWST 2013
ALMA

64 x 12m antenna’s; construction started 2003
Early observing 2010; completion 2012
Issues for this workshop

• Identify most important rates needed to address astrophysical and astrochemical questions
  – No use spending a lot of time and money on unimportant rates
  – No use spending a lot of time and money on unimportant molecules

• Quantify uncertainties as functions of parameters
  – Some easy, some difficult
  – May vary with temperature, wavelength, ….  
  – Critical evaluation of existing data (latest number is not always the best….)

• Educate astrochemists in underlying chemical physics
  – Manage their expectations of what can/cannot be achieved

• Educate (astro)chemists about proper comparison with observations
  – Make sure all relevant processes are included
  – Awareness that abundances are not constant with position
  – Sometimes physics poorly understood, not chemistry (CH+)