Radio Astronomy

PD Dr. Henrik Beuther and Dr. Hendrik Linz

MPIA Heidelberg

Tentative Schedule:
16.10. Introduction and overview (HL & HB)
23.10. Emission mechanisms, physics of radiation (HB)
30.10. Telescopes – single-dish (HL)
06.11. Telescopes – interferometers (HB)
13.11. Instruments – continuum detection (HL)
20.11. Instruments – line detection (HB)
27.11. Continuous radiation (free-free, synchrotron, dust) (HL)
04.12. Radiation transfer (HB)
11.12. Line radiation (HL)
18.12. Visit to Effelsberg (all)
08.01. Molecules and chemistry (HL)
15.01. Physics and kinematics (HB)
22.01. Applications (HL)
29.01. Applications (HB)
05.02. Exam week
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Topics for today:

- molecules in space
- rotational transitions
- astro-chemistry
- science examples
Molecules in Space

As mentioned earlier: first molecules found in the optical (CH, CH+, CN) in the 1940s

First radio detections of the molecule OH (hydroxyl) in space in the 18 cm lines in 1963

→ assumption that all interstellar molecules might be just di-atomic

But in 1968: detection of NH$_3$ (ammonia) and H$_2$O (water) at around 1.3 cm wavelength

Then in 1969: the organic molecule H$_2$CO (formaldehyde) is detected at ~ 6 cm

Finally in 1970: the very important molecule CO (carbon monoxide) is detected at 2.7 mm wavelength
Detected molecules in space (outside of stellar atmospheres): >170 (as of 11/2012)

54 molecules also detected in extragalactic systems to date ...

Taken from the CDMS (Cologne Database of Molecular Spectroscopy)

http://www.astro.uni-koeln.de/cdms
Line emission from molecules

Molecules can exhibit more degrees of freedom and more possibilities of quantised energy levels than simple atoms.

There can be energy transitions due to:

– electronic transitions
– vibrations of different kinds (bending, stretching of molecular bonds)
– molecular rotations
– inversion transitions

All will lead to line emission/absorption of one kind or the other.
A combined schematic energy diagram for the electronic, vibrational and rotational transitions

(a) **Electronic transitions** exist, like in single atoms. Their energy is often in the order of the dissociation energy of the molecules.

(b) **Vibrational transitions** within the same electronic state, at first approximation behaviour like a harmonic oscillator (equidistant energy levels)

(c) **Rotational transitions** within the same vibrational level or to a different vibrational level ("roto-vibrational" transitions)

Especially the rotational transitions occur in the (sub-)mm and cm radio regime and give access to cold dense gas!

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Rotations: the Rigid Rotor with quantised angular momentum $L = I \omega$

Diatomic or Linear Polyatomic Molecules

Energy levels

$$E_r = B J (J + 1) = \frac{L^2}{2I}$$

rotational constant

$$B = \frac{\hbar^2}{2I}$$

Moment of inertia

$$I = \sum_i m_i r_i^2$$

Quantum selection rule for permitted transitions

$$\Delta J = \pm 1$$

Large and heavy molecules have small rotational constants!
Heavy and large molecules have small rotational constants …

→ The rotational transitions with low quantum numbers carry also quite little energies then!

→ Such molecules can therefore have (many) lines at low frequencies ($\nu < 30$ GHz, $\lambda > 1$ cm), while light and small molecules just have transitions in the (sub-)millimeter

e.g.: HC$_7$N … J = 1 → 0 at around 1.130 GHz ($\lambda \sim 26.6$ cm)

HD … J = 1 → 0 at around 2.675 THz ($\lambda \sim 112$ µm)
What makes line transitions strong?

1.) The Einstein coefficient has a strong frequency dependence: \( A_{21} \sim \nu^3 \)
2.) Expression for \( A_{21} \) can be reformed in order to introduce the transition dipole moment \( \mu_{21} \)

\[
A_{21} = \frac{2\omega_{21}^3}{3\varepsilon_0 h c^3} \mu_{21}^2
\]

Linear molecules with just the same atoms as constituents in general do not have a permanent electric dipole moment! → no purely rotational transitions

Electric Dipole transitions: \( \mu_{21} \sim e a_0 \) (charge times distance/displacement) → \( A_{21} \sim e^2 a_0^2 \)

Dipole moments are measured in Debye [D], molecules with permanent dipole moments typically have 1 – 5 D \( (1 \text{ D} = 3.33564 \times 10^{-30} \text{ C m}) \)
Some remarkable transitions in Hydrogen

21 cm line
Atomic H / electron spin flip

The most famous line in radio astronomy

$F = 1$

$F = 0$

$\nu_0 = 1420 \text{ MHz}$

$\lambda_0 = 21 \text{ cm}$

Spin-Flip

Orthohydrogen

Ortho-para transition in molecular hydrogen
Nuclear spin flip

A = $2.9 \times 10^{-15} \text{ s}^{-1}$

A = $6.2 \times 10^{-14} \text{ yr}^{-1}$

Hypothetical ... not observed!
Examples for Einstein A coefficients – a proxy to the line strength

<table>
<thead>
<tr>
<th>Type</th>
<th>$A_{21}$ (s$^{-1}$)</th>
<th>Example</th>
<th>$\lambda$</th>
<th>$A_{21}$ (s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electric dipole</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>UV</td>
<td>$10^9$</td>
<td>Ly$\alpha$</td>
<td>121.6 nm</td>
<td>$2.4 \times 10^8$</td>
</tr>
<tr>
<td>Visible</td>
<td>$10^7$</td>
<td>H$\alpha$</td>
<td>656 nm</td>
<td>$6 \times 10^6$</td>
</tr>
<tr>
<td>Vibrational</td>
<td>$10^2$</td>
<td>CO</td>
<td>4.67 $\mu$m</td>
<td>34.0</td>
</tr>
<tr>
<td>Rotational</td>
<td>$10^{-6}$</td>
<td>CS</td>
<td>6.1 mm</td>
<td>$1.7 \times 10^{-6}$</td>
</tr>
<tr>
<td>Forbidden</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Opt. (el. Quadrupole)</td>
<td>1</td>
<td>[OIII]</td>
<td>436.3 nm</td>
<td>1.7</td>
</tr>
<tr>
<td>Opt. (magn. Dipole)</td>
<td>$10^2$</td>
<td>[OIII]</td>
<td>500.7 nm</td>
<td>$2 \times 10^2$</td>
</tr>
<tr>
<td>Hyperfine</td>
<td></td>
<td>HI</td>
<td>21 cm</td>
<td>$2.9 \times 10^{-15}$</td>
</tr>
</tbody>
</table>
Magnetic dipole transitions are proportional to $\mu_B$ (Bohr magneton), and are typically $10^4 – 10^5$ times weaker than electric dipole transitions. Electric quadrupole transitions are weaker by a factor of $\sim 10^8$. 

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<table>
<thead>
<tr>
<th>Electric dipole “allowed”</th>
<th>Magnetic dipole “forbidden”</th>
<th>Electric quadrupole “forbidden”</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta J = 0, \pm 1$</td>
<td>$\Delta J = 0, \pm 1$</td>
<td>$\Delta J = 0, \pm 1, \pm 2$</td>
</tr>
<tr>
<td>$0 \leftrightarrow 0$</td>
<td>$0 \leftrightarrow 0$</td>
<td>$0 \leftrightarrow 0, 1/2 \leftrightarrow 1/2, 0 \leftrightarrow 1$</td>
</tr>
<tr>
<td>$\Delta M = 0, \pm 1$</td>
<td>$\Delta M = 0, \pm 1$</td>
<td>$\Delta M = 0, \pm 1, \pm 2$</td>
</tr>
<tr>
<td>$0 \leftrightarrow 0$ when $\Delta J = 0$</td>
<td>$0 \leftrightarrow 0$ when $\Delta J = 0$</td>
<td></td>
</tr>
<tr>
<td>Parity change</td>
<td>No parity change</td>
<td>No parity change</td>
</tr>
<tr>
<td>One electron jumping</td>
<td>For all electrons</td>
<td>One electron jumping with</td>
</tr>
<tr>
<td>$\Delta l = \pm 1, \Delta n$ arbitrary</td>
<td>$\Delta l = 0, \Delta n = 0$</td>
<td>$\Delta l = 0, \Delta n = 0$</td>
</tr>
<tr>
<td>$\Delta S = 0$</td>
<td>$\Delta S = 0$</td>
<td>$\Delta S = 0$</td>
</tr>
<tr>
<td>$\Delta L = 0, \pm 1$</td>
<td>$\Delta L = 0, \pm 1, \pm 2$</td>
<td>$\Delta L = 0, \pm 1, \pm 2$</td>
</tr>
<tr>
<td>$0 \leftrightarrow 0$</td>
<td>$0 \leftrightarrow 0$</td>
<td>$0 \leftrightarrow 0 \leftrightarrow 1$</td>
</tr>
</tbody>
</table>
Molecular excitation to higher rotational levels: Collisions vs (spontaneous) radiative decay

We want to have a situation where the radiation signal we receive is a close proxy to the physical conditions in the gas (in order to derive its temperature and/or density)

In LTE the distribution of the rotational levels is governed by the Boltzmann distribution.

But in a too thin gas, there are not enough collisions per time unit to establish this distribution … the spontaneous radiative decay (governed by the Einstein coefficient $A_{UL}$) is faster.

Critical density

\[ n^* \approx \frac{A_{UL}}{\langle \sigma v \rangle} \]

cross section \( \sigma \sim 10^{-15} \text{ cm}^{-2} \)
molecular velocities \( v \sim 1 \text{ km/s} \)

At $n^*$, collisional excitation equals spontaneous radiative decay.
Connection between upper rotational energy levels and critical densities for two dense gas tracers: CS and HCN

The upper-level energy (expressed as temperatures: \( T = \frac{E_{\text{up}}}{k_B} \)) over the logarithm of the critical density. Parameter is the rotational quantum number \( J \).

Walmsley & Güsten 1994, Lecture Notes in Physics 439, 164

The upper-level energy (expressed as temperatures: \( T = \frac{E_{\text{up}}}{k_B} \)) over the logarithm of the critical density. Parameter is the rotational quantum number \( J \).
CO as a molecule with special importance for astronomy:

– CO lines are the most important cooling lines for the regime below 100 Kelvin (cooling of the molecular material in order to facilitate gravitational collapse … eventually)

– relatively light, di-atomic, simple rotational spectrum

– low dipole moment (-0.12 Debye) → easily excitable also in thinner molecular gas (1 – 0 transition is in collisional equilibrium already for $H_2$ densities of less than $10^3$ cm$^{-3}$)

– CO is the most abundant molecule after $H_2$ itself (abundance ~ $10^{-4}$)

→ Since the bulk of the cold $H_2$ molecular gas in molecular clouds is not directly accessible (no permanent dipole moment), CO is the best (?) proxy for the total amount of molecular gas in a cloud.
The next four slides are taken from a review talk

Given by Paul Goldsmith

During the 2012 EPOS conference at Schloss Ringberg
Molecular Cloud Structure: Perseus + Taurus - The Big Picture (Ungerechts & Thaddeus 1987)

$^{12}$CO integrated intensity

0.5 degree beam size and sampling

What impression do you get from this map?
Studying molecular clouds = "blobology"
Zoom into the previous map ...
Done 20 years later with a 13.7 m radio telescope + line receiver array (32 “pixels”) in on-the-fly scanning mode (Goldsmith et al. 2008, ApJ 680, 428)

Taurus 12CO Integrated Intensity

Spatial Dynamic Range = Image Size / Nyquist Interval ~ 1500 to 2000

Distance = 140 pc
1° = 2.4 pc
1' = 0.041 pc
Paradigm change in molecular cloud structure: From Blobology to Filamentology!
Molecular gas at early times of galaxy evolution ($< 1$ Gyr after the Big Bang). Even back then there was a co-evolution of the star-formation process in the host galaxy (traced by the CO) and the central black hole (evident as the action associated with the central quasar).

The CO(3 – 2) radiation associated with the quasar $J1148+5251$. The rest frequency is around 346 GHz. Due to the large redshift of $z = 6.42$, this line is shifted to much lower frequencies (46.61 GHz) accessible with the VLA.
Molecular line measurements as observational basis to study the chemistry in the interstellar medium

→ interesting in itself in order to study rare molecules in conditions that are not common on earth (low pressures, densities and temperatures)

→ chemistry as additional tool to constrain physical processes, especially relevant for star formation research

→ mixing of gas, (in)homogeneity, spatial differentiation
→ energetics (embedded heating sources)
→ influence of shocks
Astro-Chemistry: What happens?

Early theoretical investigations: at typical densities, neutral-neutral reactions are too slow to produce appreciable amounts of new molecules in less than $10^6$ years.

Solution: Ion-molecule chemistry with reaction rates a thousand times faster than neutral-neutral reactions (for these space conditions) ($\rightarrow$ ionisation in interiors of molecular cloud cores well, shielded against UV radiation, comes mainly from Cosmic Rays).

Central is the molecule $\text{H}_3^+$ as a focal point in any chemical network:

\[
\text{e.g.}: \quad \text{H}_3^+ + \text{CO} \rightarrow \text{HCO}^+ + \text{H}_2
\]

Destruction can come from recombination with electrons:

\[
\begin{align*}
\text{H}_3^+ + \text{e}^- & \rightarrow \text{H}_2 + \text{H} \\
\text{HCO}^+ + \text{e}^- & \rightarrow \text{H} + \text{CO}
\end{align*}
\]

However, for the production of $\text{H}_3^+$ one needs $\text{H}_2$. 

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Astro-Chemistry: the importance of dust grains

$H_2$ forms on dust grain surfaces!

Thermal hopping of accreted $H$ atoms on the grain surfaces until a reaction partner is met.

Also other more complex molecules like $\text{CH}_3\text{OH}$ (methanol) can be formed on grain surfaces if the conditions are sufficiently cold so that potential constituents of the final products freeze out from the gas phase onto the grains.
Astro-Chemistry: complex processes of accretion and desorption

Until recently, the situation seemed clear:

Cold conditions: many species on dust grains (formation yes, but no way back to the gas phase → not accessible via rotational gas phase transitions)

Warming up: central heating source (e.g., a protostar with a strong far—infrared radiation field) heats the grains clearly above 20 K → thermal desorption of the surface species into the gas phase → extreme objects: “Hot Molecular Cores” (HMCs) with gas temperatures of 100 – 300 K: drastic release of surface species and subsequent intense chemical reactions lead to very rich chemistry (complex molecules, saturated, methanol! and higher alcohols)
Astro-Chemistry: complex processes of accretion and desorption

New observations of cold cores (10 – 20 K):
complex species and methanol detected in the gas phase
(although the grains are not warm enough to provide normal thermal desorption)

One idea: “reactive desorption” → some grain surface reactions are slightly exothermic → reaction energy is one route to provide sufficient thrust for molecule desorption

Chemical diversity in star-forming regions (I)

An infrared-Dark Cloud (IRDC), Cold (< 20 K), mostly simple chemistry (but with some surprises ...), narrow lines

A High-Mass Protostellar Object (HMPO), elevated temperature (30 – 50 K), more complex chemistry, many methanol lines

An ultracompact HII region (UCHIIR), central massive star has ignited, hot gas, dominating ionised gas component with > 8000 K destroys most molecules, the remaining ones show broad lines

Chemical diversity in star-forming regions (II): The true molecular line factories are Hot Cores!

Hot Core: Orion KL

Hot Core: G29.96-0.02

Not (yet) a hot core: IRAS 23151+5912

Not (yet) a hot core: IRAS 05358+3543
The advantage of spatially resolved imaging spectroscopy via modern interferometers with broad immediate spectral bandpasses (SMA, PdBI, ALMA):

Chemical differentiation on small scales can be revealed!

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Scripts at: http://www.mpi-a.de/homes/beuther/lecture_ws1213.html