### **PD Dr. Henrik Beuther and Dr. Hendrik Linz** *MPIA Heidelberg*





An elective lecture course for the winter term 2012/13 at the Ruperto Carola University Heidelberg









## 01/08/2013

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**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  $\rightarrow$  assumption that all interstellar molecules might be just di-atomic But in 1968: detection of NH<sub>3</sub> (ammonia) and H<sub>2</sub>O (water) at around 1.3 cm wavelength Then in 1969: the organic molecule  $H_{g}CO$  (formaldehyde) is detected at ~ 6 cm Finally in 1970: the very important molecule CO (carbon monoxide) is detected at 2.7 mm wavelength



2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	12 atoms	>12 atoms
H2	C3*	c-C3H	C5*	C5H	C6H	CH3C3N	CH3C4H	CH3C5N	HC9N	c-C6H6*	HC11N
AlF	C2H	l-C3H	C4H	1-H2C4	CH2CHCN	HC(O)OCH3	CH3CH2CN	(CH3)2CO	CH3C6H	C2H5OCH3?	C60*
AlCl	C2O	C3N	C4Si	C2H4*	CH3C2H	СН3СООН	(CH3)2O	(CH2OH)2	C2H5OCHO	n-C3H7CN	C70*
C2**	C2S	C3O	1-C3H2	CH3CN	HC5N	C7H	CH3CH2OH	CH3CH2CHO			
СН	CH2	C3S	c-C3H2	CH3NC	СН3СНО	С6Н2	HC7N				
CH+	HCN	C2H2*	H2CCN	СНЗОН	CH3NH2	СН2ОНСНО	C8H				
CN	HCO	NH3	CH4*	CH3SH	c-C2H4O	1-HC6H*	CH3C(O)NH2				
CO	HCO+	HCCN	HC3N	HC3NH+	Н2ССНОН	CH2CHCHO(?)	C8H-				
CO+	HCS+	HCNH+	HC2NC	HC2CHO	С6Н–	CH2CCHCN	C3H6				
СР	HOC+	HNCO	НСООН	NH2CHO		H2NCH2CN					
SiC	H2O	HNCS	H2CNH	C5N							
HC1	H2S	HOCO+	H2C2O	l-HC4H*							
KC1	HNC	H2CO	H2NCN	l-HC4N							
NH	HNO	H2CN	HNC3	c-H2C3O		_				,	
NO	MgCN	H2CS	SiH4*	H2CCNH(?)	)	D	etected	molecul	les in si	pace (ou	itside of
NS	MgNC	H3O+	H2COH+	C5N-							
NaCl	N2H+	c-SiC3	C4H–			at	allor at	magnhar	$(a) \cdot (a)$		f(11/2012)
OH	N2O	CH3*	HC(O)CN			SL	char at	mospher	CS). — I	(as (	$\frac{111}{2012}$
PN	NaCN	C3N-	HNCNH								
SO	OCS	PH3?	CH3O								
SO+	SO2	HCNO									
SiN	c-SiC2	HOCN				54	1 molec	ules also	h detect	ted in ex	tragalactic
SiO	CO2*	HSCN				<u> </u>					inaganaono
SiS	NH2	H2O2					ratama 1	to data			
CS	H3+*	C3H+				S y	/stems	lo dale	•		
HF	H2D+										
HD	SICN										
FeO?	AINC										
OZ OE I	SINC					$\mathbf{T}$	aken fr	om the (	DMC (	Cologn	e Datahase
CF+	HCP					1				Cologin	
							f Malaa		atuadaa		
PU AlO	AIO⊓ ⊔2∩⊥					O I		ular Spe	ctrosce	)py)	
OH+	$H2C1 \pm$					1			• 1	1 1 1	
CN	KCN _					ht	tp://wv	vw.astro	.uni-ko	eln.de/c	ams
SH±	HO2										
SH	FeCN_										
HCl+_											
- HOL-											





## 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

Electronic Transitions: ΔE = 1-15 eV Visible-UV

Vibrational Transitions: ∆E = 0.1-1 eV Infrared

Rotational Transitions: ∆E = 0.01-0.1 eV (sub)-Millimeter



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

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

(c) <u>Rotational transitions within</u> the same vibrational level or to a

different vibrational level ("rotovibrational" 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 Rotorwith quantised angularmomentum  $L = I \omega$ 

Diatomic or Linear Polyatomic Molecules





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

Moment of inertia

$$I = \sum_{i} m_{i} r_{i}^{2}$$

Large and heavy molecules have small rotational constants!

 $\Delta J=\pm 1$ 

Quantum selection rule for permitted transitions

Heavy and large molecules have small rotational constants ...

 $\rightarrow$  The rotational transitions with low quantum numbers carry also quite little energies then!

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

e.g.:  $HC_7 N \dots J = 1 \rightarrow 0$  at around 1.130 GHz ( $\lambda \sim 26.6$  cm) HD  $\dots J = 1 \rightarrow 0$  at around 2.675 THz ( $\lambda \sim 112 \ \mu m$ )

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#### What makes line transitions strong?

The Einstein coefficient has a strong frequency dependence: A<sub>21</sub> ~ v<sup>3</sup>
 Expression for A<sub>21</sub> can be reformed in order to introduce the transition dipole moment μ<sub>21</sub>



Electric Dipole transitions:  $\mu_{21} \sim e a_0$  (charge times distance/displacement)  $\rightarrow A_{21} \sim e^2 a_0^2$ Dipole moments are measured in Debye [D], molecules with permanent dipole moments typically have 1 – 5 D (1 D = 3.33564 10<sup>-30</sup> C m)

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#### Some remarkable transitions in Hydrogen





Orthohydrogen



Parahydrogen

Ortho-para transiton in molecular hydrogen Nuclear spin flip

A = 6.2 x 10<sup>-14</sup> yr<sup>-1</sup>



Hypothetical ... not observed!

## Examples for Einstein A coefficients – a proxy to the line strength

Туре	A <sub>21</sub> (s⁻¹)	Example	λ	A <sub>21</sub> (s⁻¹)
Electric dipole				
UV	10 <sup>9</sup>	Lyα	121.6 nm	2.4 x 10 <sup>8</sup>
Visible	107	Ηα	656 nm	6 x 10 <sup>6</sup>
Vibrational	10 <sup>2</sup>	CO	<b>4.67</b> μm	34.0
Rotational	10-6	CS	6.1 mm	1.7 x 10 <sup>-6</sup>
Forbidden				
Opt. (el. Quadrupole)	1	[OIII]	436.3 nm	1.7
Opt. (magn. Dipole)	10 <sup>2</sup>	[OIII]	500.7 nm	2 x 10 <sup>2</sup>
Hyperfine		HI	21 cm	2.9 x 10 <sup>-15</sup>





## Selection rules

Electric dipole "allowed"	Magnetic dipole "forbidden"	Electric quadrupole "forbidden"
$\Delta J = 0, \pm 1$	$\Delta J = 0, \pm 1$	$\Delta J = 0, \pm 1, \pm 2$
$0 \nleftrightarrow 0$	0 ↔ 0	$0 \leftrightarrow 0, 1/2 \leftrightarrow 1/2, 0 \leftrightarrow 1$
$\Delta M = 0, \pm 1$	$\Delta M = 0, \pm 1$	$\Delta M = 0, \pm 1, \pm 2$
$0 \nleftrightarrow 0$ when $\Delta J = 0$	$0 \leftrightarrow 0$ when $\Delta J = 0$	
Parity change	No parity change	No parity change
One electron jumping	For all electrons	One electron jumping with
$\Delta l = \pm 1, \Delta n$ arbitrary	$\Delta l = 0,  \Delta n = 0$	$\Delta l = 0, \pm 2, \Delta n$ arbitrary or for all electrons $\Delta l = 0, \Delta n = 0$
$\Delta S = 0$	$\Delta S = 0$	$\Delta t = 0, \Delta h = 0$ $\Delta S = 0$
$\Delta L = 0, \pm 1$	$\Delta L = 0, \Delta J = \pm 1$	$\Delta L = 0, \pm 1, \pm 2$
0 ↔ 0		$0 \leftrightarrow 0, 0 \leftrightarrow 1$

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 ~10^8.01/08/2013Radio Astronomy

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  $A_{III}$ ) is faster.

Critical density

$$n^* pprox rac{A_{
m UL}}{\langle \sigma v 
angle}$$

cross section  $\sigma \sim 10^{-15}$  cm<sup>-2</sup> molecular velocities  $v \sim 1$  km/s

At *n*\*, collisional excitation equals spontaneous radiative decay. 01/08/2013 Radio Astronomy



# Connection between upper rotational energy levels and critical densities for two dense gas tracers: CS and HCN



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

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![](_page_14_Picture_5.jpeg)

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## 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)  $\rightarrow$  easily excitable also in thinner molecular gas (1 0 transition is in collisional equilibrium already for H<sub>2</sub> densities of less than 10<sup>3</sup> cm<sup>-3</sup>)
- CO is the most abundant molecule after H<sub>2</sub> itself (abundance ~ 10<sup>-4</sup>)
  - → 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.

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![](_page_15_Picture_8.jpeg)

### The next four slides are taken from a review talk

#### Given by Paul Goldsmith

During the 2012 EPOS conference at Schloss Ringberg

![](_page_16_Picture_3.jpeg)

![](_page_16_Picture_5.jpeg)

![](_page_17_Figure_0.jpeg)

 1.2 m radio telescope at Columbia Univ Back then done with a Zoom into the previous map ...

![](_page_18_Picture_2.jpeg)

Done 20 years later with a 13.7 m radio telescope + line receiver array<br/>(32 "pixels") in on-the-fly scanning mode (Goldsmith et al. 2008, ApJ<br/>680, 428)Distance = 140 pc<br/>1° = 2.4 pc<br/>1' = 0.041 pcDistance = 140 pc<br/>1° = 2.4 pc<br/>1' = 0.041 pc

![](_page_19_Figure_1.jpeg)

Paradigm change in molecular cloud structure : From Blobology to Filamentology!

![](_page_20_Figure_1.jpeg)

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).

![](_page_21_Figure_1.jpeg)

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.

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![](_page_21_Picture_5.jpeg)

## **Astro-Chemistry**

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)
- $\rightarrow$  chemistry as additional tool to constrain physical processes, especially relevant for star formation research
  - $\rightarrow$  mixing of gas, (in)homogeneity, spatial differentiation

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- $\rightarrow$  energetics (embedded heating sources)
- $\rightarrow$  influence of shocks

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![](_page_22_Picture_7.jpeg)

## **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<sup>6</sup> years

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

> Central is the molecule  $H_3^+$  as a focal point in any chemical network: e.g.:  $H_3^+ + CO \rightarrow HCO^+ + H_2$

**Destruction can come from recombination with electrons:** 

 $H_3^+ + e^- \rightarrow H_2^- + H_2^-$ HCO<sup>+</sup> +  $e^- \rightarrow H + CO_2^-$ 

However, for the production of  $H_1^+$  one needs  $H_2$ .

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![](_page_23_Picture_9.jpeg)

## Astro-Chemistry: the importance of dust grains

H<sub>2</sub> 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 CH<sub>3</sub>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.

![](_page_24_Picture_5.jpeg)

![](_page_24_Picture_6.jpeg)

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## Astro-Chemistry: complex processes of accretion and desorption

Until recently, the situation seemed clear:

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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)

![](_page_25_Picture_4.jpeg)

## 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

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See: Garrod, Wakelam, & Herbst 2007, A&A 467, 1103

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![](_page_26_Picture_4.jpeg)

![](_page_27_Figure_0.jpeg)

From Beuther et al. 2008, ApJ 675, L33 01/08/2013 Radio Astronomy

# 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

#### From: Beuther et al. 2009, AJ 137, 406

![](_page_28_Figure_1.jpeg)

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

![](_page_28_Picture_7.jpeg)

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!

Example: SMA interferometry at around 345 GHz for the famous Orion KL region (Beuther et al. 2005, ApJ 632, 355)

![](_page_29_Figure_3.jpeg)

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!

Example: SMA interferometry at around 345 GHz for the famous Orion KL region (Beuther et al. 2005, ApJ 632, 355)

![](_page_30_Figure_3.jpeg)

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!

Example: SMA interferometry at around 345 GHz for the famous Orion KL region (Beuther et al. 2005, ApJ 632, 355)

![](_page_31_Figure_3.jpeg)

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Scripts at : http://www.mpia.de/homes/beuther/lecture\_ws1213.html

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05.02. Exam week

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![](_page_32_Picture_7.jpeg)