Complex Molecules in Space – Present status and prospects with ALMA

(Some of) The Big Themes

### Low-mass star formation: Shifting interests

#### $\rightarrow$ Planetary system formation

- composition of gas and solids in different stages of star and planet formation
- What fraction of parental cloud goes into new solar systems
- Use molecules and dust to constrain physical conditions (*T*, *n*, *v* structure)
- Chemical diagnositics of different stages and components (outflow, infall,,disk)

#### **Observations:**

Outflows from very low luminosity objects ( $L < 0.1 L_{sun}$ )

#### Formation of complex molecules

First generation (CH<sub>3</sub>OH, H<sub>2</sub>CO) forms on grain surfaces  $\rightarrow$  evaporation  $\rightarrow$  more complex species form in gas phase

**Problem:** Necessary reactions don't occur!

Heavy radicals react on grains and form more complex molecules, which are then evaporated

#### **Complex questions:**

Where do the widespread complex molecules in the galactic center come from?

Why is it interesting to detect ever more complex molecules?

### **Line surveys**

Eminently useful tools to get

- chemical fingerprint of a region
- determine  $T, X_n, \dots$
- identify new species

LTE assumption sufficient in many interesting cases (very line-rich dense hot cores)

**THE** definitive spectral line database is urgently needed!

Concerted effort by all involved parties needed to get (at least) a smart search engine that delivers usable information

Do we need special databases for individual sources?

**Problematic** 

Rather provide source type matrices?

(which CDMS has in rudimentary form)

# **Weed control**



http://www.ph1.uni-koeln.de/cgi-bin/cdmsinfo?file=e032504.cat

#### **Exterminating weeds:**

Calculate whole spectra of all species

- what species?
- measurements at only two temperatures needed to predict spectrum at any temperature
- will enable optimum search strategy to find individually hidden, but collectively observable flowers

**Questions:** How well can whole spectrum be restored? How reliable are intensities?

Practical issues:

• How to make data available?

Lists of lines – automatic extraction mechanism

### Radiative transfer seems to be under control:

• Benchmarks  $\checkmark$ 

But, do benchmarks also for other scenarios/geometries

- disks
- circumstellar envelopes

#### **Promise and DANGER:**

Going on autopilot, without really understanding what you are doing

(also true for ALMA calibration and imaging software)

# So you've found lots of disks and hot cores – what do you do now?

**Of course: Follow up with ALMA, which can address:** 

- Efficient high resolution imaging for "plausibility" tests of new species IDs
- Energetics relation to exciting source

Example G29.96: hot molecules not associated with any continuum source

Significant offsets of ca. 0.3" (= 1500 AU) r(100 K) for L =9 10<sup>4</sup> Lsun = 4600 AU

The problem is not so much how one produces the high molecular abundances where one observes them as *why* one produces them *there* 

base of outflows

#### How are bipolar outflows launched?







**Chemical Diversity: The W3(OH) Region** 

(Wyrowski et al. 1999)

#### W3(OH)-H<sub>2</sub>O



Hachisuka et al. (2006)

 $\Rightarrow$  D = 2.04 +/- 0.07 kpc





Chandler, Greenhill, et al.

#### Even a region as thorougly studied as Orion-KL has many mysteries left!

- SiO outflow and rotating/expanding disk
- (Unrelated) Large scale H2O outflow
- (Unrelated) Smaller scale CO outflow
- How many outflows, originating from where?
- Shock-excited H<sub>2</sub> "explosion" related to multiple merger event?
- Any evidence for H<sub>2</sub> explosion in (sub)mm emission?
- HH-objects

**Promises and Challenges of ALMA observations:** 

- structure on many scales from <0.01"</li>
  - to tens of arc seconds (continuum) or
  - to arcseconds (hot lines)
- $\Rightarrow$  multi-configuration imaging

**EVEN THEN:** 

**Severe 0-spacing problems:** 

Current interferometers often only see 10 – 20% of total flux

Very many lines from many molecules: • One doesn't want maps of S (or  $T_B$ ) but • maps of  $T_{kin}$ , n, X and fit dynamical models



# *To do science* with (3D) line surveys one needs very advanced data analysis tools:

- Automatic line identification and information extraction (fluxes, velocities)
  - requires up-tp-date "living" molecular spectroscopy database
- LTE analysis
  - $\rightarrow$  maps of N(X), T<sub>rot</sub>
- non-LTE analysis (LVG/Monte Carlo least sqares method; see Leurini et al. 2004 for CH<sub>3</sub>OH)

 $\rightarrow$  maps of *n*, *T*<sub>kin</sub>, [X/H<sub>2</sub>]

• Fit dynamical models

Astronomical Data Analysis Software and Systems XV ASP Conference Series, Vol. XXX, 2005 C. Gabriel, C. Arviset, D. Ponz and E. Solano, eds.

# Advanced Science Analysis Package and the prototype DALIA **=** Direct Approach to Line Analysis

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Figure 1. "Model Editor" window generated from the XML description of the model, in this case a galactic disk kinematic model. To create a model instance make the choices allowed for the model and edit the parameters to give a first guess.

**P98** 

# What do we have now?

- Not even a software package that provides basic imaging capability!
- Dispersed (and very low manpower level) efforts to develop data modeling and smart analysis tools
- Not yet the optimal solution for spectroscopy databases

# Even more basic...

Apart from smart data analysis tools, we need:

## For observing, calibration, & imaging:

- computer-aided observation preparation
  \* (semi)automatic setup tools for frequency selection, mosaicing, ...
- (largely) automatic
  - \* calibration
  - \* imaging + selfcalibration,
  - \* mosaicing, multi-configuration combination, 0spacing addition

# ... and we don't even have *aips++* working!

On a more *positive* note...

# Considerable effort is put into Herschel/HIFI observing and data analysis software

#### Even ALMA will not be able to do everything!



#### **JCMT Heterodyne Array Receiver Programme**

- 16 elements
- 325 375 GHz
- 14" FWHM

Will not only map very large areas in CO, but could also be used for finding interesting new hot cores





Exploring the formation of galaxies and stars Découvrir la formation des galaxies et des étoiles

Astronomers' website: http://www.rssd.esa.int/herschel

# Even ALMA can't do everything!

 $H_2O!$ 

# **Politics:**

Do we really need multiple European ARC nodes?

If we think so, who will coordinate furthergoing software developments?

- within Europe
- in Coordination with N.A. and Japan

Thank you