

Complex organic molecules in hot cores

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High-Resolution Submillimeter Spectroscopy of the Interstellar Medium and Star Forming Regions – From Herschel to ALMA and Bevond

Zakopane, 14 May 2015





Collaborators:

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Complex organic molecules in the ISM

Search for interstellar COMs: line surveys!

COMs in hot cores

Outlook

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Complex organic molecules in the ISM

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Meteorites and comets

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Basic questions

- are meteoritic amino acids and cometary glycine pristine interstellar molecules? Did the ISM contribute to seeding life on Earth?
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- what is the degree of chemical complexity in the ISM?



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- COMs in prestellar cores at low temperature (Öberg+ 2010, Bacmann+ 2012, Cernicharo+ 2012):
 - reactive desorption of COM precursors followed by radiative association? (Vasyunin & Herbst 2013b)
 - non-thermal desorption in core outer layers? (Vastel+ 2014, Bizzocchi+ 2014)
 - revision/expansion of gas-phase reaction network? (Balucani+ 2015)

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⇒ predictions of chemical models need to be tested observationally!

Hot cores

(in the perspective of understanding interstellar chemistry of COMs)

- hot core: early evolutionary stage during formation of a high-mass star, when protostar starts to heat up its envelope (promoting COM formation and desorption from grain surfaces), but before ionization sets in
- rare objects ⇒ distant ⇒ interferometry essential to probe individual protostellar objects and resolve their structure (envelope, outflows)

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Despite their scarcity and large distance:

- ► high column densities of hot cores ⇒ key advantage for COM detection
- most COMs first detected in hot cores, mainly Sgr B2 and Orion KL
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⇒ hot cores excellent targets to test chemical models

Chemistry in hot cores (and corinos)

Three-phase scenario: (Herbst & van Dishoeck 2009)

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 Example: methanol CH₃OH, by surface hydrogenation of carbon monoxide CO

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 Example: methyl formate CH₃OCHO
- second-generation species: COMs formed in gas phase after sublimation of grain mantles

Search for interstellar COMs: line surveys!

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The need for interferometric line surveys

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Secure identification of a COM requires: (see, e.g., Snyder+ 2005, Halfen+ 2006)

- ► identification of a large number of lines ⇒ large frequency coverage
- ▶ no missing line ⇒ unbiased survey
- ► consistent relative line intensities ⇒ radiative transfer modeling
- ▶ no conflict with other molecules ⇒ model emission of all molecules
- ▶ all lines of a molecule should peak at the same position ⇒ interferometry

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Advent of broadband backends at (sub)mm interferometers (8 GHz@ALMA + soon 16 GHz@NOEMA) ⇒ efficient line surveys at high angular resolution!

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ALMA: sensitivity and resolution!



(SMA, Qin+ 2011)



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Line survey of Sgr B2(N) with ALMA (EMoCA, Belloche+ 2014)

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Modeling of spectral line surveys

Assumptions:

Collision rates missing for many COMs ⇒ LTE often remains unique solution (but see, e.g., Faure+ 2014 for non-LTE analysis of methyl formate CH₃OCHO, Crockett+ 2014 for methyl cyanide CH₃CN)

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Modeling tools:

- spectroscopic databases: mainly CDMS and JPL, + other contributions from lab spectroscopists
- predictions for isotopologues and vibrationally excited states of known COMs essential to perform line identification and prevent misassignments
- radiative transfer codes to model emission of each COM: e.g., XCLASS (Schilke+), Weeds (Maret+ 2011), CASSIS (Caux+), MADEX (Cernicharo+)

COMs in hot cores

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COMs tracing different "temperature" regimes



JCMT/IRAM 30 m survey of COMs toward 7 hot cores: (Bisschop+ 2007)

- COMs classified as either "cold" (T_{rot} < 100 K) or "hot" (> 100 K)
 - ⇒ two distinct regions (N-containing COMs only in "hot" region)
- "hot" species: high abundances, similar T_{rot} , correlations between COMs \Rightarrow common solid state formation scheme

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But some of the "hot" species do also exist in colder regions:



- NH₂CHO and CH₃C(O)NH₂ in Sgr B2(N) with ARO 12 m and SMT (Halfen+ 2011):
 - both molecules trace two "temperature" components
 - see also GBT detections of COMs in Sgr B2 with low T_{rot} (Hollis+ 2004, Remijan+ 2008, Zaleski+ 2013, Loomis+ 2013)

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- significant contribution of colder, extended envelope for HNCO and CH₃OH in "line-poor" massive YSOs (Fayolle+ 2015)

Chemical differentiation in Orion-KL

N- and O-bearing COMs at different locations (Blake+ 1987): different thermal history (Caselli+ 1993)? different grain mantle composition (Charnley+ 1992)?



Orion KL, ALMA-SV (Crockett+ 2014)

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 acetone CH₃C(O)CH₃ distribution more related to N-bearing COMs (Peng+ 2013), same conclusion for ethanol C₂H₅OH (Feng+ 2015)

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- acetone CH₃C(O)CH₃ distribution more related to N-bearing COMs (Peng+ 2013), same conclusion for ethanol C₂H₅OH (Feng+ 2015)
- Analysis of Herschel/HIFI line survey based on velocity components (HEXOS, Crockett+ 2014): additional component, hot core (S), with O-bearing species

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 single-dish attempt to probe N/O differentiation in 12 other hot cores inconclusive due to lack of angular resolution (Fontani+ 2007)

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Sgr B2(N), PdBI (Belloche+ 2008)

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 $\Rightarrow~$ detailed understanding of N/O chemical differentiation will benefit a lot from ALMA

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Constraints on chemistry from series of COMs

Series of alkyl cyanides in Sgr B2(N): (Belloche+ 2009)

▶ detection of normal-propyl cyanide n-C₃H₇CN toward Sgr B2(N) with IRAM 30 m telescope ⇒ column density ratios CH₃CN/C₂H₅CN/C₃H₇CN = 108/80/1

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⇒ expanding COM series sets constraints on their formation process

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- [*i*-C₃H₇CN]/[*n*-C₃H₇CN] well reproduced by hot-core chemical model of R. Garrod (First inclusion of branched alkyl molecules in a chemical network!)



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- dominant route for *i*-C₃H₇CN: ĊN + CH₃ĊHCH₃
 (addition of H to propene CH₂=CHCH₃ strongly favors CH₃ĊHCH₃ over ĊH₂CH₂CH₃, Curran 2006)

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• α -amino acids have a branched heavy-atom backbone:

 \Rightarrow detection of *i*-C₃H₇CN **bodes well for presence of amino acids** in the ISM!

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Outlook

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- ► ALMA: broad bandwidth, high sensitivity, high angular resolution, excellent data quality ⇒ perfect machine to test predictions of chemical models:
 - search for new COMs in the ISM (branched molecules? chiral molecules? glycine?), in particular expand series of COMs
 - map chemical differentiation in large sample of hot cores
 - ALMA+ACA ideal to map radial distribution of COM emission

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- ► NOEMA: survey mode: 250 kHz channels over 16 GHz bandwidth ⇒ excellent line survey machine for northern sources!

(+ band 1 down to 72 GHz? \Rightarrow lower line confusion!)

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one (of many) challenge(s): accurate spectroscopic predictions needed!
 Example: ethanol C₂H₅OH

ALMA helps improving spectroscopic predictions!

LTE model with official JPL entry of ethanol on top of ALMA Sgr B2(N) spectrum:



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ALMA helps improving spectroscopic predictions!

LTE model with official JPL entry of ethanol on top of ALMA Sgr B2(N) spectrum:



New predictions with gauche a-dipole components turned positive:

⁽H. Müller, priv. comm.)

