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Why studying COMs?

Complex Organic Molecules (COMs): C-bearing molecules with 6 or more atoms

→ classics like methanol (CH₃OH) or methyl cyanide (CH₃CN), but also more complex: Di-methyl ether (CH₃OCH₃), methyl formate (CH₃OCHO), or Acetaldehyde (CH₃CHO)

In our case: investigation of COMs **NOT** for reasons of establishing astro-biology (COMs → pre-biotic molecules → pre-conditions for life)

Instead: COMs as astro-chemical tools to constrain physical conditions and evolution of higher-mass star-forming regions

Early stages of higher-mass SF

Infrared-dark clouds (IRDCs) still a good hunting ground to look for these stages

Important: IRDCs are a heterogeneous class of objects!

Besides a large variety of shapes, sizes and contrasts, also differences in properties of embedded objects

MPIA has a Herschel Key Program to investigate the FIR continuum properties of such early stages: EPoS (PI: O. Krause)

→ many sources for our line investigation drawn from the EPoS sample

Early studies of the gas content

Single-dish studies to check for (dense) gas content:

Carey et al. 1998: H₂CO Teyssier et al. (2002): ¹³CO + C¹⁸O Pillai et al. (2006): NH₃



The Brick G0.253+0.016



The Snake G11.11-0.12





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Early studies of the gas content

H₂E⁺ Contours 33⁺ 34⁺ 35⁺ 35⁺



(using the 14-m FCRAO telescope \rightarrow beam size of ~45")

Ragan et al. 2006:

with 41 IRDCs in

C¹⁸O(1-0)

N₂H⁺(1-0), CS(2-1),

Observational paper

→ Gibson et al. 2009 used this data set, enhanced by additional pointed observations in higher CS transitions

One of Sarah Ragan's IRDCs in N₂H⁺ and CS

→ First application of a chemical evolution code (Calgary) → studied IRDCs are chemically young ($10^{4.5} - \tau - 10^{5.5}$ years)

Advent of broad-band for receivers and backends

Mopra antenna in Australia



22-m antenna for observations up to 116 GHz (3-mm band) (beam size of ~36")
8 GHz bandwidth and up to 16 spectral zoom windows → used by many groups in the typical 90 GHz set up (86-94 GHz) mainly tracing the "big four": HCO^+ , HCN, HNC, N_2H^+

Vasyunina et al. 2011

Sanhueza et al. 2012

Hoq et al. 2013

Miettinen 2014

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Advent of broad-band for receivers Average spectrum



→ used by many groups in the typical 90 GHz set up (86-94 GHz) mainly tracing the "big four": HCO⁺, HCN, HNC, N₂H⁺

Vasyunina et al. 2011 single points

Sanhueza et al. 2012 single points

Hoq et al. 2013 MALT90 maps

Miettinen 2014 MALT90 maps

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Tentative trends with evolutionary state



from Sanhueza et al. 2012

Note: While n_{crit} is very similar for HCO⁺(1-0) and N₂H⁺(1-0), n_{eff} is >10 x higher for N₂H⁺(1-0) than for HCO⁺(1-0) (Shirley 2015).

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Our single-dish study of southern IRDCs

Test case for the modelling: Vasyunina et al. 2012

Model: 0-D model (constant density and temperature over time) + complete chemical network with adsorption / desorption and grain surface reactions

Results:

- 0-D model can reproduce all simple molecules
- Surface reactions are important at the temperatures of 20-30K, especially for N₂H⁺

"Warm" cloud IRDC321.73-1 T = 22K



Vasyunina et al. 2014: Detection of COMs



Telescopes: Mopra, APEX, IRAM (20 – 100 mK rms) Species: CH3OH, CH3CCH, CH3CHO, CH3OCHO, CH3OCH3

Model: 0-D model + warm-up + complete network + reactive desorption

Results:

• One promising way to explain abundances of COMs in IRDCs is to warm-up the environment.

• Detailed shape of warm-up profile less important than duration of cold phase and final temperature level.

Work in progress: high-sensitivity multi-line study

Telescope: IRAM-30m Frequency: 99 – 107 GHz (5-6 mK); 218 – 225 GHz (14 mK)

Species: more than 25

Objects: 7 quiescent and intermediate IRDC sub-regions,

2 active IRDC sub-regions,

 \rightarrow often, a phenomenological classification is used depending on the presence of 8-µm and/or 24-µm compact emission sources within the IRDCs, and the detection of "green fuzzies" at 4.5 µm as shock indicators (implying star-formation activity)

see, e.g., Chambers et al. 2009

→ ad-hoc evolutionary sequence from <u>Quiescent</u> over <u>Intermediate</u> to <u>Active</u> IRDCs

Target Examples (I): quiescent IRDC locations



EPOS: Henning et al. 2010; Ragan et al. 2015

EPOS: Pitann et al. 2013

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Target Examples (II): quiescent and active IRDC locations



Sanhueza et al. 2013 See also their poster P38



e.g., Wang+ 2006; Rathborne+ 2006; Zhang+ 2009; EPOS: Tackenberg et al. 2014

Target Examples (III): transition sources



Pre-EPOS: Birkmann et al. 2007 EPOS: Ragan et al. 2012; Bihr et al. 2015a

Bontemps et al. 2010, Fechtenbaum et al. 2015

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Target Examples (IV): IR-bright high-mass protostellar objects (HMPOs)



e.g., Zhang et al. 2007, Araya et al. 2007

e.g., Cesaroni et al. 2014, Johnston et al. 2011

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High-sensitivity multi-line study II

Detected in quiescent IRDCs:

HCNH+, H2CS, SO, SO2(5), CCS, HC3N, CH2CO, CH3CCH, CH3OCH3(2), CH3OH(4), CF+(2), c-C3H2, C4H(2), I-C3H2(2), c-C3HD(2)

Detected in active IRDCs and HMPOs:

HCNH+, H2S, H2CS, SO, SO2, CCS, OCS, HC3N, HC5N, CH2CO, CH3OH, CH3CHO, CH3OCH3, CH3OCHO, HNCO, CH3CCH, CH3CN, c-C3H2, t-CH3CH2OH, NH2CHO, CH2CN, CH2NH, DC3N, CF+(4)

High-sensitivity multi-line study II

Detected in quiescent IRDCs:

HCNH+, H2CS, SO, SO2(5), CCS, HC3N, CH2CO, CH3CCH, CH3OCH3(2), CH3OH(4), CF+(2), c-C3H2, C4H(2), I-C3H2(2), c-C3HD(2)

Detected in active IRDCs and HMPOs:

HCNH+, H2S, H2CS, SO, SO2, CCS, OCS, HC3N, HC5N, CH2CO, CH3OH, CH3CHO, CH3OCH3, CH3OCHO, HNCO, CH3CCH, CH3CN, c-C3H2, t-CH3CH2OH, NH2CHO, CH2CN, CH2NH, DC3N, CF+(4)

High-sensitivity multi-line study III

Active IRDC: G28.34 P2

Quiescent IRDC: G28.34 C1



Chemical modelling: G28.34-C1 (quiescent)

Chemical code "ALCHEMIC" (Semenov et al. 2010) 1-D model (density and temperature structure)

Parameters of the best fit model:

Out of 21 species, 2 are not reproduced: CCS,H2CS Agreement: 83% Age ~60,000 yr

Modeling results:

• With 21 molecules, a 0-D model is not sufficient anymore even for a quiescent IRDC.

 Elevated temperature at the inner radius might indicate beginning of star formation. Hence, IRDC028-C1S might be in a more evolved phase than a starless core.

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Chemical modelling: G28.34-C1 (quiescent)



On all panels the grey area corresponds to observed value +/- error margin. Bottom right panel presents temperature and density profiles.

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Interferometers peek into the inner spatial structure of the clumps



Galactic longitude

The fine structure of the G28.34 **IRDC cloud complex**

I (degrees)

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Tan et al. 2013

ALMA Cycle-0 study toward one of the supposedly quiescent IRDC clumps: G28.34-C1, mainly using deuterated species



FOV shown is around 34" ... our IRAM high-sensitivity observations with HPBW~27" (16") are centred on C1-S

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Summary

Chemistry in IRDCs is far from boring! → beside the typical high-abundant dense-gas tracers, much more can be found In particular: complex organic molecules

→ inclusion of such tracers in chemical evolution codes can constrain better the chemical and thermal history of the IRDCs

→ multi-line studies also important to trace different physical conditions in an IRDC and hence to constrain the chemico-spatial structure

→ ALMA gives access to low-excitation transitions of complex molecules in the bands (1+2+)3 - 6

- → ALMA is incredibly sensitive: a prerequisite to detect rarer molecules in the typical kpc distances of most IRDCs
- → ALMA brings sufficient spatial resolution to distinguish different constituents (massive prestellar cores, deeply embedded protostars and hot cores) on a core scale (0.1 pc) → lift the degeneracy of the observational data which limits the complexity of chemical modelling