Molecular Spectroscopy with SKA

What are the pathways from atoms to simple diatomics to complex species?

What is the interplay between gas phase and solid phase synthesis?

What is the origin of organic matter in solar system and how is it related to the ISM? (meteorites, comets, planets & satellites)
• Over 170 species, most detected in the radio (cm to submm) domain; not including isotopologues

• Molecular line spectra depend on the environment: molecular abundances vary depending on the source properties & history
<table>
<thead>
<tr>
<th>2 atoms</th>
<th>3 atoms</th>
<th>4 atoms</th>
<th>5 atoms</th>
<th>6 atoms</th>
<th>7 atoms</th>
<th>8 atoms</th>
<th>9 atoms</th>
<th>10 atoms</th>
<th>11 atoms</th>
<th>12 atoms</th>
<th>&gt;12 atoms</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>C₃</td>
<td>c-C₃H</td>
<td>C₅</td>
<td>C₆H</td>
<td>C₆H</td>
<td>CH₃C₃N</td>
<td>CH₃C₄H</td>
<td>CH₃C₅N</td>
<td>H₂C₆N</td>
<td>c-C₆H₆</td>
<td>HC₁₁N</td>
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<td>C₂H</td>
<td>t-C₃H</td>
<td>C₄H</td>
<td>t-H₂C₄</td>
<td>CH₂CHCN</td>
<td>HC(O)OC₃H</td>
<td>CH₃CH₂CN</td>
<td>(CH₃)₂CO</td>
<td>CH₃C₆H</td>
<td>C₂H₆OC₃H</td>
<td>C₆₈* 2012</td>
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<td>C₃N</td>
<td>C₄Si</td>
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<td>CH₃C₂H</td>
<td>CH₃COOH</td>
<td>(CH₃)₂O</td>
<td>(CH₂OH)₂</td>
<td>C₂H₆OC₂H</td>
<td>n-C₃H₇CN</td>
<td>C₇₀*</td>
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<tr>
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<td>C₃O</td>
<td>t-C₃H₂</td>
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<td>HC₆N</td>
<td>C₇H</td>
<td>CH₃CH₂OH</td>
<td>CH₃CH₂CHO</td>
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<tr>
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<td>c-C₃H₂</td>
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<td>CH₃CHO</td>
<td>Ce₂H</td>
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<td>CH₃NH₂</td>
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<td>CH₄*</td>
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<td>t-H₂CHO</td>
<td>CH₃C(O)NH₂</td>
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<td>CO</td>
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<td>HC₃N</td>
<td>HC₃NH⁺</td>
<td>H₂CCOH</td>
<td>CH₂CHCHO</td>
<td>C₈⁻</td>
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<td>HCS⁺</td>
<td>HCNH⁺</td>
<td>HC₂NC</td>
<td>HC₂CHO</td>
<td>C₈H⁻</td>
<td>CH₂CCHCN</td>
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<td>C₈H⁻</td>
<td>H₂NCH₂CN</td>
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<td>HNCS</td>
<td>H₂CNH</td>
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<td>H₂S</td>
<td>HOCO⁺</td>
<td>H₂C₂O</td>
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<td>t-H₂C₄N</td>
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<tr>
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<td>HNO</td>
<td>H₂CN</td>
<td>HNC₃</td>
<td>c-C₃H₃O</td>
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<td>MgCN</td>
<td>H₂CS</td>
<td>SiH₄*</td>
<td>H₂CCNH(?)</td>
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<tr>
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<td>MgNC</td>
<td>H₃O*</td>
<td>H₂COH⁺</td>
<td>C₈N⁻</td>
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Molecular Spectroscopy with SKA

A few basic numbers:

Rotational lines → The line frequencies scale with the rotational constant $B \propto h/l$ ($\propto 1/\mu$ for a diatomic species) where $I$ the inertia momentum and $\mu$ is the reduced mass

$\text{CO} : B = 57 \text{ GHz}$

$\text{HC}_3\text{N} : B = 4.5 \text{ GHz}$

$\text{HC}_{11}\text{N} : B = 0.17 \text{ GHz}$

Rotational transitions in the SKA baseline domain → «heavy molecules» with $B \sim$ few GHz
Molecular Spectroscopy with SKA:
Other types of molecular transitions

- Rotational level splitting due to couplings of rotation with other properties (e.g., fine, hyperfine structure, $\Lambda$ doubling, etc.)

- Relatively low energies → transitions at GHz frequencies

Examples: OH, CH, NH$_3$
Lessons from spectral surveys

- Arecibo 4-6 GHz & 8-10 GHz (Kalenskii et al 2004)
  - needs <5mK sensitivity.
  - The line density is higher in the 8 - 10 GHz window and above.
- GBT PRIMOS (A. Remijan et al) 0.5 – 50 GHz
  - Several detections of new species towards SgrB2 (ethanimine, E-cyanomethanimine E-NHCHCN)
Sensitivity issues

- Thermal emission & line strengths
  - Brightness temperature limited by the kinetic/excitation temperature: 5 - 300 K
  - Small source sizes for complex molecules & warm regions: few arcsec
  - Line width: few km/s → high spectral resolution
  - Non LTE effects, masers
- Most suitable windows for complex species above 10 GHz
- NB: Even with the VLA imaging NH3 at high spatial resolution is not easy (Conf C with 0.9" 2mJy or 6 K rms at 0.2 km/s resolution in |5 hr)
A few important spectral diagnostics below 8 GHz

- OH 1.7 GHz (ground state) + excited lines (6 GHz, 13 GHz)
  - From diffuse to dense molecular gas + Masers & mega-masers
  - A good probe of $\text{H}_2\text{O}$ desorption (e.g. PDRs, comets)
- CH 3.3 GHz
  - A good probe of diffuse molecular gas with a constant abundance relative to $\text{H}_2$
  - Non LTE Excitation (weak maser)
OH FIR emission in the Orion Bar

Goicoechea et al 2011
Herschel PACS with ~10'' resolution
CH in molecular gas

Nakai et al. 2013, Effelsberg

Liszt & Lucas; comparison visible & radio data
A few important spectral diagnostics below 8 GHz

- $\text{H}_2\text{CO} \, ^{11}\text{CO}^{10} \, 4.8 \text{ GHz}$
  - Sensitive probe of molecular cores (absorption of the CMB)
  - Maser in star forming regions
- $\text{CH}_3\text{OH} \, 6.7 \text{ GHz}$
  - Maser in high mass star forming region: high angular resolution probe, proper motions
- Carbon chains ($\text{C}_8\text{H}, \text{C}_8\text{H}^-$) and cyanopolyynes ($\text{HC}_{11}\text{N}$)
  - Building molecular complexity
- Recombination lines ($\text{H, C, S,...}$)
  - Interfaces of ionized and neutral gas
Understanding the connection from ISM to the solar system

NH₃, NH₂D, ND₂H, ND₃, ¹⁵NH₃, ¹⁵NH₂D

Inversion lines in the cm regime for ND₃
Magnetic Field probes (Zeeman effect)

OH:
well demonstrated for ground state lines (~1.7 GHz);
can use the excited levels at eg 6GHz for probing high densities in star forming regions?

CH & Carbon chains (eg C₄H Turner & Heiles):
Similar sensitivity than OH but weaker lines. Not demonstrated yet: can provide complementary probes for different density or ionization fraction regimes.

Requires a very high S/N
OH in M17 (Brogan & Troland 2001)

VLA, 26'', ~ 12 hrs, 10mJy/beam