Millimeter and submillimeter tracers

- Remote sensing: no in-situ measurement possible
- Use information on
  - Images: Geometry, Structure
  - Spectrum: SED (photometry), lines
    - Physical conditions (T, n)
    - Velocity field
    - Chemical composition
  - Polarization
    - Magnetic field
  - Time Variability
    - Distance (parallax)
  - Evolution & Dynamics
The spectral energy distribution (SED)

- Continuum: dust thermal emission (+ other mechanisms)
- Spectral lines from
  - Molecules (mostly rotational transitions)
  - Atoms (fine structure lines)
  - Atoms (recombination lines)
  - Solids (ices), mostly in the IR
Dust emission (very simplified)

- At FIR and submillimeter wavelengths: modified blackbody with an emissivity $\varepsilon(\lambda)$

- $\varepsilon(\lambda)$ contains all the information on the dust composition. 
  $\varepsilon(\lambda) = \varepsilon_0(\lambda_0)(\lambda/\lambda_0)^{-\beta}$  $\beta \sim 2$ (can depend on $\lambda$, $T_d$, structure ...)

- $T_d$ is set by equilibrium between heating (FUV radiation) and cooling (FIR emission)
  
  $T_d \sim 16.4 \left(\frac{a}{0.1\mu m}\right)^{-1/15} U^{1/6}$ silicate $0.01 < a < 1 \mu m$
  
  $T_d \sim 22.3 \left(\frac{a}{0.1\mu m}\right)^{-1/40} U^{1/6}$ graphite $0.005 < a < 0.15 \mu m$

  $u^* = \text{energy density } ; U = u^*/\text{ISRF}$

Draine 2011
Dust emission (very simplified)

- Warmer grains for higher radiation fields
- The peak of the SED shifts to shorter wavelengths
- The PAH emission at short wavelengths scales with \( U \to \) can be used to trace the SFR

Draine 2011
FIR & submm fine structure lines - I

- “Forbidden” lines; collisional excitation is dominant
- [CII] $^2P_{3/2} \rightarrow ^2P_{1/2}$ 1.9 THz (158µm)
- [OI] $^3P_1 - ^3P_2$ (63µm) & ($^3P_0 - ^3P_1$) (145µm)

Draine 2011, Langer, Goldsmith, Pineda et al.; The Herschel GotC+ project, 2010 ... 2015
“Forbidden” lines; collisional excitation is dominant

Cooling lines → The energy input from massive stars (FUV radiation, mechanical heating) is balanced by gas cooling → Tracers of star formation rate

- [CII] 1.9 THz (158µm)
  Contribution from different ISM phases

- [OI] 63µm & 145µm
  - Gas cooling for higher density gas (as compared with [CII])
  - More violent phenomena: shocks, outflows?

*Langer, Goldsmith, Pineda et al.; The Herschel GotC+ project, 2010 … 2015*
FIR & submm fine structure lines - III

- [NII] Ionized gas $^3P_2 -^3P_1$ (205µm) & $^3P_1 -^3P_0$ (122µm)
  - N ionization potential is > 13.6eV → N$^+$ is mostly present in ionized gas: from HII regions to warm ionized medium
  - The ratio of the 2 lines is sensitive to the electron density

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Langer, Goldsmith, Pineda et al.; The Herschel GotC+ project, 2010 ... 2015
Fine structure lines in galaxies

Gracia-carpio et al., 2011
Gas pressure using carbon fine structure lines

- [CI] neutral/molecular gas $^3P_1 - ^3P_0$ (492 GHz) & $^3P_2 - ^3P_1$ (809 GHz)

Population fraction in the 1st excited level

Population fraction in the 2nd excited level

Jenkins & Tripp (2011)
Gas pressure from [CI] and [CII]

Gerin et al. 2015, Jenkins & Tripp (2011)
The variety of available molecular spectral lines

Guzman et al. 2014
Spectroscopic diagnostics

- Physical information from
  - Line intensities (eg SFR from [CII], masses, chemical diagnostics)
  - Line ratios (temperature, density, pressure, sizes)
  - Line profiles (velocity field, geometry, B)

- Radiative transfer (cf F Levrier's talk)
- Source Models (MHD, chemistry ...
Line identification – Preparation of observations

- Spectral line catalogs/data bases
  - Cologne Data base for Molecular Spectroscopy (CDMS)
    http://www.astro.uni-koeln.de/cdms
  - JPL http://spec.jpl.nasa.gov/
- Interfaces, combination of catalogs
  - Virtual Atomic and Molecular Data Center
    http://portal.vamdc.eu
  - Splatalogue http://www.cv.nrao.edu/php/splat/
- Collision cross sections
  - BASECOL http://basecol.obspm.fr/
  - LAMDA http://home.strw.leidenuniv.nl/~moldata/
Line identification – Preparation of observations: tools & package

- **CLASS/WEEDS**
- **CASSIS**
- **X-CLASS**
- Model of line emission/absorption using data base & “simple” radiative transfer
- Find “U” lines
- Identification of new molecules

*Iso-propyl-cyanide Belloche et al. 2014*
Computation of molecular line intensities

\[ T_R = f \left[ J_\nu(T_{ex}) - J_\nu(T_{bg}) \right] \left[ 1 - \exp(-\tau_\nu) \right], \]

- \( T_R \): observed line brightness temperature
- \( f \) source filling factor = \( \Omega s/\Omega b \sim (r/\text{HPBW})^2 \)
- \( \tau_\nu \): line opacity. Contains all information on spectroscopy + molecule density along the line of sight
- \( J(T_{ex}) = h\nu/k \left( 1/\exp(h\nu/kT_{ex}) - 1 \right) \)
- \( T_{bg} \): CMB, plus eventually the ambient radiation

\[ B_\nu(T) \equiv \frac{2h\nu^3}{c^2} \left[ \exp \left( \frac{h\nu}{kT} \right) - 1 \right]^{-1}. \]
Excitation temperature

- $T_{ex}$ defined for a transition as:
  
  \[ \frac{N_u}{N_l} \sim \frac{n_u}{n_l} = \frac{g_u}{g_l} \exp(-hv/kT_{ex}) \]

- $T_{ex} \rightarrow T_K$ at high density (Local Thermodynamic Equilibrium)

- $T_{ex} \rightarrow T_{bg}$ (2.73 K) for low densities

- $T_{ex}$ may be different for different lines. Out of LTE

- Some lines can have negative $T_{ex}$ (masers) or $T_{ex} < T_{bg}$ for specific excitation conditions leading to an excess population in the upper level (masers)
Computation of molecular line intensities

II

- For optically thin lines, $\tau_\nu \ll 1$ … … with a single $T_{ex}$
- $N_u$: colon density in the upper level, of energy $E_u$
- $N_{tot}$: total column density, $Q_{rot}$: rotational partition function at $T_{ex}$

\[
N_u = \frac{3h}{8\pi^3 |\mu_{lu}|^2} \left[ \exp \left( \frac{h\nu}{kT} \right) - 1 \right]^{-1} \int \tau_\nu d\nu.
\]

\[
N_{tot}^{thin} = \left( \frac{3h}{8\pi^3 S\mu^2 R_i} \right) \left( \frac{Q_{rot}}{gJgKg_l} \right) \exp \left( \frac{E_u}{kT_{ex}} \right) \left[ \exp \left( \frac{h\nu}{kT_{ex}} \right) - 1 \right]^{-1} \int \frac{T_R d\nu}{f \left( J_\nu(T_{ex}) - J_\nu(T_{bg}) \right)}.
\]

Simple LTE predictions in line identification softwares like CLASS/WEEDS, CASSIS ...
Molecule excitation

● Collision excitation & de-excitation (H₂, He, H, e-)

● Radiative excitation: same frequency + pumping at shorter wavelengths through vibrational or other rotational lines

● Chemical pumping (excess energy in the molecule formation process)

● Radiative de-excitation (line emission)

\[
A_{ul} \equiv \frac{64\pi^4\nu^3}{3hc^3} |\mu_{lu}|^2.
\]

\[
n_i \left[ \sum_j \left( n_{\text{collider}} C_{ij} + B_{ij} \int_0^\infty J_\nu \phi_{ij}(\nu) d\nu \right) + \sum_{j<i} A_{ij} \right] \\
= \sum_j n_j \left( n_{\text{collider}} C_{ij} + B_{ji} \int_0^\infty J_\nu \phi_{ji}(\nu) d\nu \right) \\
+ \sum_{j>i} n_j A_{ji}. \tag{3}
\]

Shirley & Mangum 2015
Excitation temperature & critical density

The critical density $n_{\text{crit}}$ is defined as:

$$n_{\text{thin, no bg}}^{\text{crit}} = \frac{A_{jk}}{\sum_{i \neq j} \gamma_{ji}} = \frac{A_{jk}}{\sum_{i<j} \gamma_{ji} + \sum_{i>j} \frac{q_i}{g_j} \gamma_{ij} e^{-(E_i-E_j)/kT_k}}.$$  

- $n_{\text{crit}}$ depends on the line, on $T_K$.
- $n_{\text{crit}}$ defines the regime where $T_{\text{ex}}$ starts to approach $T_K$.
- It does not define the density regime where a specific line is emitted.
- Shirley defines $n_{\text{eff}}$, the density corresponding to a 1Kkm/s line intensity for a reference column density: $n_{\text{eff}} \ll n_{\text{crit}}$.

Maret et al., Shirley 2015
$n_{\text{eff}}$ and $n_{\text{crit}}$
The limit of low collisional excitation

- For gas with low densities, $T_{ex}$ is close to $T_{bg}$, so most molecules are in the ground state.
- In this limit, every upward collision will trigger the emission of a photon which will eventually escape the medium. The intensity scales with $N_{mol}$ and $n(H_2)$
- For example: extended H$_2$O ground state emission with $n_{crit} \sim 10^8$ cm$^{-3}$

Melnick et al. 2011, Linke et al. 1977
CO Rotational lines: I

- Low dipole moment (0.1D), the ground state transition is easily thermalized ($n_{\text{crit}} \sim 10^3 \text{ cm}^{-3}$)

- A large number of transitions from low $T_{\text{ex}}$ material (cold and/or diffuse) to high $T_{\text{ex}}$ (warm and dense)

- Each transition is most sensitive to the regions with $T_{\text{ex}} \sim E_u$
CO rotational lines II

- 5 Isopologues with similar spectroscopic properties & different abundances → lines with different opacities.

\[ {}^{12}\text{CO}:{}^{13}\text{CO}:{}^{18}\text{O}:{}^{17}\text{O}:{}^{13}\text{C}^{18}\text{O} \sim 500:8:1:0.4:0.02 \]

- \(^{12}\text{CO}\) transitions have high opacities → The line brightness can be used to get \( T_{ex} \sim T_K \)

- Use \( T_{ex} \) from \(^{12}\text{CO}\) to derive the opacity of the \(^{13}\text{CO} \) .. or \(^{18}\text{O}\) lines assuming the molecules are co-spatial and have the same excitation

\[
T_{ex} = \frac{h\nu/k}{\ln \left( 1 + \frac{h\nu/k}{T_R/f + J_\nu(T_{cmb})} \right)} \quad \text{(if} \ \tau \gg 1) \]

Application, CO excitation in the Galactic Center: a template for external galaxies?

Hot CO: $T \sim 1000$ K, $n \sim 5000$ cm$^{-3}$

Goicoechea et al 2013
Other temperature diagnostics: \( \text{NH}_3 \)

- Symmetric top molecule \((J, K)\) with inversion (~23 GHz)
- The lowest level of K-ladder is metastable
- The ratio of the populations of the 1,1 and 2,2 levels is determined by collisions and therefore measures the kinetic temperature

\[
T_{1,2} = -\frac{T_0}{\ln \left[ \frac{9}{20} \times \frac{\tau(2_2)}{\tau(1_1)} \right]}
\]

\( T_0 \approx 41.7\text{K} \)

“Mangum & Shirley 2015, Maret et al. 2009”
Other temperature diagnostics: \( \text{NH}_3 \)

Knowing the collision cross sections, \( T_K \) can be deduced from \( T_{\text{rot}} \).

The excitation can be sensitive the \( \text{H}_2 \) spin state: o-H\(_2\) or p-H\(_2\).

\[
T_{1,2}^A = T \left\{ 1 + \frac{T}{T_0} \ln \left[ 1 + \frac{C (2 \rightarrow 2_1)}{C (2 \rightarrow 1_1)} \right] \right\}^{-1},
\]

Maret et al. 2009
Other temperature & density probes

- Symmetric top molecules ($\text{CH}_3\text{CN}$, $\text{CH}_3\text{CCH}$, ...) series of JK-J-1K transitions at the same frequency → $T$ probes

- $\text{H}_2\text{CO}$ : pairs of transitions can be used to probe either the density or the temperature

- $\text{CH}_3\text{OH}$ : bands

Wang et al. 2011
**CH$_3$OH**

- Single temperature models
- Temperature gradient

Wang et al. 2011
Sounding the gas content : HI 21cm

- Optically thin gas for $N$(HI) $\leq 10^{20}$ cm$^{-2}$

$$\tau_\nu = 2.190 \frac{N(HI)}{10^{21}\text{ cm}^{-2}} \left( \frac{100K}{T_{spin}} \right) \left( \frac{1\text{ kms}^{-1}}{\sigma_V} \right) e^{-u^2/2\sigma_V^2}$$

$$\int (T_A - T_A^0) du = \int \frac{c^2}{2kBv^2} [I_\nu - I_\nu^0] \frac{c}{\nu} dv = \frac{3h\nu^2\chi_{ul}}{32\pi k_B} A_{ul} N(HI)$$

$$N(HI)\text{ (cm}^{-2} = 1.82 \times 10^{18} \int T_A dv K\text{ kms}^{-1}$$

- $T_{spin}$ = excitation temperature. $n_u/n_l = g_u/g_l e^{-hv/kT_{spin}} = 3 e^{-hv/kT_{spin}}$

Efficient thermalization of the hyperfine levels, given the low difference in energy

- The HI column density from emission is independent of $T_{spin}$ (in the optically thin limit) $\rightarrow$ both phases (CNM + WNM) contribute to the emission

- The opacity scales inversely with $T_{spin}$ : the CNM dominates the absorption
Derivation of the HI spin temperature

Comparison of spectra towards a bright continuum source (ON) and nearby (OFF)

Assumption: same properties along both sight-lines

ON source:

\[ T_{A}^{on}(v) = T_{S}e^{-\tau(v)} + T_{spin}(1 - e^{-\tau(v)}) \]

OFF source:

\[ T_{A}^{off}(v) = T_{CMB}e^{-\tau(v)} + T_{spin}(1 - e^{-\tau(v)}) \]

These 2 equations can be solved to determine \( \tau(v) \) and \( T_{spin} \):

\[ \tau(v) = \ln\left[ \frac{T_{S} - T_{CMB}}{T_{A}^{on}(v) - T_{A}^{off}(v)} \right] \]

\[ T_{spin} = \frac{T_{A}^{off}(v)T_{S} - T_{A}^{on}(v)T_{CMB}}{[T_{S} - T_{CMB}] - [T_{A}^{on}(v) - T_{A}^{off}(v)]} \]
• HI Spin Temperature:
• CNM: 30 – 150 K; WNM > 2000 K;
• unstable phase ~ 500 K

*Murray et al., 2014, Heiles & Troland 2003*
Sounding the gas content: \( \text{H}_2 \)

- \( \text{H}_2 \) is difficult to detect
  - Electronic transition in the FUV (from space)
  - Rotational transition in the MIR (12, 17, 28 \( \mu \text{m} \)) (space, marginally from the ground). Not sensitive to cold gas
  - Ro-vibrational transitions in the NIR (2.1 \( \mu \text{m} \)). From the ground. Emission is mostly pumped by FUV absorption → very specific regions (PDRs)
- Finding alternate tracers of \( \text{H}_2 \)
Sounding the gas content: \( \text{H}_2 \) from CO J = 1-> 0 emission

- CO is relatively easily formed, and excited. CO excitation depends most on the gas pressure.

- Empirical factor \( W_{\text{co}} = \frac{N(\text{H}_2)}{I_{\text{co}}} \sim 2 \times 10^{20} \text{ cm}^{-2}/\text{Kkm}s^{-1} \) calibrated by observations, and chemical models.

- Still some molecular gas is not fully traced by CO “CO-dark” gas.
Sounding the gas content: other $\text{H}_2$ tracers

- $[\text{CH}] \sim 3.5 \times 10^{-8}$
  Lines in the visible, FIR & cm ($\Lambda$ doubling 3.3 GHz)
- $\text{OH} \sim 10^{-7}$ (TBC)
  Lines in the near UV, FIR and cm ($\Lambda$ doubling 1.7 GHz)
- $\text{HF} \sim 1.2 \times 10^{-8}$
  FIR lines. At high redshift $\text{F}$ abundance?
- CCH, HCO$^+$, CF$^+$ absorption

Checking the consistency

- Comparison of CO emission with HI, CH (H$_2$), C+ (H+H$_2$) absorption along a sight-line in the Galactic plane
- $W_{CO} \sim 1 - 2 \times 10^{20}$ cm$^{-2}$/Kkms$^{-1}$

Liszt & Gerin 2015
Chemical diagnostics: “snow line”

- Molecules freeze on dust grains in cold & UV-shielded regions
- Low ionization fraction \( \text{ne}/n(H_2) \sim 10^{-8} \), maintained by CR ionization of \( H_2 \rightarrow H_3^+ \)
- Protonated molecular ions are formed from \( H_3^+ \). (e.g. \( N_2H^+ \))
  Destruction by dissociative recombination with electrons and by reactions with neutrals (e.g. CO) → higher abundance when CO is frozen → indirect probe of the snow lines
- Strong enhancement of deuterated species through reactions like \( H_3^+ + HD \rightarrow H_2D^+ + H_2 \ldots H_2D^+ + N_2 \rightarrow N_2D^+ + H_2 \)
- Target species: \( N_2H^+ \), DCO\(^+\), \( N_2D^+ \)
Some examples of “snow line”

$^{13}\text{CO}$  \hspace{2cm} \text{HCO}^+$  \hspace{2cm} \text{N}_2\text{H}^+$

$^{13}\text{CO}(1-0)$ \hspace{2cm} \text{HCO}^+(1-0) \hspace{2cm} \text{N}_2\text{H}^+(1-0)$

$K \ (T \text{mb})$

$\delta_1 \ (\degree)$

$0.1 \ 1 \ 10$

$0.1 \ 1$

$N_2H^+$ appears only in the filaments while HCO$^+$ is very extended:

strong variation of abundances

Pety et al., in prep
Measurement of the depletion factor using DCO\(^+\) and N\(_2\)D\(^+\) in the L183 dense core

- Several transitions
- LVG models
- Chemical model

Pagani et al. 2011
The snow line in disks

Oberg et al., 2015
● O chemistry initiated by CR ionization of H ; followed by the charge transfer reaction: $\text{H}^+ + \text{O} \rightarrow \text{O}^+ + \text{H}$

● Series of hydrogen abstraction reactions $\text{OH}_{n-1}^+ + \text{H}_2 \rightarrow \text{OH}_n^+ + \text{H}$

● $\text{OH}^+$, $\text{H}_2\text{O}^+$, $\text{H}_3\text{O}^+$ : present in gas with increasing $\text{H}_2$ content; with abundances scaling with $\zeta$

_Hollenbach et al. 2012_
Chemical diagnostics: CR ionization rate

\[ \zeta \sim 2 \times 10^{-16} \text{ s}^{-1} \]

OH+ : gas with a low \( f(H_2) \sim 5\% \)

\[ f(H_2) = \frac{2n(H_2)}{n(HI) + 2n(H_2)} \]

- Indriolo et al. et al. 2015
- Gonzalez-Alfonso et al.
- Spliker et al. (ALMA)
Chemical diagnostics: isotopic ratios

- Use Molecules with different isotopes (CO, CS, ...) to determine isotopic ratios:
  - $^{12}\text{C}/^{13}\text{C}$ ; $^{14}\text{N}/^{15}\text{N}$ ; $^{16}\text{O}/^{18}\text{O}$ ; $^{32}\text{S}/^{34}\text{S}$ ; $^{28}\text{Si}/^{29}\text{Si}$ ; $^{35}\text{Cl}/^{37}\text{Cl}$; $^{36}\text{Ar}/^{38}\text{Ar}$ …
- Constraints on chemical evolution

Muller et al. 2014
Using the velocity information

- Infall signature: optically thick line with blue shifted emission peak and redshifted absorption
- The line profiles depend on the excitation gradient along the line of sight & velocity field

Caselli et al. 2012
Using the velocity profile: outflows and shocks

- Line wings up to high velocities → shock velocity
- Using CO lines, comparisons with shock models: determination of mass, momentum & energetics
- Rotational excitation up to very large quantum numbers (~40!)
- Shocks show up more clearly for high $J_u$ (eg $>6$)
- CO lines can be optically thick even in the wings

Gusdorf et al.
Accretion shock

IRAS 04368+2557: a protostar with a disk / envelope structure
Strong change of chemistry at the envelope/disk transition: signature of the accretion shock?

Sakai et al. 2014
MHD Collapse models

Formation of a pseudo-disk

Accretion & Ejection: molecular outflow

Ciardi & Hennebelle
Commercon et al.
Chemical information: comparison of CH$_3$OH with H$_2$O & CO

- CH$_3$OH seen at less extreme velocities than H$_2$O
- CH$_3$OH abundance lower than in ice
- CH$_3$OH destruction in the sputtering process more efficient than for H$_2$O
- Fast H$_2$O formed in the gas

Suutarinen et al. 2014
Time variability

- IRC+10216, the brightest carbon star
- Strong variation in the IR
- 1st evidence for variation in spectral lines.

Teyssier et al. 2014
Some References

Draine 2011 Book “Physics of the interstellar and intergalactic medium”
Mangum & Shirley arXiv1501.01703
Atmospheric transmission

Excellent at millimeter wavelengths
More restricted at submillimeter wavelengths
The important parameters