Radiative transfer & molecular data for far-infrared astrophysics

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Goals of radiative transfer calculations

- Dust continuum: estimate mass
  - input: temperature (assumed or calculated from $L$)
  - dust opacity parameter: e.g. Shirley et al 2011

- Line shape: kinematics
  - tools: line profiles, channel maps, P-V diagrams ..

- Line ratio: physical conditions
  - excitation model: thermal / statistical equilibrium
  - radiative & collisional contributions

- Line intensity: molecular column density
  - alternative mass estimate (especially CO)
  - need physical conditions first
  - compare abundance with chemical model: age, $\zeta_{\text{CR}}$ ..
Radiative transfer: limitations

- Resolution mismatch
  - emission vs absorption

- Unresolved substructure
  - clumps

- Incomplete coverage
  - spatially
  - energy levels

- Missing molecular data
  - spectroscopy
  - collisions
Basic radiative transfer: single-\( T_{\text{ex}} \) ("LTE")

- Estimate excitation temperature & column density
  - straightforward, only need spectroscopic data
  - assume Boltzmann distribution (HIFI can test this!)
  - full-spectrum version: line survey (e.g., Crockett / Neill)
Correction for optical depth & source size

- SMA observations
  - CH$_3$CN 18$_K$-17$_K$ band
  - dense clumps in Orion-KL
- Detect 9+3 lines in 5 clumps
  - 3 show 2 V-components
  - assume single size, $T$
  - fit $N$, $T$, $\tau$, size

Goldsmith & Langer 1999; Wang et al 2010
Semi-advanced RT: Statistical equilibrium

- Uniform medium, constant level populations
  - global (not detailed) balance
  - radiative & collisional processes
  - breaks down e.g. for reactive species (CH$^+$, OH$^+$)
- Treat line opacity with LVG (?) or escape probability method
  - estimate $T_{\text{kin}}$, $n(\text{H}_2)$ & $N(\text{mol})$ for $\tau < \sim 100$
  - need collision data
Example: Molecular line ratios

- RADEX program: Van der Tak et al 2007
  - input: molecular spectroscopic & collision data
  - calculate line ratios as function of $n$ & $T$
  - CS often probes $n$, NH$_3$ & H$_2$CO probe $T$

JCMT observations of H$_2$CO in W49A: Nagy et al 2012
Advanced RT: Non-local methods

- Excitation and radiation field mutually dependent
  - solve statistical equilibrium locally
  - shoot rays / propagate photon packages through model
  - iterate toward solution
- Common assumption: spherical / cylinder symmetry
  - many-level problem: slow convergence
  - and uncertain convergence
- Methods: iteration / Monte Carlo / multi-zone esc. prob.
  - test / constrain physical / chemical model
  - many parameters: need detailed observations
Example 1D: High mass protostar

- Detect 14 (isotopic) H$_2$O lines
  - envelope / outflow / foreground
  - physical structure from continuum
  - Ratran modeling of lines
- Kinematics
  - turbulence increasing outward
  - infall speed increasing outward (?)
  - high accretion rate
- Chemistry
  - outer envelope: most H$_2$O frozen out
  - inner envelope: all O in H$_2$O

Herpin et al 2012
Example full radiative transfer calculation (2D)

• **SMA spectral images**
  • CO, $^{13}$CO, C$^{18}$O lines
  • protoplanetary disk IM Lup

• **Test two models to uv data**
  • old model: small emission
  • need to extend the disk
  • density drop at 400 AU

*RATRAN program*

Hogerheijde & van der Tak 2000; Panič et al 2009
Example full radiative transfer calculation (3D)

- **Galaxy merger at** $z=3.26$
  - SPH simulation (N=2M) (Sommer-Larsen)
  - CO line profile and map

*LIME code: Brinch & Hogerheijde 2010*
Molecular input data

- **Spectroscopy**: >500 entries in JPL/CDMS catalogs
  - energy levels, statistical weights
  - line frequencies, Einstein A coefficients
  - many species / isotopes / vibrational states
  - **Most data at low frequencies:**
    - high frequency predictions uncertain / unavailable
    - especially HIFI above 1 THz

- **Collisions**: >32 entries in LAMDA/BASECOL catalogs
  - only most common molecules: scalings like $\text{H}_2\text{O}$ to $\text{H}_2\text{S}$
  - limited isotope coverage: effect neglected ($\text{C}^{34}\text{S}$ vs HDO)
  - limited vibrational excitation: neglected / LTE assumed
  - limited state / energy coverage: extrapolation
  - sometimes He as proxy for $\text{H}_2$
Collision calculations: status

- Early work (<2000, Green et al):
  - closed shell molecules (CO, CS, ...)
  - He as collision partner
  - simplified PES

- More resources (both CPU and €) recently:
  - collision partner $\text{H}_2$ (rates $\sim 3\times$ larger)
  - accurate PES, dynamics at close coupling level
  - open shell molecules (CN)

- But: $>170$ molecules known in space, have CRC for $\sim 30$
  - detection rate $\approx$ calculation rate (few/yr)
  - gap widening, convergence unlikely
Recent collision calculations

- **HCN, HNC – He**: Sarrasin, Dumouchel et al 2010
- **CH$_3$OH – He, H$_2$**: Rabli & Flower 2010, 2011 (incl torsion)
- **H$_2$O– H$_2$**: Dubernet, Daniel et al 2009 – 2011 (complete!)
- **HDO– H$_2$**: Wiesenfeld et al 2011
- **SO$_2$ – H$_2$**: Cernicharo et al 2011
- **HF – H$_2$**: Guillon & Stoecklin 2011
- **C$_2$H – He**: Spielfiedel et al 2012
- **HCl – He**: Lanza & Lique 2012
- **HCN – H$_2$**: Ben Abdallah et al 2012 (incl hyperfine)
- **CN – H$_2$**: Kalugina et al 2012 (incl hyperfine)

Expensive calculations: first PES, then dynamics

$\approx$1 man-year per molecule (isotopes faster)
only a few specialists can do this
A well-studied case: $\text{H}_2\text{O}$

- Quantum rates now available for wide $T$-range
  - 45 rotational levels = up to bending mode
  - ortho & para $\text{H}_2$ and $\text{H}_2\text{O}$
- Pre-2011 work often uses quasi-classical rates
  - usually OK within factor of 2
  - low density, low abundance: up to factor of 3

F. Daniel et al 2012
A rare case: experimental verification

- Pressure broadening coefficient
  - same PES as for CRCs
  - can be measured in lab
- Good agreement at $T > 80$ K
  - verifies PES
  - o/p $\approx 3$ (black)
- Sharp drop at lower $T$
  - impact approximation?
  - ortho-para conversion!
  - $T$(ice) $< 40$ K
  - also in ISM?

Drouin & Wiesenfeld 2012; also s2s by Yang et al 2012
Hyperfine selective collisions: CN and HCN

- Non-zero nuclear spin causes “hyperfine” splitting
  - most common cases: $^{14}\text{N}$ and $^2\text{D}$
  - ratios often assumed in LTE ... is that true?
- Consider 3 sets of collision rates:
  - close coupling (solid)
  - IOS (dashed)
  - statistical (dotted)
- Assumption fine for $\tau < 10$
  - else underestimate $\tau$ by $\sim 2x$
  - ratios $\sim$statistical, not LTE
  - example: $N(\text{HCN}) = 10^{15} \text{ cm}^{-2}$
Future developments

- **Automated data fitters**
  - crucial for large data streams
  - still limited to level-2 RT ...

- **Coupling of gas and dust RT**
  - thermal balance + chemistry
  - making model takes ~1 yr ...

- **Merging / streamlining of databases**
  - spectroscopy: merged into Splatalogue
  - ongoing effort = VAMDC (careful: updates / credits)

- **Collision data for other molecules / more (IR) lines / high \( E,T \)**
  - CH, p-H\(_2\)CO, NH\(_3\) on o-H\(_2\) (incl hyperfine), e\(^-\) ... organics ...