Splinter on PDR/XDR models

Background:

The differences in the model comparison are totally dominated by gas temperature differences. **The heating efficiency is the critical parameter for the CO ladder.**

Effects of debated microphysics/chemistry:

Fixed processes with unknown/uncertain parameters

Convergence/major progress on:

- Coolants
  - traditional coolants; OI, CII, H_2, Ly α, CO, H_2O, ^{13}CO, OH, ...
    - should take full rotational or ro-vib description
  - Ionic coolants important in case of significant hard radiation: NeIII, OIII, MgII …
    - needed in case of XDR contributions or enhanced CR
- IR/UV pumping
  - Approximations/omissions in molecule description and RT
    - use full ro-vib description for affected molecules
  - relevant if UV input is large enough that thermal re-emission creates significant MIR/FIR field
    - pumping of H_2O, OH, …
    - CO only in extreme cases
- H_2 formation rate
  - Hot-dust H_2 formation needed
    - Formalism based on Cazaux & Tielens
    - Consistency with Jura (1974) to be checked
  - Major boost of warm gas temperature and resulting high-J CO
- H_2 level treatment → vibrational heating
  - H_2* is essential for chemistry
  - many levels needed if chemistry depends on particular levels
    - in most cases reduced set accurate enough

Remaining main uncertainty on:

- Gas-grain thermal coupling
  - Accomodation coefficient unknown
    - stick to “standard value”
  - Affects temperature of dense regions
- CO collisional excitation
  - H_2 well established now (Yang 2010)
  - H still uncertain
    - wait for new results from Phil Stancil
  - electrons and formation excitation relevant in extreme cases
- Ices, grain surface chemistry
  - important if cold
  - not that relevant for warm CO in PDRs/XDRs
- PAH physics
  - To large degree unknown
  - Does H_2 form on PAHs?
    - May significantly change gas temperature and CO excitation!

Variable parameters/processes to be set per source

- Elemental abundances:
  - Galactic gradient, “There is more than a single metallicity number.”
    - Main effect: e^- density, chem. Network
  - potentially significant impact on temperature
- SED of illuminating UV field
  - Uncertainty: Spectral shape of input UV field at short wavelengths from HII/HI layer
  - Proposed solution: treat by tabulated UV from HII region
    - Suppression of high-J CO at moderate UV fields
- Turbulent velocity
  - Current models inconsistent with turbulence models
    - Implement variable, Larson-type relation as function of depth
  - small impact on CO ladder expected
- PAH abundance
  - major impact on e^- density
    - changes PE efficiency and resulting gas temperature
- Dust grain distribution
  - UV/IR connection
    - affects all major heating processes