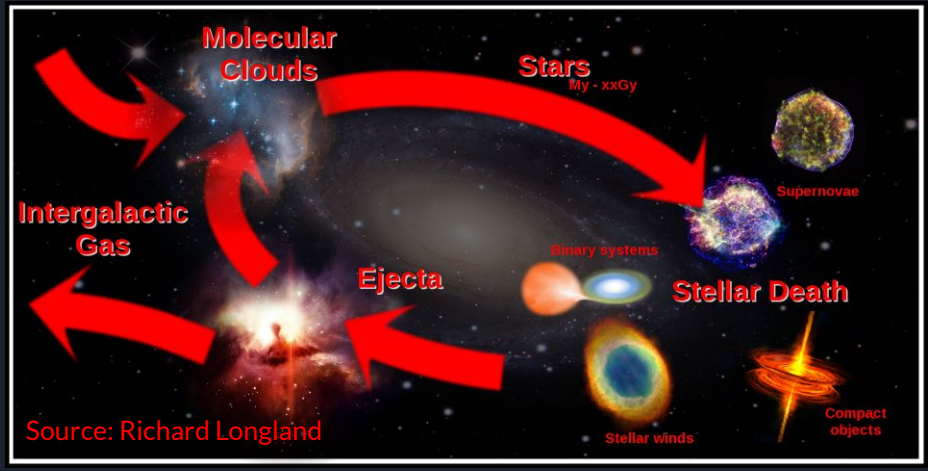
Molecular transitions in supernova spectra

From quantum chemistry to astrophysics

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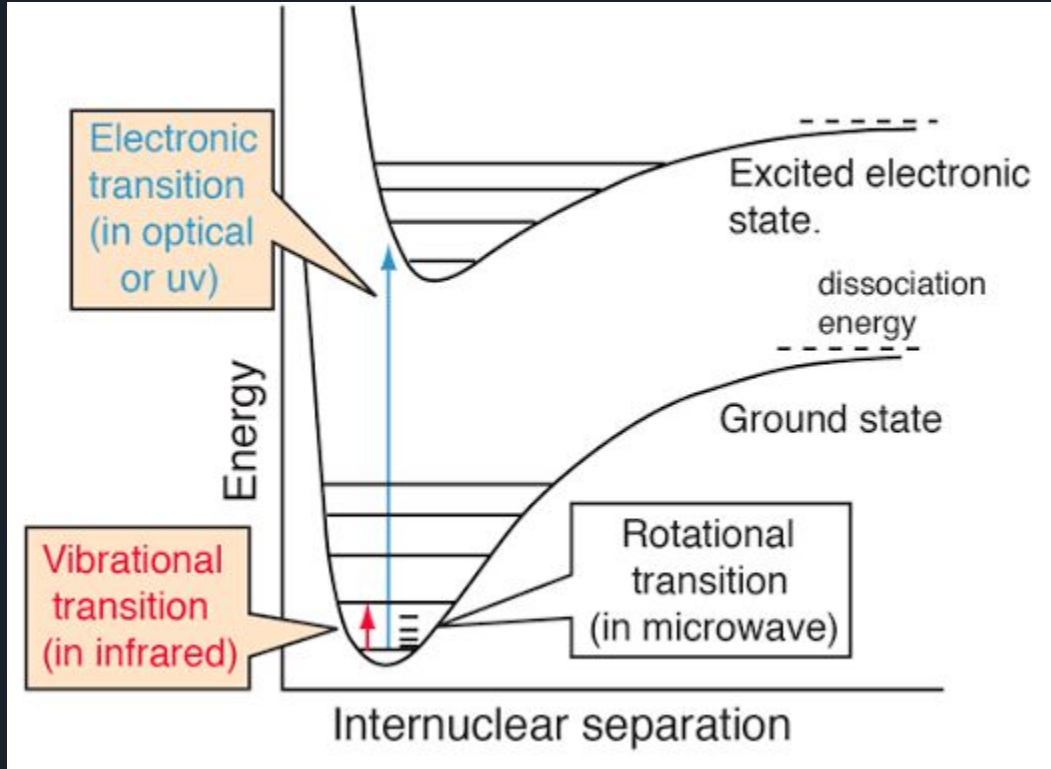
Supernovae in galactic evolution

- Supernovae (SNe) play an important role in galactic chemical evolution
- We found a lot of molecular lines and dust
- Molecular research is a new topic in supernovae (high temperature, high energies)



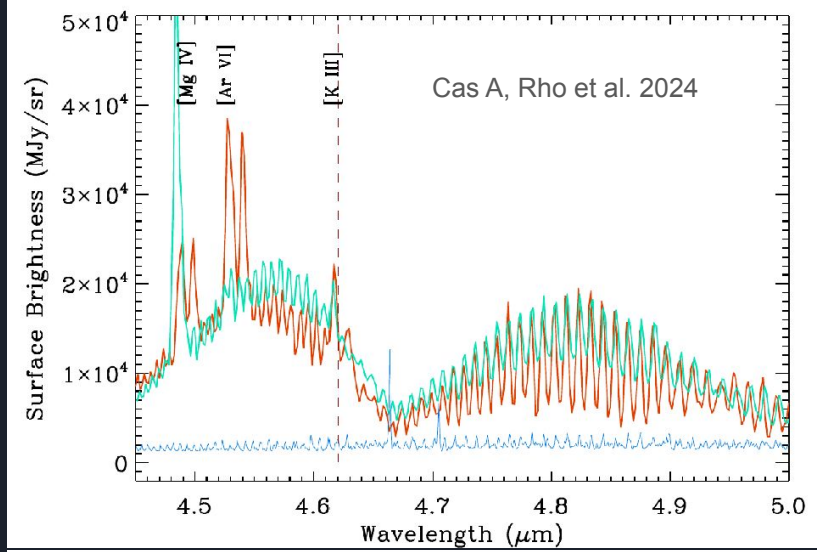
Molecular transitions

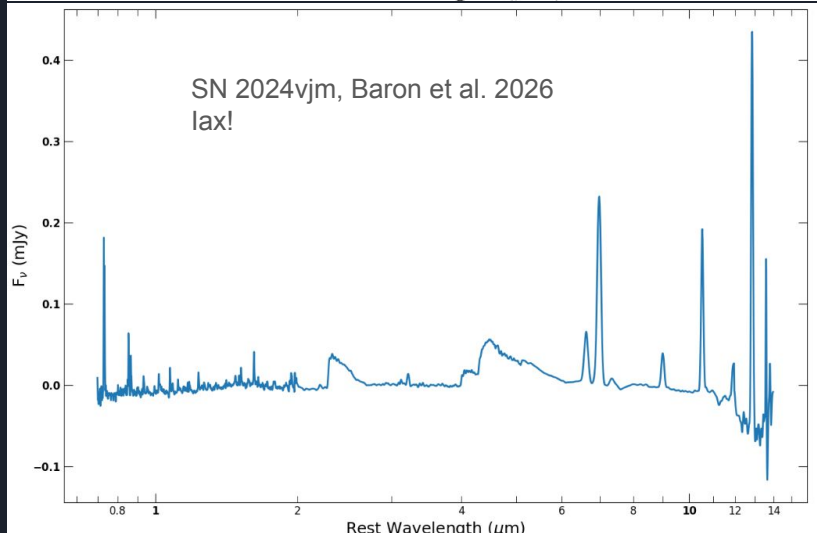
- 3 types of transitions:
  - Electronic
  - Vibrational
  - Rotational



Observations

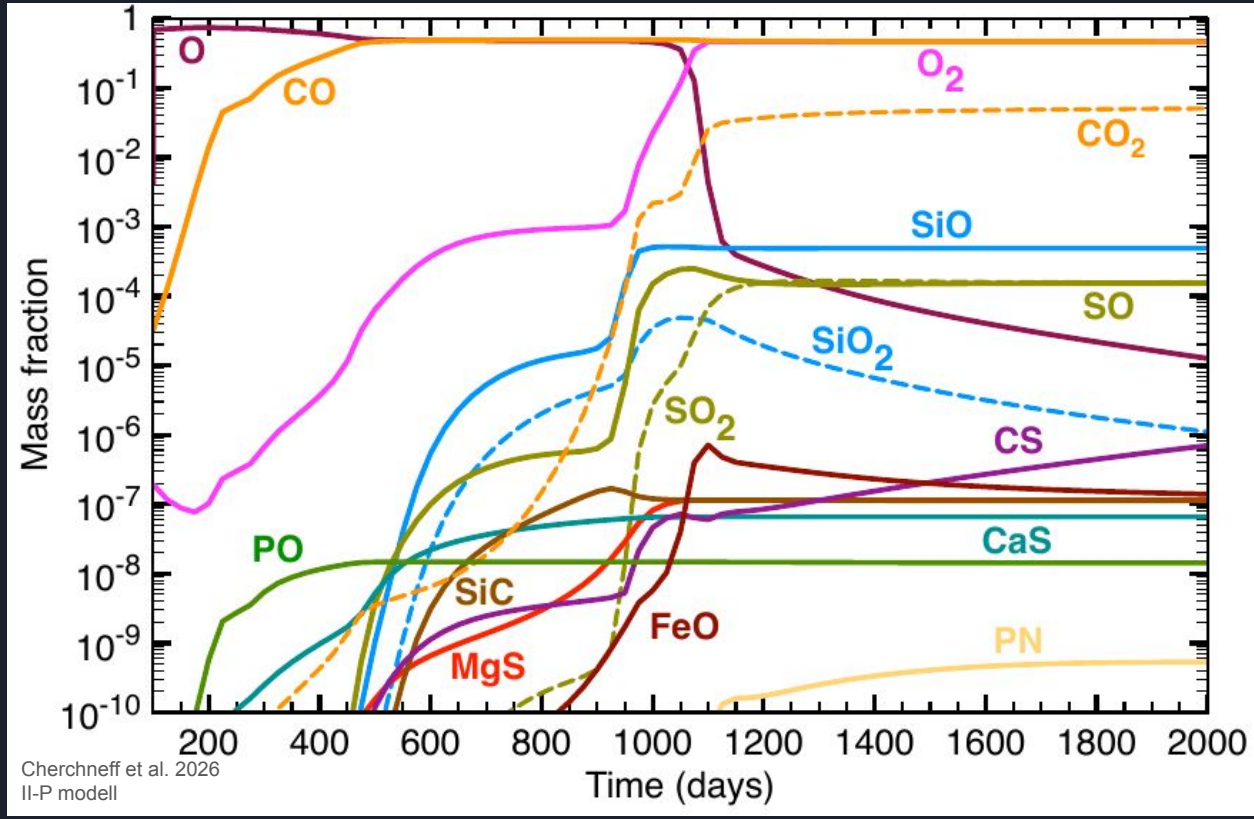
- Since the JWST we have high resolution observations of vibrational bands of molecules
- We have molecular data from young supernovae





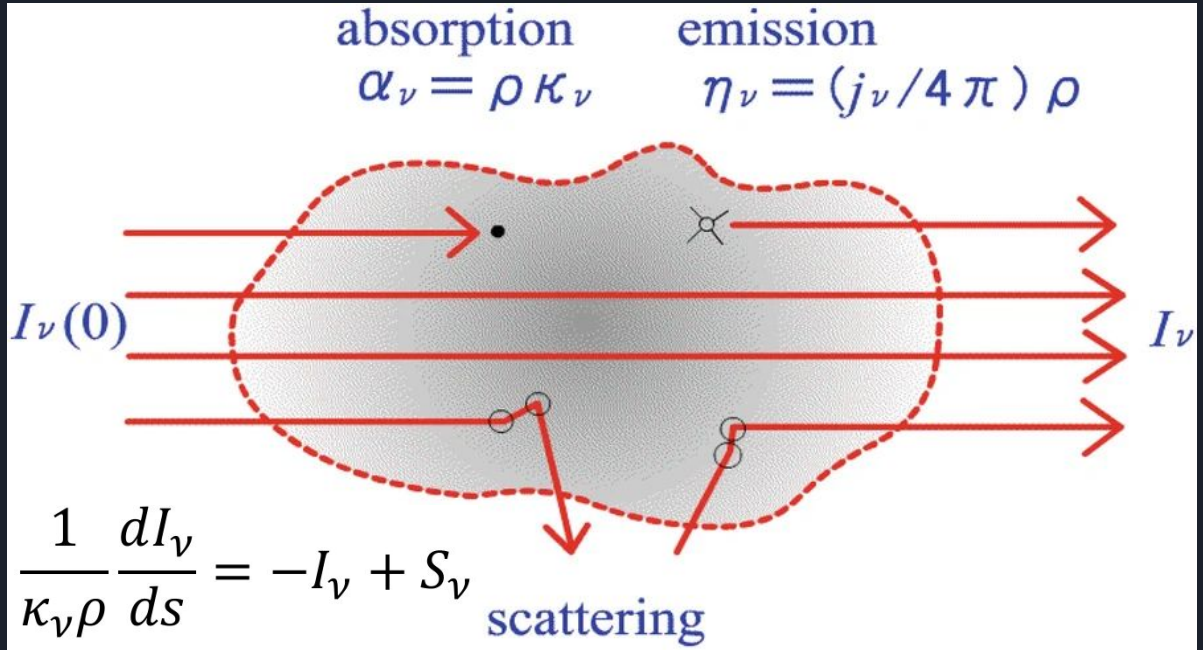
Molecular models for supernovae

- Young SNe: CO and O
- Older SNe: CO and O_2



Radiative transfer

- Describes the interaction between light and matter
- Local thermodynamic equilibrium



Collisional Transfer Rates

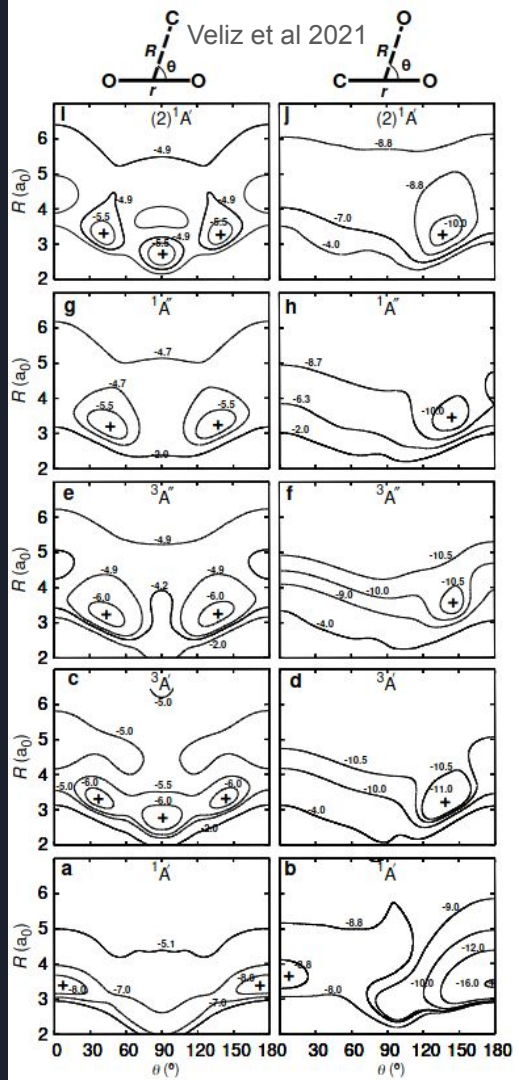
- Describes the probability of transition from i to j states on a specific temperature
- This has to be calculated for all transitions, on a wide temperature scale and for different collisional partners
- These are usually calculated for protoplanetary disks and interstellar media, and typically for rotational lines
- Some databases: LAMBDA, EMAA, BASECOL

Quantum scattering

- The scattering cross-sections are behind the collisional transfer rates
- There are a lot of different models, from full dimensional close coupled methods to the quasi classical trajectories methods
- All of the methods require potential energy surfaces
- One of the widely used scattering code: Molscat
- Collaboration: Sándor Demes, ATOMKI

Potential Energy Surfaces

- The Potential Energy Surface (PES) describes the interacting system of molecules
- These are often complex, strongly anisotropic, and varies greatly on the electric states
- The calculations usually use proprietary softwares, like MolPro or Gaussian



In process: CO - O collision

- The typical collisional partners in young supernovae
- Rovibrational scattering calculations using the BIGOS scattering code
- Currently making convergence tests
- Problem: the PES I use has a larger uncertainty, which may hinder convergence
- In the near future I will calculate a new PES
  collaboration: Gábor Czakó, SZTE
- The calculations will require supercomputer time

Takeaway

- Molecular modelling in supernovae, more and more measurements with JWST
- Non-LTE radiative transfer: populations unknown, needs collisional data
- Collisional data only exists for ISM and protoplanetary disks: DIY needed
- Current project: CO - O scattering, collaborations, potential energy surface development