Collisional Excitation Processes

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Astrophysical Observations

- Infrared Space Observatory (ISO)
- Submillimeter Wave Astronomy Satellite (SWAS), ODIN : 1 line of H_2O and O_2
- Future Herschel Space Observatory (HSO) : Heterodyne Instrument for the Far-Infrared (HIFI)
  - Unprecedent sensitivity in different environments, from ISM to the stellar or planetary atmospheres
  - Water Survey for many rotational lines in v=0, and some in v=1
  - Other molecules
- Future ALMA (ground based millimeter interferometer) : higher spatial resolution

$\Rightarrow$ More accurate molecular data : 10% to 20%

Collisional Excitation Processes

A selection of work for FP6 : rotational and ro-vibrational excitation

- H_2O, HDO + H, He, H_2 : Meudon, Grenoble, Oxford, Nijmegen
- N_2H^+ + He, H_2 : Meudon, Basel
- HC_3N + He : Rennes, Grenoble, Varsow
- NH_2D, ND_2H + H_2 : Grenoble, Meudon
- H_2CO, HDCO + H_2 : Grenoble, Varsow
- CH^+ + H_2 : Basel, Meudon, Rennes, Oxford, Götteborg, Göttingen
- SO, SiO, SO_2 + He, H_2 : Durham, Madrid, Meudon

Rate coeFFicients

$$k_{\alpha\to\beta}(T) = \int_0^\infty \sigma_{\alpha\to\beta}(E)\, E e^{-E/kT}\, dE \qquad (1)$$

Cross-sections

$$\sigma_{\alpha\to\beta} = y * \sum_{Jtot} (2 * Jtot + 1) |1 - S^{Jtot}_{\alpha\to\beta}|^2 \qquad (2)$$

Scattering matrix elements obtained from solving Schrödinger Equation :

$$H\Psi = E\Psi$$

Hamiltonian

$$H = -\frac{\hbar^2}{2\mu} R^{-1} \frac{\partial^2}{\partial R^2} R + \frac{\hbar^2 \hat{\mathbf{L}}^2}{2\mu R^2} + H_{\text{at/mol2}} + H_{\text{mol1}} + V_{\text{inter}} \qquad (3)$$

exemple : N_2H^+ + He

$$H_{\text{mol}} = B\hat{\mathbf{j}}^2 + H_{hfs} \qquad H_{hfs} = H_Q + H_{mag}$$

Angular momentum coupling :

$$\hat{\mathbf{j}} + \hat{\mathbf{I}}_1 = \hat{\mathbf{F}}_1 \qquad \hat{\mathbf{F}}_1 + \hat{\mathbf{I}}_2 = \hat{\mathbf{F}}$$

Best basis set for calculations of hyperFine levels of N_2H^+

$$|jI_1F_1I_2F\rangle$$

$$\hat{\mathbf{L}} = \hat{\mathbf{J}}_t - \hat{\mathbf{j}} - \hat{\mathbf{I}}_1 - \hat{\mathbf{I}}_2 = \hat{\mathbf{J}}_t - \hat{\mathbf{j}} - \hat{\mathbf{I}}$$

Dynamical methods in order to get $\sigma_{\alpha\rightarrow\beta}(E)$?

- Most reliable methods : Quantum with no approximation
  - the method we use : Close Coupling (N^3)
  - other possibilities : wavepackets
- Angular momentum decoupling approximations in CC
  - Coupled states (CS) , Infinite Order Sudden (IOS)
  - allow to reach higher temperatures
- Semiclassical Methods
  - Minimum assumption : translational motion treated classically
  - Quasi-Classical Trajectories (QCT)
  - Other methods implemented by various groups

Solving CC equations

$$\left[\mathbf{I}\frac{d^2}{dR^2} + \mathbf{W(R)}\right]\mathbf{F(R)} = 0, \tag{4}$$

$$\mathbf{W(R)} = \mathbf{k}^2 - \mathbf{l}^2 - \mathbf{V(R)} \tag{5}$$

Propagation of log-derivative matrix $Y(R) = F'(R)F(R)^{-1}$

At Short range : solution following method, i.e, approximate the matrix of solutions F(R) by a power series and then solve Eq. (4) exactly. Similar in spirit to usual numerical techniques for solution of ordinary differential equations (Runge-Kutta..)

At Long range : potential-following method, i.e. approximate matrix **W(R)** by a series of constant or linear segments. In local regions, CC eq. are solved exactly.

State of the Art

2 packages : MOLSCAT and HIBRIDON (same propagators)
Complexity increases with

- number of internal states of molecules (rot., vib., fine structure)
- higher energy, this implies summing over more total angular momenta, including more closed channels

Simple Solution for CC:
Parallelization of loops over energy, parity, J_{tot}