COLLISIONAL ENERGY TRANSFER IN THE CO-CO SYSTEM

M. Żółtowski[1,2], F. Lique[2], J. Loreau[3]

1. *LOMC - UMR 6294, CNRS-Université Le Havre Normandie*
2.Univ Rennes, CNRS, IPR (Institut de Physique de Rennes) - UMR 6251, F-35000 Rennes, France
3. KU Leuven, Department of Chemistry, B-3001 Heverlee, Belgium
Email: michal.zoltowski@univ-lehavre.fr

Context and Motivation

- Accurate determination of the physical conditions in comets can be inferred from the modelling of observational spectra
- The full exploitation of these spectra requires going beyond the local thermodynamic equilibrium
  - Radiative and collisional properties are needed
- CO, CO_2, and H_2O are the most abundant molecules in comets
- For comets at large heliocentric distances, production of CO significantly exceeds production of H_2O [1]
- Accurate rate coefficients for CO-CO collisional system are essential for proper astrophysical modelling of comets

Details of the calculations

- The 4D Potential Energy Surface (PES) calculated by Visser et al. [2] was used in our calculations
- Calculations were performed within the coupled states (CS) approximation using the MOLSCAT scattering code [3]
- Molecules were treated as distinguishable ones for the purpose of astrophysical applications
- Cross sections were calculated for transitions between rotational levels of CO molecules up to $j_1 = j_2 = 10$
- From calculated cross-sections, we provide rate coefficients for temperatures up to 150 K
- Statistical Adiabatic Channel Model (SACM) was investigated to extend calculations to higher rotational levels [4]

Propensity rules

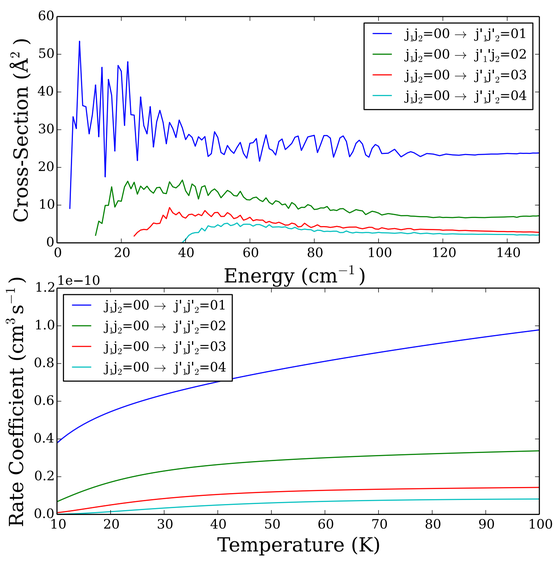

Fig.1 Cross-sections and rate coefficients of no-pair (only one CO is excited) transitions

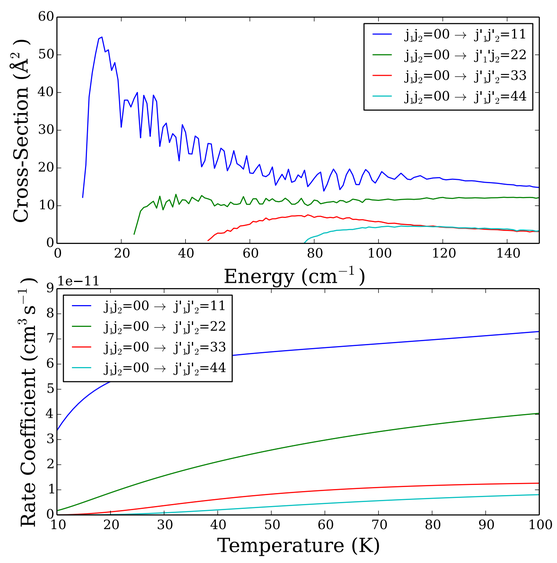

Fig.2 Cross-sections and rate coefficients of pair (both CO are excited) transitions

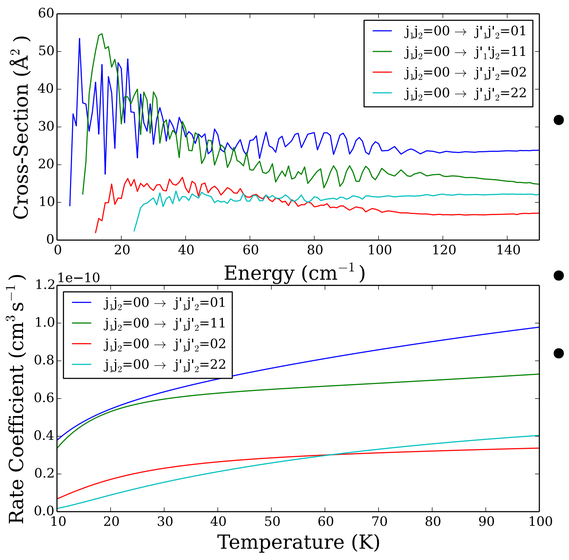

Fig.3 Comparison of cross-sections and rate coefficients between pair and no-pair transitions

- Strong propensity rules toward no pair transitions with $\Delta j_2 = 1$ (Fig.1)
  - Cross sections decrease while Δj_2 increases
- Same behaviour for pair transitions (Fig.2)
- Similar magnitude of cross-sections and rate coefficients for pair and no pair transitions (Fig. 3)

Comparison with previous study

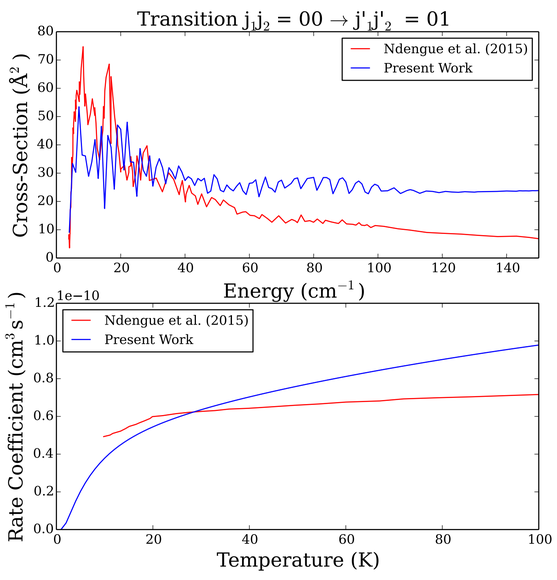

Fig.4 Comparison of cross-section and rate coefficients for first no-pair transitions

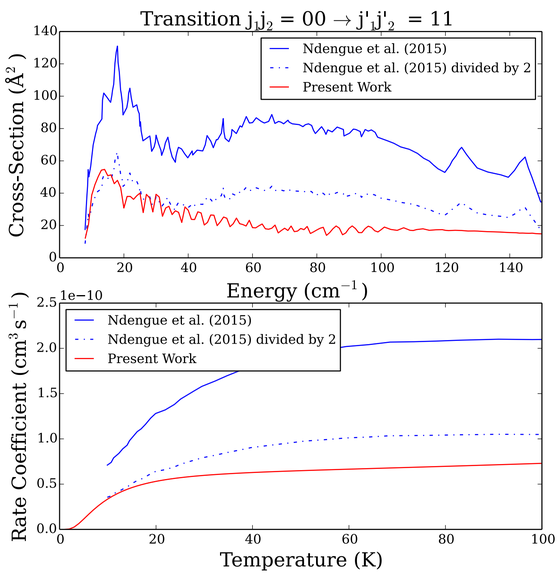

Fig.5 Comparison of cross-section and rate coefficients for first pair transitions

We observe differences due to:

- PESs used in calculations [2,6]
- Calculation method: close coupling (CC) + Multi Channel Time Depended Hartree (MCTDH) in previous work [5], coupled states approximation in this work
- Size of rotational basis: $j_1 = j_2 = 7$ in previous work [5], $j_1 = j_2 = 15$ in this work
- Error in the MOLSCAT code - overestimation of pair transitions (Fig 5.)

Statistical approach

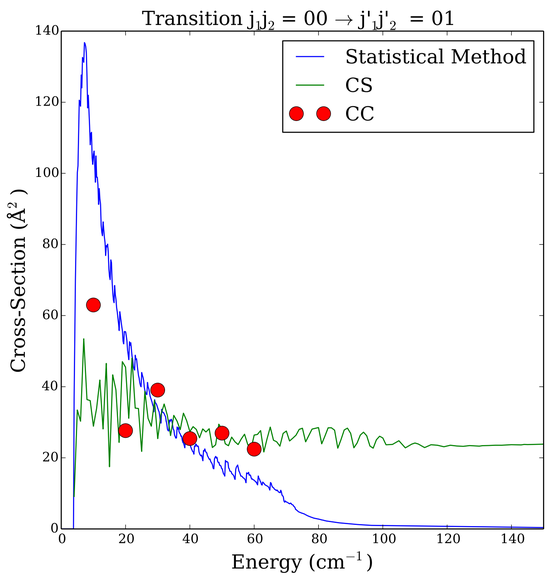

Fig.6 Comparison of cross-sections using different scattering methods

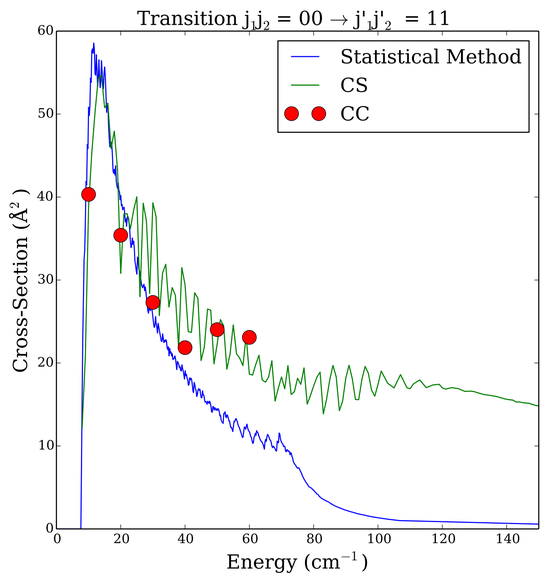

Fig.7 Comparison of cross-sections using different scattering methods

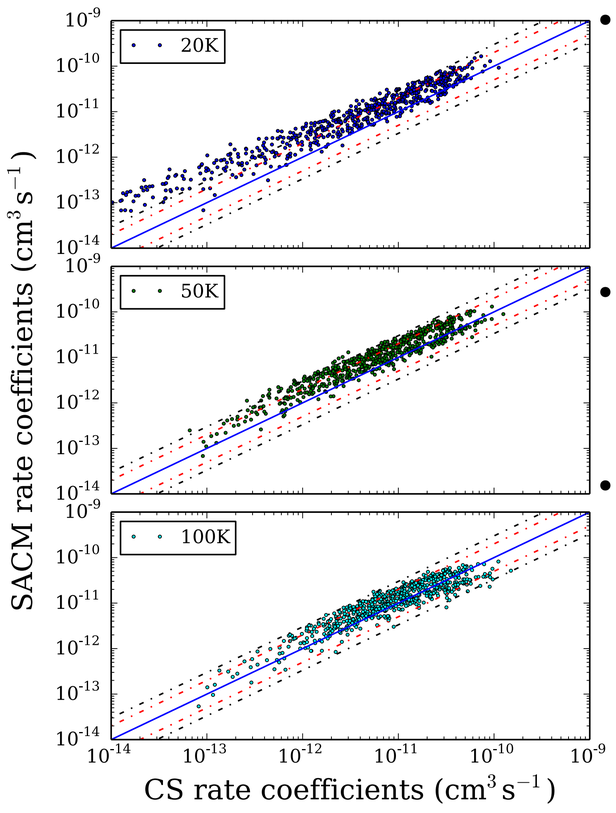

Fig.8 Systematic comparison of the rate coefficients for different temperatures. Blue line: identical results, red dashed line: factor of 2 difference, green dashed line: factor of 3 difference

- SCAM cross-sections are compared to the CS results
  - Up to a factor of 3 of differences observed at low energy (Fig.6)
  - Good agreement for part of the transitions at medium energy range (Fig. 7)
- Sudden decrease of cross-sections is observed above 60 cm^{-1} (Fig. 6 and 7).
  - Due to high density of accessible channels
- Systematic comparison of rate coefficients at 3 different temperatures (Fig. 8)
  - 20K - Part of the transitions exceeds a factor of 3 differences
  - 50K - Acceptable agreement within a factor of 3
  - 100K - Good agreement but rather fortuitous at this temperature

Summary and Future plans

- We calculated rate coefficients for temperatures up to 150K for transitions between CO rotational levels $j_1 = j_2 = 10$
- Comparison with previous study uncover error in the MOLSCAT scattering code
  - The cross-sections are overestimated for pair transitions in icollisional systems involving identical molecules
- SACM method does not work for the CO-CO system
  - Density of accessible channels is too high
- The new data will be used in the modelling of the CO rich comets

References

[1] D. Bockelée-Morvan, J. Crovisier, M.J. Mumma, H.A. Weaver, *Univ. Arizona Press*, (2004)

[2] G. W. M. Vissers, et. al. *J. Chem. Phys.* **122,** (2003)

[3] J. M. Hutson and S. Green, MOLSCAT computer code, version 14 (1994)

[4] J. Loreau *et al, ApJL* **853** L5 (2018)

[5] S. Ndengué, R. Dawes, F. Gatti, *J. Chem. Phys.* **119,** (2015)

[6] R. Dawes, X.G. Wang, T. Carrington *J. Chem. Phys.* **117,** (2013)