

State-to-State Rotational Energy Transfer in CO – Ar and CO – H₂ Collisions at Very Low Temperatures

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Rotational energy transfer plays a key role in a variety of astrophysical environments. Radio astronomical observations of dipolar molecules often require radiative transfer calculations to obtain reliable estimations of densities and state populations. These calculations require robust state-to-state rate constants for rotational energy transfer in collisions between the observed molecules, and the most abundant collider species (usually H₂, He, H). CO is the most abundant molecule in the Interstellar Medium after H₂ with a ratio of [CO]/[H₂] $\approx 10^{-4}$,¹ and is widely used to locate and map dense molecular clouds in galaxies owing to its large dipole moment. It is also used to measure temperature and density in these regions. Collisions between CO and noble gases, such as He and Ar, provide an ideal testing ground for comparisons between theory and experiment, in which the potential energy surface can be calculated with high accuracy.

Using an Infrared Vacuum Ultraviolet Double Resonance (IRVUVDR) method developed in previous work on CO – He collisions,² combined with the CRESU technique (a French acronym for reaction kinetics in uniform supersonic flow) to provide extremely cold Ar or H₂ collider gas, we present experimental state-to-state rate coefficients and thermally averaged cross sections for rotational energy transfer in CO ($v = 2, j_{\text{initial}} = 0, 1, 4, 6$) collisions with Ar at temperatures down to 30 K, and CO in collisions with the most abundant partner in the interstellar medium, H₂, at temperatures down to 5 K. The experimental results for CO($v = 2$) – Ar will be compared to close-coupling calculations employing the Newmat package recently used in the study of vibrating NO⁺ with He,³ on the new three-dimensional potential energy surface for the Ar-CO complex of Sumiyoshi and Endo.⁴ Some preliminary results are shown in the figure below.

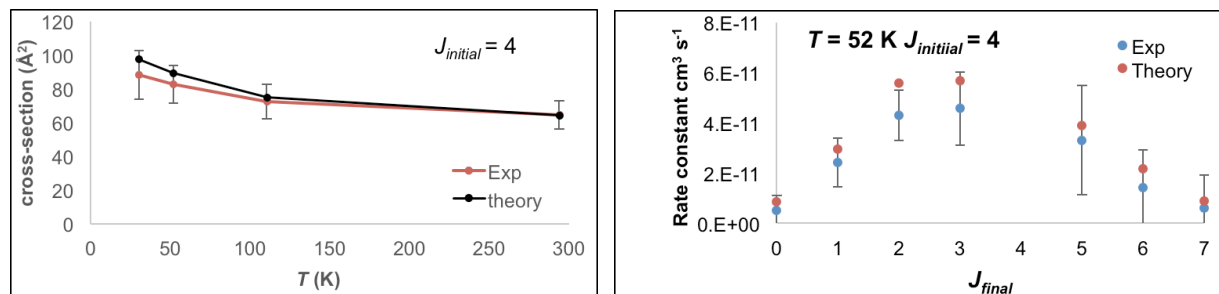


Figure 1: preliminary results for total relaxation cross sections (30—300 K) and state-to-state rate coefficients (52 K) for CO – Ar collisions

References

- (1) Liu, T.; Wu, Y. F.; Zhang, H. W. *Astrophys. J. Lett.* **2013**, 775.
- (2) Carty, D.; Goddard, A.; Sims, I. R.; Smith, I. W. M. *J. Chem. Phys.* **2004**, 121, 4671-4683.
- (3) Denis-Alpizar, O.; Stoecklin, T. *Mon. Not. R. Astron. Soc.* **2015**, 451, 2986-2990.
- (4) Sumiyoshi, Y.; Endo, Y. *J. Chem. Phys.* **2015**, 142, 024314.