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Vibrational and rotational quenching of CO by collisions with H, He, and H₂

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ABSTRACT

Collisional quenching of molecular species is an important process in a variety of astrophysical environments including interstellar clouds, photodissociation regions, and cool stellar/planetary atmospheres. In this work, quantum mechanical scattering calculations are presented for the rotational and vibrational relaxation of rotationally-excited CO due to collisions with H, He and H₂ for collision energies between 10⁻⁶ and ~15000 cm⁻¹. The calculations were performed using the close-coupling approach and the *l*-labeled form of the coupled-states approximation. Cross sections and rate coefficients for the quenching of the *v*=0-2, *j*=0-6 levels of CO are presented and comparisons with previous calculations and measurements, where available, are provided.

1. Introduction

Due to their astrophysical importance as these species are the most common ones in a wide range of astronomical sources, collisions of CO with H, He, and H₂ have been the subject of numerous experimental (1-6) and theoretical studies (7-13). Accurate data for state-to-state cross sections and rate coefficients for these systems are crucial to quantitative models of astrophysical environments. Accurate potential surfaces are needed for reliable theoretical simulations of energy transfer in collisions of CO by H, He, and H₂. To date, impressive progress has been made in the construction of potential energy surfaces (PESs) for neutral H-CO. In our calculations, we adopted the WKS PES (13; 14) for H-CO, Heijman *et al.*'s PES (15) for He-CO, and the PES by Jankowski and Szalewicz (16) for H₂-CO scattering. Theoretical calculations for rovibrational excitation have been used to obtain rate coefficients needed to interpret astrophysical data, and the present work is part of a project aimed at calculating the required rate coefficients for CO excited by H, He and H₂.

2. Results

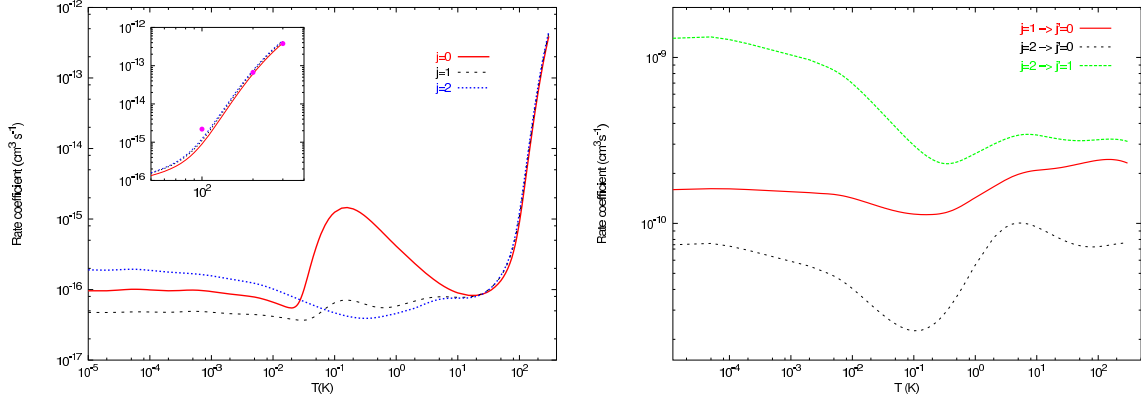


Fig. 1.— Left panel: Rate coefficients for the quenching of $v=1$, $j=0, 1$, and 2 for CO scattering by H. Symbols are IOS results (8). Right panel: Rate coefficients for the rotational quenching of $v=1$ for CO scattering with H.

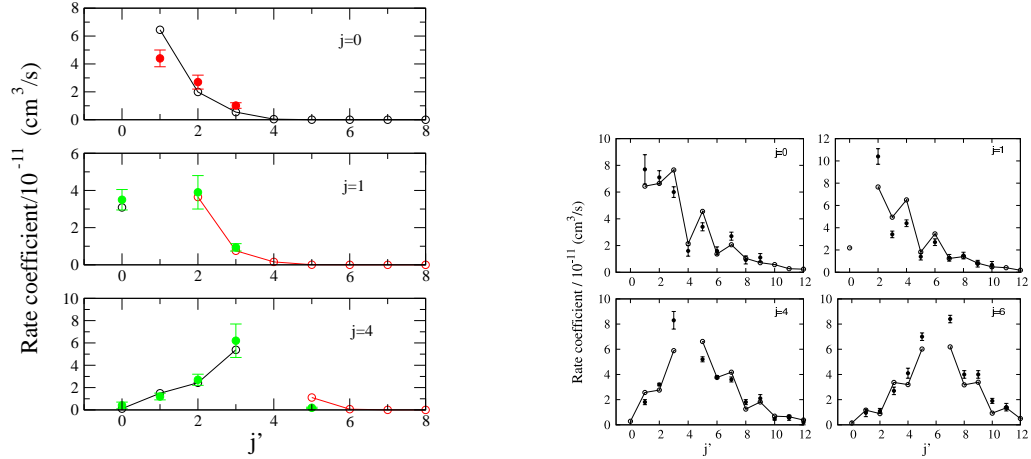


Fig. 2.— State-to-state rate coefficients for rotationally inelastic collisions of CO($v=2$) with He atom. Left panel: at 15 K, (a) $j = 0$, (b) $j = 1$, (c) $j = 4$. Right panel: at 294 K, (a) $j = 0$, (b) $j = 1$, (c) $j = 4$, (d) $j = 6$. Lines with open circles: current CC calculations; solid circles with error bar: measurements (4).

Calculations were done with the molecular scattering program MOLSCAT (17) to generate integral state-to-state cross sections. The coupled-channel equations were integrated using the modified log-derivative Airy propagator of Alexander and Manolopoulos (18). Calculations were performed for collision energies between 10^{-6} cm^{-1} and 15000 cm^{-1} in order to present accurate thermally averaged rate constants from 10^{-5} to 3000 K. At each energy a sufficient number of total angular momentum partial waves has been included to secure convergence of the cross sections. Examples of our results are shown in Figs. 1, 2 and 3 for CO scattering with H, He and H_2 .

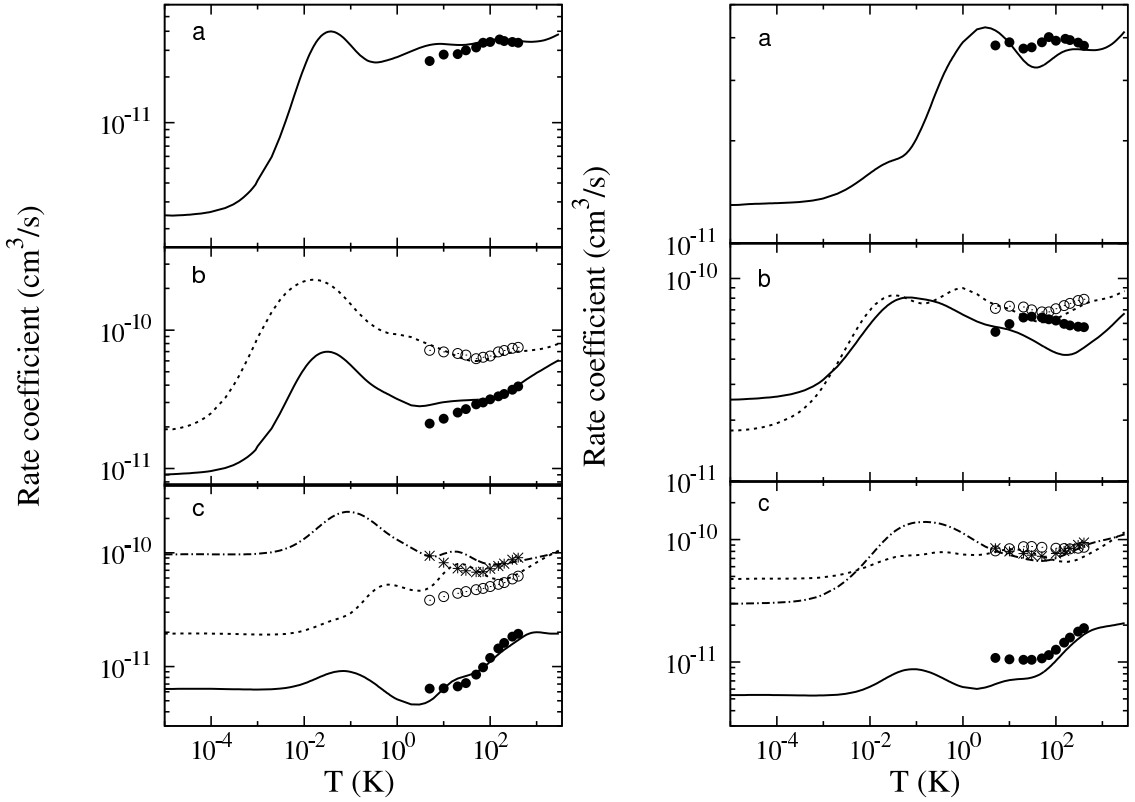


Fig. 3.— Rate coefficients for the quenching of CO by collisions with para- H_2 (Left panel) and orth- H_2 (Right panel) as functions of the temperature. Lines indicate current calculations. Symbols denote Flower’s results (11). (a) $j_2 = 1 \rightarrow j'_2 = 0$. (b) solid line: $j_2 = 2 \rightarrow j'_2 = 0$, dashed line: $j_2 = 2 \rightarrow j'_2 = 1$, solid circles: $j_2 = 2 \rightarrow j'_2 = 0$, open circles: $j_2 = 2 \rightarrow j'_2 = 1$; (c) solid line: $j_2 = 3 \rightarrow j'_2 = 0$, dashed line: $j_2 = 3 \rightarrow j'_2 = 1$, dash dotted line: $j_2 = 3 \rightarrow j'_2 = 2$, solid circles: $j_2 = 3 \rightarrow j'_2 = 0$, open circles: $j_2 = 3 \rightarrow j'_2 = 1$, stars: $j_2 = 3 \rightarrow j'_2 = 2$.

3. Summary

Rotational and vibrational quenching cross sections have been presented for a range of initial rotational states j and initial vibrational levels $v = 0, 1, \text{ and } 2$. Good agreement was found with most other calculations where overlap exists and available experimental data. Future calculations will be performed to attempt to extend the range of v and j .

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