

INELASTIC SCATTERING OF H+CO: INFLUENCE OF RENNER-TELLER COUPLING

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Carbon monoxide is after molecular hydrogen the second most abundant molecule in the interstellar medium (ISM) and also an important molecule for processes occurring in the atmosphere, and hydrocarbon combustion. The rate coefficients of CO in collision with dominant species like H, H₂, He, etc are common keys to understand the CO emission spectrum or to model combustion chemistry processes. The inelastic scattering of H+CO has indeed been intensively studied in the past decades, using mainly the so-called WKS PES developed by Werner et al or recently a modified version by Song et al. Though the spectroscopic agreement of the WKS surface with experiment is known to be quite good, there is no experimental evidence that the dynamics of the system is correctly reproduced by the surface. We will present in this talk new results on a set of HCO surfaces of the ground and the excited Renner-Teller coupled electronic states with the principal objective of studying the influence of the Renner-Teller coupling on the inelastic scattering of H+CO. Our calculations done using the MCTDH algorithm cover the 0-2 eV energy range and allow one to interpret the effect of the Renner-Teller coupling on the rovibrational inelastic scattering. Additionally, vibrational bound and resonance state calculations on this new PES and comparisons with available experimental data will be presented.