INFLUENCE OF THE RENNER-TELLER COUPLING IN CO+H COLLISION DYNAMICS

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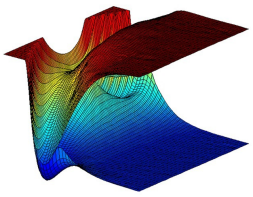

Carbon monoxide is after molecular hydrogen the second most abundant molecule in the universe and an important molecule for processes occurring in the atmosphere, hydrocarbon combustion and the interstellar medium. The rate coefficients of CO in collision with dominant species like H, H_2, He, etc are necessary to understand the CO emission spectrum or to model combustion chemistry processes. The inelastic scattering of CO with H has been intensively studied theoretically in the past decades,[1] mostly using the so-called WKS PES[6] developed by Werner et al. or recently a modified version by Song et al.[2] Though the spectroscopic agreement of the WKS surface with experiment is quite good, so far the studies of scattering dynamics have neglected coupling to an electronic excited state. We present new results on a set of HCO surfaces of the ground and the excited Renner-Teller coupled electronic states[3] with the principal objective of studying the influence of the Renner-Teller coupling on the inelastic scattering of CO+H. Our calculations done using the MCTDH[4] algorithm in the 0-2 eV energy range allow evaluation of the contribution of the Renner-Teller coupling on the rovibrationally inelastic scattering and discuss the relevance and reliability of the calculations.

References:

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