

Abstract Submitted
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Theoretical study of vibrational (de-)excitation of NO₂ and N₂O by low-energy electron impact¹ HAINAN LIU, MEHDI AYOUB, PIETRO CORTONA, CentraleSupélec, SAMANTHA FONSECA DOS SANTOS, Rollins College, CHI HONG YUEN, VIATCHESLAV KOKOULINE, University of Central Florida — We present cross sections for vibrational (de-)excitation of NO₂ and N₂O by low-energy electron impact. Calculations are performed using a theoretical approach based on a combination of the normal mode approximation for vibrational states of the target molecule, fixed-nuclei electron-target scattering matrices and the vibrational frame transformation employed to evaluate the scattering matrix for vibrational transitions. Results are presented for excitations between the ground and first two excited vibrational states for NO₂, and between the ground and first excited vibrational state for N₂O in all the vibration modes for both target molecules. Thermally-averaged rate coefficients are derived from the obtained cross sections for temperatures in the 10-10000 K interval. For NO₂, a comprehensive set of calculations are performed for assessing the uncertainty of the present calculations. The uncertainty assessments indicate that the computed observables for vibrational (de-)excitation is reasonable for later use in NO₂-containing plasma kinetics modeling. For N₂O, the NO and NN stretching modes cross-section behavior agrees reasonably well with the available experimental data.

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