Abstract Submitted
for the DAMOP19 Meeting of
The American Physical Society

Theoretical study of vibrational excitation and dissociative electron attachment of NO2 by an electron impact[1] HAINAN LIU, SPMS, CentraleSuplec, Universit Paris-Saclay, 8-10 rue Joliot-Crurie, 91190 Gif-sur-Yvette, France, SAMANTHA FONSECA DOS SANTOS, Rollins College, Winter Park, FL, USA, CHI HONG YUEN, Department of Physics, University of Central Florida, Orlando, FL 32816, USA, PIETRO CORTONA, SPMS, CentraleSuplec, Universit Paris-Saclay, 8-10 rue Joliot-Crurie, 91190 Gif-sur-Yvette, France, VIATCHESLAV KOKOOULINE, Department of Physics, University of Central Florida, Orlando, FL 32816, USA, MEHDI AYOUZ, LGPM, CentraleSuplec, Universit Paris-Saclay, 8-10 rue Joliot-Crurie, 91190 Gif-sur-Yvette, France, PIETRO CORTONA COLLABORATION, SAMANTHA FONSECA DOS SANTOS COLLABORATION, VIATCHESLAV KOKOOULINE COLLABORATION, MEHDI AYOUZ COLLABORATION — The NO2 molecule plays a critical role in modeling atmospheric processes. However, the theoretical description of the vibrational excitation and dissociative electron attachment (DEA) for this open-shell molecule is still an extremely challenging task to date. In this study, we use a theoretical approach that combines the normal modes approximation, the R-matrix formalism, and the vibrational frame transformation to compute the cross sections for electron-impact vibrational excitation of NO2. The cross sections for DEA to NO2 are estimated through a simplified approach which is based on the fact that the resonance energy only varies substantially over a subset of normal coordinates, and compared to available experimental data. Thermally-averaged rate coefficients are obtained from the cross sections for the temperatures 10 K-10000 K.

[1]This work is supported by the Chinese Scholarship Council

Hainan LIU
SPMS, CentraleSuplec, Universite Paris-Saclay

Date submitted: 06 Feb 2019 Electronic form version 1.4