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Dissociative electron attachment of NO_2 molecule at low collision energies[1] EMILY HENDRIX, SAMANTHA FONSECA DOS SANTOS, Rollins College, NICOLAS DOUGUET, Kennesaw State University, CHI HONG YUEN, VIATCHESLAV KOKOOULINE, University of Central Florida, ASA LARSON, Stockholm University, ANN OREL, University of California Davis — The work focuses on the theoretical study of dissociative electron attachment (DEA) of nitrogen dioxide, NO_2, which is a part of undesired air pollutants in the atmosphere produced from combustion processes. NO_2 molecules are emitted from combustion processes and can react with oxygen and water present in the atmosphere resulting in the formation of nitric acid that can be detrimental for the environment. Therefore, it is important to not only understand the formation mechanism of NO_2 molecules but also its destruction mechanisms. We investigate whether DEA is an efficient process to remove the unwanted NO_2 molecules at combustion level before being emitted into the environment. We report here the results of our ab initio quantum chemical studies of the geometrical and electronic structure of the NO_2 and and its negative ion NO_2^- in our theoretical study of DEA in NO_2. The scattering calculations are carried out using the complex Kohn variational method. The nuclear dynamics, including dissociation, will later be treated using the MCTDH code with a three-dimensional potential energy surface.

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