INELASTIC COLLISION DYNAMICS OF O_3+Ar

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Collisional energy transfer between a metastable ozone molecule and an inert collider such as an argon atom is a key step in the formation process of ozone. Understanding these collisional cooling dynamics may provide insight into the "ozone isotopic anomaly", which is the observation of larger than expected concentrations of certain heavy ozone isotopologues in the atmosphere. Although many explanations to understand this phenomenon have been put forward previously, quantitative prediction/understanding is still lacking. One of the major reasons is the lack of an accurate potential energy surface (PES) for the system. We have recently constructed a new and accurate 3D PES of O_3+Ar and computed bound states of the complex within the rigid rotor approximation.[a] In this work, we now present the dynamics of collisions between this triatomic asymmetric top molecule and a heavy atom: O_3–Ar. The MultiConfiguration Time Dependent Hartree (MCTDH) method was used to study the scattering between the O_3 molecule and Ar atom. The state-to-state probabilities from the 0_{00} rotational state to low lying excited rotational states as well as the state-to-state cross sections are determined for the system. The rate coefficients obtained for $^{16}O^{16}O^{16}O$–Ar, are compared with the rate coefficients obtained for the $^{16}O^{16}O^{18}O$–Ar isotopologue. The lowered symmetry in $^{16}O^{16}O^{18}O$–Ar results in roughly double the density of allowed states due to nuclear spin statistics for bosons, which impacts the scattering dynamics.

[a] S. Sur, E. Quintas-Sánchez, S. A. Ndengué, R. Dawes "Development of a potential energy surface for the O_3–Ar system: Rovibrational states of the complex", Submitted, PCCP (2019)