INELASTIC COLLISIONS OF Ar AND O_3

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According to the Chapman cycle, during formation, metastable ozone can be stabilized by a third body (M) collision (buffer gas) in the atmosphere. The stabilization occurs through an energy transfer (ET) mechanism from O_3^* to M. The details of this ET are not well known and one of the reasons is the lack of an accurate potential energy surface (PES) including the collision partner. The PES of the O_3-Ar complex is a 6D problem in full-dimensionality, or 3D for rigid O_3. Here we present a global 3D PES for O_3 fixed at equilibrium, interacting with Ar. Highly accurate Davidson-corrected multi-reference configuration interaction (MRCI-f12) energies were computed at 2112 data points. The AUTOSURF code was used to construct the PES automatically, represented by a local interpolating moving least-squares (L-IMLS) method. A global RMS fitting error of 0.6 cm^{-1} was obtained. Symmetry equivalent minima with a well depth of -229 cm^{-1} are located above and below the plane of O_3. We present here bound vdW states of the O_3-Ar complex obtained by variational rovibrational calculations, as well as quantum scattering cross-sections for rotationally inelastic collisions.