Abstract Submitted
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Theoretical predictions of imaging initial vibrational wave functions of H_2O^{++} after one-photon double ionization[1] Z. L. STREETER, C. W. MCCURDY, U. C. Davis and Lawrence Berkeley National Laboratory, R. R. LUCCHESE, Lawrence Berkeley National Laboratory — Previous analysis of the dissociative dynamics of the H_2O^{++} ion following one-photon double ionization for all eight experimentally observed states [Phys. Rev. A 98, 053429 (2018)] provided a clear picture of the breakup mechanisms for $H_2O^{++} \rightarrow O + H^+ + H^+$ and showed that sampling from the Wigner phase space distribution for the *ground* vibrational state produced classical trajectories that agree extremely well with COLTRIMS observations. The question arises of how different the momentum imaging observations would be for vibrationally *excited* water. Here, we explore this question using the Wigner distributions for excited vibrational states of water in all three modes for classical trajectories on the 2^1A_1, 1^1B_1, and 1^1A_2 states of H_2O^{++} and the ideas of E. J. Heller and coworkers from the 1970s and 80s. We find that the initial vibrational states, with their nodes, can be imaged in the final momentum plane of the three-body breakup. A separatix dividing 2- and 3-body dynamics in phase space is revealed for the 2^1A_1 state. For one quantum of excitation of the asymmetric mode the branching ratios for this state flip from 67.3% 3-body to 64.5% 2-body.

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