

Abstract Submitted  
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**Sequential dissociation of  $\text{H}_2\text{O}^{++}$  following double photoionization**<sup>1</sup> Z. L. STREETER, C. W. MCCURDY, U. C. Davis and Lawrence Berkeley National Lab., R. L. LUCCHESI, Lawrence Berkeley National Lab., T. SEVERT, I. BEN-ITZHAK, Kansas State University — A recent analysis of momentum imaging experiments on the dissociation of the  $\text{H}_2\text{O}^{++}$  ion following one-photon double ionization [Phys. Rev. A 98, 053429 (2018)] elucidated the dynamics of direct three-body dissociation to  $\text{H}^+ + \text{H}^+ + \text{O}$ , but also suggested that in one ionization channel a sequential mechanism is involved. Analysis of the momentum imaging data in the native frames of reference associated with each break step confirms sequential dissociation dynamics. A previous study of three-body breakup of  $\text{H}_2\text{O}^{++}$  showed sequential dissociation of the  $2^1A_1$  state by  $\text{H}_2\text{O}^{++}(2^1A_1) \rightarrow \text{OH}^+(^1\Sigma^+) + \text{H}^+$  followed by spin-orbit coupling of the  $^1\Sigma^+$  and the  $^3\Pi$  hydroxyl cation states leading to  $\text{OH}^+(^3\Pi) \rightarrow \text{O}(^3P) + \text{H}^+$ . Here we present a theoretical determination of the rovibrational populations of the  $\text{OH}^+(^1\Sigma^+)$  state from classical trajectories on the  $\text{H}_2\text{O}^{++}(2^1A_1)$  surface. For two-body dissociation, the resulting internal energy distribution of the  $\text{OH}^+(^1\Sigma^+)$  cation is binned quasi-classically. The resulting vibrational distribution and coupling to the dissociative  $\text{OH}^+(^3\Pi)$  state allow comparison with the experimental native frames analysis.

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