Abstract Submitted
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Classical trajectory studies of the dynamics of one-photon double photionization of H_2O[1] ZACHARY STREETER, University of California, Davis, FRANK YIP, California State University, Maritime Academy, ROBERT R. LUCCHESE, Lawrence Berkeley National Lab., BENOIT GERVAIS, CIMAP, Unité Mixte CEA-CNRS-ENSICAEN-UCBN, C. WILLIAM MCCURDY, University of California, Davis and Lawrence Berkeley National Lab. — The triple differential cross section in the body frame for double photoionization of water, $H_2O + h\nu \rightarrow 2e^- + H^+ + H^+ + O$, can be measured in principle by detecting the protons and photoelectrons in coincidence – but only if the dynamics of dissociation of the doubly charged molecular ion are known. A classical trajectory study of the nine lowest states of the water dication is presented using *ab initio* potential energy surfaces, and sampling from a semiclassical initial distribution of positions and momenta. Excellent agreement with preliminary experimental momentum imaging measurements of double photoionization of water show that eight dication states can be unambiguously identified in the experiment with the aid of theory. The theoretical trajectory results will allow body frame measurements of double photoionization to yield all eight states even though the usual assumption of direct dissociation, the "axial recoil" approximation, breaks down for three of the dication electronic states seen in the experiment, opening the door for the first kinematically complete double photoionization experiments on a polyatomic molecule.

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