FORMATION OF EXCITED H_3O STATES BY CHARGE TRANSFER FROM Cs

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Charge transfer (CT) probability between Cs and H_3O^+ was studied. In the experiment a Rydberg type H_3O molecule is formed in electronically excited state after CT from Cs, following by the dissociation to H_2O+H. However it is not clear which excited state is a precursor of the dissociation. Electronic structure of H_3O molecule was investigated by ab initio methods. Couplings between initial and target states were calculated, and charge transfer probabilities were estimated. Calculations show that 4s Rydberg state of H_3O molecule is the most likely state to be populated in the experiment.