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Ultracold atom-molecular ion systems: a photo-asisted spin-dependent polyatomic chemical reaction[1] IONEL SIMBOTIN, JOHN A. MONTGOMERY, JR., ROBIN CÔTÉ, Department of Physics, University of Connecticut, Storrs — In recent years, rapid progress in cooling and trapping of hybrid atom-ion systems has led to studies of atom-ion processes. These range from charge transfer, recombination, internal state conversion, to the possibility of changing cross sections and corresponding rates with tunable Feshbach resonances. A recent experiment from the group of Eric Hudson at UCLA explored how ultracold Ca atoms interact with a trapped polyatomic molecular ion, namely $BaOCH_3^+$. We computed stationary points of the potential energy surface (PES) for this complex system, and reaction paths for different spin states, and found that a large barrier prevents the reaction to form $BaOCa^+$ and CH_3 in the singlet channel. We also found a barrier corresponding to a transition state for the triplet channel corresponding asymptotically to $Ca(^3P) + BaOCH_3^+$, but low enough to allow reactions. We computed reaction rates based on a Langevin model, taking into account the different J values of the initial ^3P_J state of Ca, and found that this photo-assisted reaction depends not only on the singlet/triplet spin state, but also on the fine structure of the initial reactants.

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