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Mutual neutralization of H^- with H^+ and H_2^+[1] MARJAN KHAMESIAN, MICHAEL SAHLIN, PATRIK HEDVALL, Department of Physics, Stockholm University, ANN E. OREL, Department of Chemical Engineering, University of California, Davis, ÅSA LARSON, Department of Physics, Stockholm University, LARSON COLLABORATION — We have previously studied the low energy mutual neutralization reaction in collisions of H^+ and H^- using an ab initio molecular close-coupling approach. The reaction is driven by non-adiabatic couplings between the ion-pair state and the $n = 2$ and $n = 3$ covalent states at large internuclear distances. In present work we have calculated all states of $^1\Sigma_g^+$, $^1\Pi_g$, $^1\Sigma_u^+$ and $^1\Pi_u$ symmetries associated with the limits $n \leq 4$ including the ion-pair states. We have computed adiabatic potential energy curves, non-adiabatic couplings, as well as the rotational couplings between the Σ and Π states. The goal is to perform a detailed study and investigate the importance of the higher lying states, rotational couplings as well as non-zero asymptotic non-adiabatic couplings. These effects have previously not been considered. To perform an ab initio study of mutual neutralization in collisions of H^- with H_2^+ is a challenge. The multi-dimensional potential energy surfaces as well as non-adiabatic couplings for many excited electronic states have to accurately be computed. We perform full configuration interaction calculations of the states to identify the important avoided crossings/conical intersections driving the reaction.

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