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Dissociative recombination of HCl+: direct an indirect mechanisms ASA LARSON, Stockholm University, SAMANTHA FONSECA, NICOLAS DOUGUET, Drake Univ, ANN OREL, UCDavis — We present the study of the Dissociative Recombination (DR) of HCl^+ treating both the direct and indirect dissociation mechanisms. The relevant electronic states are calculated from ab initio principles by combining electron scattering calculations to obtain resonance positions and autoionization widths with multi-reference configuration interaction calculations of the ion and Rydberg states. Direct and indirect DR cross sessions were calculated independently and added incoherently. The former was obtained by solving the time-dependent Schrodinger equation and propagating the wave packets along the resonant states, while the latter was computed using a theoretical model. In this model, an upper bound for the indirect process is obtained using a vibrational frame transformation of the elements of the scattering matrix at energies just above the ionization threshold. Vibrational excitations of the ionic core from the ground vibrational state to the first three excited states are considered and autoionization is neglected. The calculated cross section is compared to measurements.

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