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Complete theoretical treatment of Dissociative Recombination of $\mathbf{LiH^+}$ and $\mathbf{LiH_2^+}$ DANIEL HAXTON, University of Colorado, Boulder and JILA, ROMAN CURIK, University of Colorado, Boulder and JILA; and the J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic, CHRIS GREENE, University of Colorado, Boulder and JILA — Studies of LiH^+ and LiH_2^+ ions are motivated by their role in the chemistry of the early universe. They are diatomic and triatomic prototypes of of the indirect dissociative recombination (DR) process, in which a colliding electron destroys the molecule through Rydberg capture pathways. We apply ab-initio multi-channel quantum defect theory in combination with ro-vibrational frame transformation techniques to calculate DR for these fundamental ions. Alternate versions of the vibrational frame transformation employing either Siegert states or Exterior Complex Scaling are employed. In both cases every rovibrational degree of freedom is included in the calculations, without approximation to the nuclear kinetic energy operator. In case of the LiH^+ ion we identify the underlying mechanism behind the suprisingly high DR rate recently measured in storige-ring experiments. Calculated DR rate coefficients are in a good agreement with the experimental data. This work is supported in part by the NSF.

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