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Abstract for an Invited Paper
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Gas-Phase Theoretical Kinetics for Astrochemistry

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We will survey a number of our applications of ab initio theoretical kinetics to reactions of importance to astrochemistry. Illustrative examples will be taken from our calculations for (i) interstellar chemistry, (ii) Titan's atmospheric chemistry, and (iii) the chemistry of extrasolar giant planets. For low temperature interstellar chemistry, careful consideration of the long-range expansion of the potential allows for quantitative predictions of the kinetics. Our recent calculations for the reactions of H_3^+ with $O(^3P)$ and with CO suggest an increase of the predicted destruction rate of H_3^+ by a factor of 2.5 to 3.0 for temperatures that are typical of dense clouds. Further consideration of the interplay between spin-orbit and multipole terms for open-shell atomic fragments allows us to predict the kinetics for a number of the reactions that have been listed as important reactions for interstellar chemical modeling [V. Wakelam, I. W. M. Smith, E. Herbst, J. Troe, W. Geppert, et al. Space Science Rev., 156, 13-72, 2010]. Our calculations for Titan's atmosphere demonstrate the importance of radiative emission as a stabilization process in the low-pressure environment of Titan's upper atmosphere. Theory has also helped to illuminate the role of various reactions in both Titan's atmosphere and in extrasolar planetary atmospheres. Comparisons between theory and experiment have provided a more detail understanding of the kinetics of PAH dimerization. High level predictions of thermochemical properties are remarkably accurate, and allow us to provide important data for studying P chemistry in planetary atmospheres. Finally, our study of $O(^3P) + C_3$ provides an example of a case where theory provides suggestive but not definitive results, and further experiments are clearly needed.