IAU LabAstro Symposium
Proceedings IAU Symposium No. xxx, 2019
A.C. Editor, B.D. Editor & C.E. Editor, eds.

DOI: 00.0000/X000000000000000X

Low Temperature Gas Phase Reaction Rate Coefficient Measurements: Toward Modeling of Stellar Winds and the Interstellar Medium.

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Abstract. Stellar winds of Asymptotic Giant Branch (AGB) stars are responsible for the production of ∼85% of the gas molecules in the interstellar medium (ISM), and yet very few of the gas phase rate coefficients under the relevant conditions (10 - 3000 K) needed to model the rate of production and loss of these molecules in stellar winds have been experimentally measured. If measured at all, the value of the rate coefficient has often only been obtained at room temperature, with extrapolation to lower and higher temperatures using the Arrhenius equation. However, non-Arrhenius behavior has been observed often in the few measured rate coefficients at low temperatures. In previous reactions studied, theoretical simulations of the formation of long-lived pre-reaction complexes and quantum mechanical tunneling through the barrier to reaction have been utilized to fit these non-Arrhenius behaviours of rate coefficients.

Reaction rate coefficients that were predicted to produce the largest change in the production/loss of Complex Organic Molecules (COMs) in stellar winds at low temperatures were selected from a sensitivity analysis. Here we present measurements of rate coefficients using a pulsed Laval nozzle apparatus with the Pump Laser Photolysis - Laser Induced Fluorescence (PLP-LIF) technique. Gas flow temperatures between 30 - 134 K have been produced by the University of Leeds apparatus through the controlled expansion of N_2 or Ar gas through Laval nozzles of a range of Mach numbers between 2.49 and 4.25.

Reactions of interest include those of OH, CN, and CH with volatile organic species, in particular formaldehyde, a molecule which has been detected in the ISM. Kinetics measurements of these reactions at low temperatures will be presented using the decay of the radical reagent. Since formaldehyde and the formal radical (HCO) are potential building blocks of COMs in the interstellar medium, low temperature reaction rate coefficients for their production and loss can help to predict the formation pathways of COMs observed in the interstellar medium.

Keywords. methods: laboratory, ISM: molecules, molecular processes, kinetics

1. Introduction

Formaldehyde, CH_2O, is a key molecular species in the InterStellar Medium (ISM) and it was first observed in the ISM in 1969 (Snyder *et al.* (1969)). The chemistry of CH_2O is important for the understanding of the formation of Complex Organic Molecules (COMs). A few of the radical species that have the possibility of undergoing fast neutral-neutral reactions with CH_2O at low temperatures and are measurable in the laboratory via laser induced fluorescence include OH, CN, and CH.

2. Method, Results, Discussion, and Future Work

The pulsed Laval apparatus coupled with PLP-LIF was utilized at the University of Leeds to measure low temperature rate coefficients. It has been described in detail previously (Caravan *et al.* (2015); Heard (2018); Martin *et al.* (2014); Shannon *et al.* (2014); Shannon *et al.* (2010); Taylor *et al.* (2008)) and will not be described here.

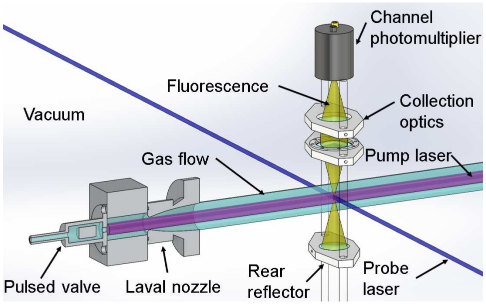

Figure 1. Experimental schematic. Reprinted and adapted with permission from D. E. Heard, Accounts of Chemical Research 51, 2620 (2018). Copyright 2018 American Chemical Society.

The pseudo first order coefficients for the loss of the radicals OH, CN, and CH were measured individually in an excess of CH_2O via PLP-LIF in low temperature gas flows produced from a pulsed Laval nozzle apparatus at the University of Leeds. Rate coefficients for OH + CH_2O agreed with the modified Arrhenius fit of those measured previously by Jiménez and co-workers to within one σ error bars(Ocana *et al.* (2017)). Preliminary temperature dependent rate coefficients of CN + CH_2O showed a negative temperature dependence between 30 - 103 K and preliminary temperature dependent rate coefficients of CH + CH_2O showed a positive temperature dependence between 30 - 133 K. The relatively large low-temperature rate coefficients for the reaction of CH + CH_2O were found to have reached the collision limit as calculated by classical capture theory.

In future work, temperature dependent rate coefficients will be collected at additional temperatures for the above reactions. Preliminary work has also been done to determine the impact of these new rate coefficients in astrochemical systems such as dark clouds and Asymptotic Giant Branch (AGB) stellar winds.

3. Acknowledgements

Niclas West is grateful to the OU, RAS, and RSC for the funds provided to assist his attendance at the IAU S350. Funding for the low temperature kinetics studies was provided by ERC Consolidator Grant 646758 AEROSOL 2016-2020.

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