Rate Coefficient Determination of $NH_3 + CH_3 \rightarrow NH_2 + CH_4$

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Abstract: As global warming mitigation occurs, there is an emphasis on limiting the amount of greenhouse gases released to the environment by attempting to find environmentally friendly alternatives for common fuels such as methane. One possible replacement is ammonia. Ammonia has a lower flame speed and adiabatic flame temperature compared to current fuels such as methane. However, creating a hydrocarbon-ammonia mixture could provide satisfactory combustion properties while curbing greenhouse emissions. There have been many prominent studies on measuring NH_3, N_2O, and H_2O concentrations, but no information on intermediates such as NH_2 in ammonia-hydrocarbon mixtures is available. Furthermore, key chemical kinetics reaction rates for ammonia chemistry are still unknown since intermediates are not well researched. One key reaction in hydrocarbon-ammonia chemistry is $NH_3 + CH_3 \leftrightarrow NH_2 + CH_4$. Directly measuring the rate coefficient of this reaction using ammonia or methane provides some difficulties due to the fast decomposition during ammonia-ethane pyrolysis. Observing NH_2 instead of NH_3 or CH_4 would significantly improve the accuracy of the reaction measurement due to the limited number of competing reactions. The only other sensitive reactions for NH_2 in this system are $NH_3 + M \rightarrow NH_2 + H + M$ and $C_2H_6 + M \rightarrow CH_3 + CH_3 + M$, both of which are well studied. To this end, an NH_2 laser absorption diagnostic outlined by Abulail et al. 2025 is being used alongside an NH_3 laser diagnostics defined in Alturaifi et al. 2022 to gather simultaneous measurements during ammonia-ethane pyrolysis in 97% argon dilution behind reflected shock waves in a shock tube between 1365 to 2389 K. The resulting NH_3 data are being used to verify initial ammonia concentrations, and the NH_2 data are used to obtain the reaction rate coefficient for $NH_3 + CH_3 \rightarrow NH_2 + CH_4$.

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