Comparison of ion-molecule reactions in cyclohexane, methylcyclohexane and ethylcyclohexane\textsuperscript{1} CHARLES JIAO, UES, STEVEN ADAMS, Air Force Research Laboratory — Cyclohexanes including cyclohexane (C\textsubscript{6}H\textsubscript{12}), methylcyclohexane (C\textsubscript{7}H\textsubscript{14}) and ethylcyclohexane (C\textsubscript{8}H\textsubscript{16}) are significant components of many practical fuels. C\textsubscript{6}H\textsubscript{12} and C\textsubscript{7}H\textsubscript{14} have been chosen as representative cycloalkanes in several proposed surrogate mixtures for jet fuels. In this study, the gas-phase ion-molecule reactions in these three cyclohexanes are examined, and comparison of the reaction channels in each of the cyclohexanes are made. A variety of reaction channels has been observed, which include charge transfer, H\textsuperscript{-} transfer, H\textsubscript{2}\textsuperscript{-} transfer, H\textsubscript{3}\textsuperscript{-} transfer, hydrocarbon anion transfer, and association with concerted fragmentation. Among these channels, H\textsuperscript{-} transfer is the most prevalent in the three cyclohexanes and, for many reactant ions, is the exclusive channel. Also observed is that H\textsubscript{3}\textsuperscript{-} transfer occurs only in C\textsubscript{6}H\textsubscript{12} while C\textsubscript{3}H\textsubscript{7}\textsuperscript{-} transfer occurs only in C\textsubscript{8}H\textsubscript{16}.

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