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Comparison of ion-molecule reactions in cyclohexane, methylcyclohexane and ethylcyclohexane[1] CHARLES JIAO, UES, STEVEN ADAMS, Air Force Research Laboratory — Cyclohexanes including cyclohexane (C_6H_{12}), methylcyclohexane (C_7H_{14}) and ethylcyclohexane (C_8H_{16}) are significant components of many practical fuels. C_6H_{12} and C_7H_{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^- transfer, H_2^- transfer, H_3^- transfer, hydrocarbon anion transfer, and association with concerted fragmentation. Among these channels, H^- transfer is the most prevalent in the three cyclohexanes and, for many reactant ions, is the exclusive channel. Also observed is that H_3^- transfer occurs only in C_6H_{12} while $C_3H_7^-$ transfer occurs only in C_8H_{16}.

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Charles Jiao
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