Formation of positive ions of quadricyclane

C.Q. JIAO, Innovative Scientific Solutions, Inc., Dayton, OH, C.A. DEJOSEPH, JR., R.H. LEE, A. GARSCADDEN, Air Force Research Laboratory, Wright-Patterson AFB, OH — Quadricyclane (QC) is one of the strained hydrocarbons that have potential as high-energy density materials used as aerospace fuel or as additives to kerosene rocket fuel. We have studied the formation of positive ions of QC by electron impact and by charge-transfer reactions, using Fourier-transform mass spectrum (FTMS) techniques. The electron ionization cross sections in the energy range of 10-200 eV have been measured. The total cross section reaches a maximum of $2.3 \times 10^{-15}$ cm$^2$ at 60 eV. Parent ion C$_7$H$_8^+$ and 21 fragment ions including C$_5$H$_6^+$ and C$_5$H$_5^+$ that dominate the dissociation channels at low energies (<25 eV) are observed. Ar$^+$ charge-transfer reaction with QC produces C$_5$H$_5^+$ and C$_7$H$_7^+$ as the major ionic species. Some selected hydrocarbon ions, i.e., C$_3$H$_3^+$, C$_5$H$_3^+$, C$_5$H$_5^+$ and C$_5$H$_6^+$, which are formed from QC by electron ionization, are found to react with QC forming C$_7$H$_7^+$ and C$_7$H$_8^+$ as the major product ions, while the latter two ions are unreactive with QC. The relative rates of the hydrocarbon ion reactions, compared to the Ar$^+$ charge-transfer reaction, are rather low; while the rate for C$_3$H$_3^+$ is less than 20 percent of the Ar$^+$ reaction rate, the rates for C$_5$H$_3^+$, C$_5$H$_5^+$ and C$_5$H$_6^+$ are less than 3 percent.

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