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Controlling Ionic Dissociations Reactions with Isotopic Labeling: Methane Loss in Acetone DAVID KLECYNGIER, JIM KERCHER, ANDRAS BODI, TOMAS BAER, DAN FAKOURY, None — Acetone-h_6 and acetone-d_6 were fragmented by low energy mass spectrometer to observe the formation of methane and methyl radicals. Methyl and methane loss are competing parallel reaction with activation energies of 78 ± 2 kJ mol^{-1} and 75 ± 2 kJ mol^{-1}, respectively. The dissociation thresholds for the fragment ions were measured from 10.200 eV to 10.700 eV. A hydrogen transfer is necessary to form CH_4; this requires tunneling through the potential barrier modeled by the Eckart barrier. The tunneling process was effectively shut off when acetone-d_6 was used, resulting in only methyl loss. This is due to the isotope effect, given that heavier matter is less likely to tunnel. The measured dissociations were then modeled with theoretical rates determined with high level quantum calculations using the approximate Eckart barrier, thermal energy, and dissociation rates. Time of flight, TOF, files were required to accurately model the dissociation of methane because it is a slow reaction, it dissociates while in flight, this leads to the development of asymmetric peaks in the spectra. A 1-dimensional Eckart barrier was determined to be effective as a rough analysis of this kind of reaction.

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None

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