Decomposition Kinetics of Nitroglycerine·Cl\textsuperscript{(g)} in Air at Ambient Pressure with a Tandem Ion Mobility Spectrometer

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Abstract:

Gas ions derived from the ionization of nitroglycerine (NG) vapor with chloride anions in air at ambient pressure included two adduct ions NG·Cl\textsuperscript{−} and NG·NO\textsubscript{3}\textsuperscript{−}. The chloride adduct of NG was isolated in a tandem ion mobility spectrometer with synchronized dual ion shutters and characteristic mobility of the ion peak for NG·Cl\textsuperscript{−}. Decomposition of NG·Cl\textsuperscript{−} in a second mobility stage occurred though a loss of nitrate with an activation energy of 80 ± 3 kJ mol\textsuperscript{−1} and a pre-exponential factor of 1.3 x 10\textsuperscript{12} s\textsuperscript{−1}. The reaction was seen as a displacement reaction from ab-initio calculations and the standard enthalpy change was measured as 83.3 ± 3 kJ mol\textsuperscript{−1} at 116.5 °C, the mid-point of the experimental range. Decomposition could occur from an initial NG·Cl\textsuperscript{−}* species from a collision stabilized NG·Cl\textsuperscript{−} or though an adduct of dinitrochloropropane·NO\textsubscript{3}\textsuperscript{−}, distinguishable neither by model nor measurement. Variations in temperature within the tandem IMS drift tube would create an error of only 0.5% in E\textsubscript{a}. Resolving power was 25 to 30 with shutter pulse widths of 300 µs sufficient to isolate NG·Cl\textsuperscript{−} from NG·NO\textsubscript{3}\textsuperscript{−}. Ionization chemistry was controlled by excluding impurities in the sample using heart-cutting techniques with a gas chromatograph inlet permitting selective measurements of explosives even in a mixture.

KEYWORDS: explosives, ab-initio, gaseous ions, drift tube, dual shutter