

Abstract: NeSA202100oral-07: A cross flow design of a tandem ion mobility spectrometer for the study of the thermal decomposition of the chloride and nitrate adducts of pentaerythritol tetranitrate in air at ambient pressure

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The thermal decomposition of chloride and nitrate adduct of pentaerythritol tetranitrate (PETN) has been measured using cross flow design dual shutter ion mobility spectrometer (IMS). The reaction region of IMS is a reservoir of chloride ion. It reacts with PETN sample, introduced using a nebulizer with heated system, to form both $\text{PETN}\cdot\text{Cl}^-$ and $\text{PETN}\cdot\text{NO}_3^-$ ion. $\text{PETN}\cdot\text{Cl}^-$ decomposes at a temperature range of 145°C - 165°C forming nitrate ion through $\text{S}_{\text{N}}2$ displacement mechanism. The activation energy is calculated to be 80 ± 7 kJ/mol. Similarly, $\text{PETN}\cdot\text{NO}_3^-$ decomposes to form nitrate ion at 175°C - 200°C with an activation energy of 92 ± 8 kJ/mol. Theoretical calculations are used to find the pathway of decomposition and support the experimental results.

Keywords: IMS, PETN, thermal decomposition