The Research of well-known Explosive RDX by Thermal Decomposition Technique by the means of Ion Mobility and Mass spectrometry

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1.Introduction

Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) is an explosive widely used as a major ingredient of solid propellants in military applications. Many effective techniques have been used for a thermal decomposition of RDX. Among them, ion mobility spectrometry (IMS) has proved to be one of the best methods for the detection of low concentration of explosives.

In this study, we have focused on reactions of RDX with reactant ions (RI) produced in negative corona discharge (CD) and formed ions after thermal decomposition at melting point 473 K. The ions have been detected by IMS coupled with orthogonal acceleration time of flight (oaTOF). The nature of observed ions RDX was abundant.

2. Experiment

The CD-IMS-oaTOF was described in detail in work [1]. It can be operated in three different regimes: in single IMS, TOF regime and in two-dimensional (2D) regime, where both devices work simultaneously, which allows us to gain 2D spectra. The IMS device was working in reverse gas flow mode during the entire experiment [2]. The 38 mg of RDX was inserted into a container placed out of the IMS and heated by heating patrons to reach its melting point, thus its decomposition could have started [3].

3. Results and discussion

The dominant RI present in zero air are O_2^- with m/z = 32 Da, $O_2^-(H_2O)$ of m/z = 50 Da, $N_2O_2^-$ of m/z = 60 Da, $O_2^-(H_2O)_2$ of m/z = 68 Da and $N_2O_3^-(H_2O)$ of m/z = 94 Da.

The 2D map allowed us ascribed peaks detected in IMS and MS spectra measured individually. The ions of m/z = 42 Da were assigned to $(NCO)^-$. The ions of m/z = 46 Da have been observed in previous researches and were assigned to NO_2^- [3].

Another generated ions of m/z = 59 Da were ascribed to $(CH_3NHCHO)^-$ or $(CH_3CONH_2)^-$ ions. The observed NO_3^- of m/z = 62 Da is a common fragment of thermal decomposition of RDX. The ions of m/z = 85 Da were asigned to triazine $(C_3H_7N_3)^-$. The response of RDX with reduced mobility 1.85 $cm^2V^{-1}s^{-1}$ has been corresponded to the ions of m/z = 105 Da. Since there are not any relevant references, we assumed they were formed by attachment of observed product ions of m/z = 59 Da $(CH_3NHCHO)^-$ or $(CH_3CONH_2)^-$ with another dominant product, NO_2^- ions, and generated clusters $(CH_3NHCHO+NO_2)^-$ or $(CH_3CONH_2+NO_2)^-$. The product ions of m/z= 89 Da originated from fragmentation of ions $(CH_3NHCHO+NO_2)^-$ or $(CH_3CONH_2+NO_2)^-$ of m/z = 105 Da by cleavage of oxygen atom either from triazine or from NO_2 under the influence present ions in CD. The ions with mass m/z = 221 Da were ascribed to $(RDX-H)^-$.

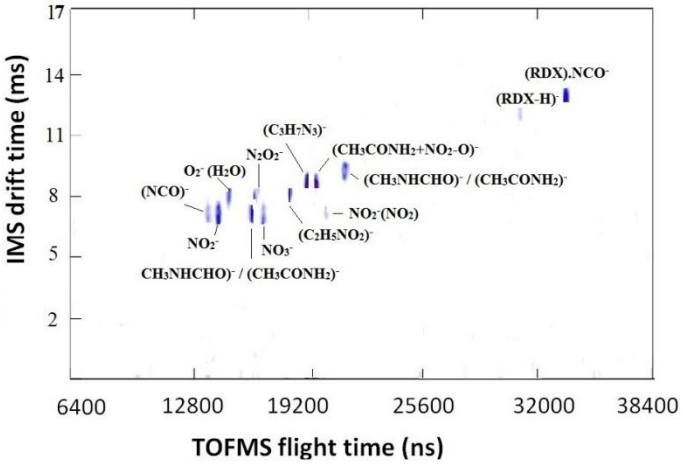

Fig.1: The two dimentional IMS-MS spectrum for 1.66 ppb concentration of RDX

References

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