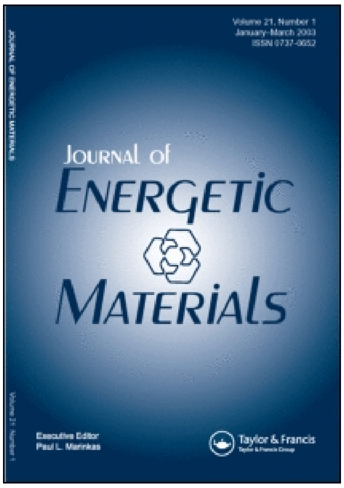

Journal of Energetic Materials
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713770432

Analysis of rdx vapors in pre- and postdetonations using the ion mobility spectrometer under field conditions

B. J. Yelverton[a]
[a] Sandia National Laboratories, Systems Engineering Div. 5248, Albuquerque, NM

To cite this Article Yelverton, B. J.(1988) 'Analysis of rdx vapors in pre- and postdetonations using the ion mobility spectrometer under field conditions', Journal of Energetic Materials, 6: 1, 73 — 80

To link to this Article: DOI: 10.1080/07370658808017237

URL: http://dx.doi.org/10.1080/07370658808017237

ANALYSIS OF RDX VAPORS IN PRE- AND POST-DETONATIONS USING THE ION MOBILITY SPECTROMETER UNDER FIELD CONDITIONS

B. J. Yelverton*

Systems Engineering Div. 5248

Sandia National Laboratories

Albuquerque, NM 87185

ABSTRACT.

The purpose of this work was threefold: To determine if the presence of RDX vapors could be detected both before and after an explosion in an enclosed area; to determine if this could be done with an ion mobility spectrometer(IMS) in the field; and to test the concept of using a 6-in. quartz tube(0.25-in. od) as a preconcentrator in the field. All three purposes were fulfilled.

INTRODUCTION.

The illegal use of explosive materials has created the need for analysis of both pre- and post-detonation of explosives. The first would be part of the effort to prevent life-threatening use of explosives; the second would be to verify the identity of the explosive(s) used in an incident.

Journal of Energetic Materials vol. 6, 073-080 (1988)

Published in 1988 by Dowden, Brodman & Devine, Inc.

This investigation, performed during the summer of 1986, is part of the broad spectrum of ongoing work at this laboratory dealing with the vapor detection of explosives. The purpose of the study was three-fold: (a) to determine if the presence of explosive vapors could be detected both before and after an explosion within an enclosed area; (b) to test if this could be done using an ion mobility spectrometer(IMS); and (c) to test the concept of using a 6-in. long quartz tube(0.25-in. od) as a preconcentrator in the field. The first has been generally demonstrated, primarily with nitrated dynamite and TNT[1-5]. Although recent studies indicate that quartz would be a good preconcentrator surface[6], a field demonstration of its utility has not been done. The use of a quartz tube preconcentrator in conjunction with an IMS in the field also has not been demonstrated.

EXPERIMENTAL.

Explosive.

The explosive used was RDX in the form of 0.5 lb. of PBX-9404 with a Reynolds Exploding Bridge Wire attached. This was supported by a 4-in. styrofoam block hollowed to fit the device. The assembly was set over the shot pad in a basket-like container constructed of a 2.25-in. plastic mesh lined with plastic sheeting. The entire container then was filled with AFC-172 aqueous foam.

Containment.

Detonations were done in a hemispherical, dome- shaped, inflatable building, 25-ft. tall and 50-ft. diameter. An air flow sufficient to maintain a one-inch pressure was used to fill the building. The entire dirt floor of the structure, including the metal shot pad, was covered by a thin sheet of polyethylene or polyvinyl.

Sampling.

Pre-detonations vapor sample collection was accomplished in the following manner: one end of an 18-in. length of polyvinyl tubing was attached to a Fixt-Flow pump(Model No. 1) and the other end was fitted with a swagelok containing a teflon ferrule. In each experimental run, the preconcentrator was a 0.25-in. od quartz tube, 6-in. long, which had been cleaned prior to use by heating to 300-400 ^{o}C for several minutes until extraneous peaks were not apparent in the IMS. It was locked in place and the pump turned on to draw air and any explosive vapor through the quartz tube by sweeping above the explosive at a distance of 0.50 to 1.00 in. for 30-sec.

Post-detonation samples were obtained using similar equipment approximately 30-min. after detonation in the volume above the shot pad. Sampling times again were about 30-sec. In one instance, a series of post-detonation samples were collected at varying intervals for 30-hours.

To determine if any explosive vapors had been collected, the preconcentrator was detached from the polyvinyl tubing and inserted into a swagelok(graphite ferrule) attached to an SNLA modified PCP-100 IMS. The IMS was operated in the negative ion mode. Explosive vapors adsorbed on the inner wall of the tube were removed by resistive heating of a nichrome wire coiled around the length of the preconcentrator tube. Ion mobility spectra were sequentially averaged over a 64-sec. interval and stored in the memory of a Sony Tektronix 336 Digital Storage Oscilloscope. Subsequently, the spectra were recalled, photographed, and any RDX peaks were identified.

Background Studies.

Background studies were made by obtaining the spectra from a quartz tube which had been attached to the IMS overnight. Any vapors collected within the tube were desorbed by resistive heating as described previously. Similar studies were made using a quartz tube that had not been attached to the IMS overnight. Open air environmental samples were also taken.

Ion Mobility Spectrometer(IMS).

The PCP-100 IMS was operated in the negative mode. Through secondary, tertiary, etc. ionizations, radioactive sources(e.g.^{63}Ni) in the IMS provide very low energy electrons. Subsequently, these can become attached to electronegative entities in air to form three major negative reactant ions, viz. $O_2(H_2O)^-$, O_2^-, $O(H_2O)^-$ (and perhaps some NO_2^-). Explosive molecules are more electronegative than any of the reactant ions. TNT, for example, will undergo charge transfer reactions: $TNT + A^- = TNT^- + A$. RDX enters into ion-molecule reactions with the reactant ions, viz. $RDX + A^- = (RDX\text{-}A)^-$.[7] The reduced ion mobility times correspond to the molecular weights of the addition compounds, e.g.$[RDX\text{-}O(H_2O)]^-$, $[RDX\text{-}O_2]^-$, etc. and, therefore, the resultant IMS spectra of RDX contains three distinct peaks (see Figure 1).

RESULTS.

The presence of small, sharp peaks were observed in the background studies. For quartz tubes left attached to the IMS overnight, the peak heights were in the range of 32-54 mV and the reduced ion mobility times were between 1.56-1.57. Quartz tubes not subjected to continuous attachment to the IMS produced peaks with amplitudes of 10-12 mV and reduced ion mobilities between 1.40-1.62. Ignoring the reactant ions, environmental samples yielded small peaks(10-12 mV height) with reduced ion mobilities between 1.36-1.49(Figure 1a).

All of the pre-detonation samples contained three distinct peaks(10-26 mV height) which had reduced ion mobilities of 1.49, 1.58 and 1.62(Figure 1b). Post-detonation samples produced the same three distinct peaks(18-34 mV height)(Figure 1c). The spectra in Figure 1d illustrates that the presence of RDX can be ascertained as long as 30-hrs. after detonation under the conditions of these tests.

As discussed above, the three peaks noted in Figure 1b-d result from the interaction between RDX and negative reactant ions and are characteristic of RDX. The reduced ion mobilities agree with those determined for RDX in the laboratory using the same IMS[8].

DISCUSSION

The results indicate that:

a) The IMS can be used for obtaining information in the instance of both pre- and post-detonation examination;

b) A quartz tube can be used as a preconcentrator in the field in conjunction with an IMS;

c) There is sufficient unexploded RDX in the post-detonation atmosphere to be collected and recognized.

Additional work should be done in this area to determine the sensitivity of the quartz tube/IMS detection system used under the conditions of this work. It also is desirable to know if other explosive compounds, such as PETN, can be detected prior to detonation and if they also leave traces of undetonated explosive in a blast area. Finally, a more efficient, and perhaps more sophisticated, preconcentrator system might prove to be quite useful in this type of study.

ACKNOWLEDGEMENT.

The author expresses appreciation to F. J. Conrad, B. T. Kenna and R. L. Schellenbaum, of Sandia National Laboratories, for their guidance and many helpful discussions in this work.

REFERENCES.

1. R. Jenkins and H. J. Yallop, Explosivestoffe Nr, 6, 139(1970).
2. C. R. Midkiff and W. D. Washington, Journal of the AOAC, 57, 1092(1974).
3. H. Forestier, Internat. Criminal Police Review, 277, 99(1974).
4. K. Bratin, P. T. Kissinger, R. C. Briner and C. S. Bruntlett, Anal. Chim. Acta, 130, 295(1981).
5. J. Yinon and S. Zitrin, "The Analysis of Explosives", Chap. 14, Pergamon Press, NY(1981).
6. B. T. Kenna and F. J. Conrad, "Studies on The Adsorption/Desorption Behavior of Explosive Molecules", to be published.
7. J. Yinon and S. Zitrin, Ibid., Chap. 13.
8. B. T. Kenna, Unpublished Data, July(1986).

* Summer appointment at Sandia National Laboratories; Ms. Yelverton is a chemistry teacher at Manzano High School, Albuquerque, NM.

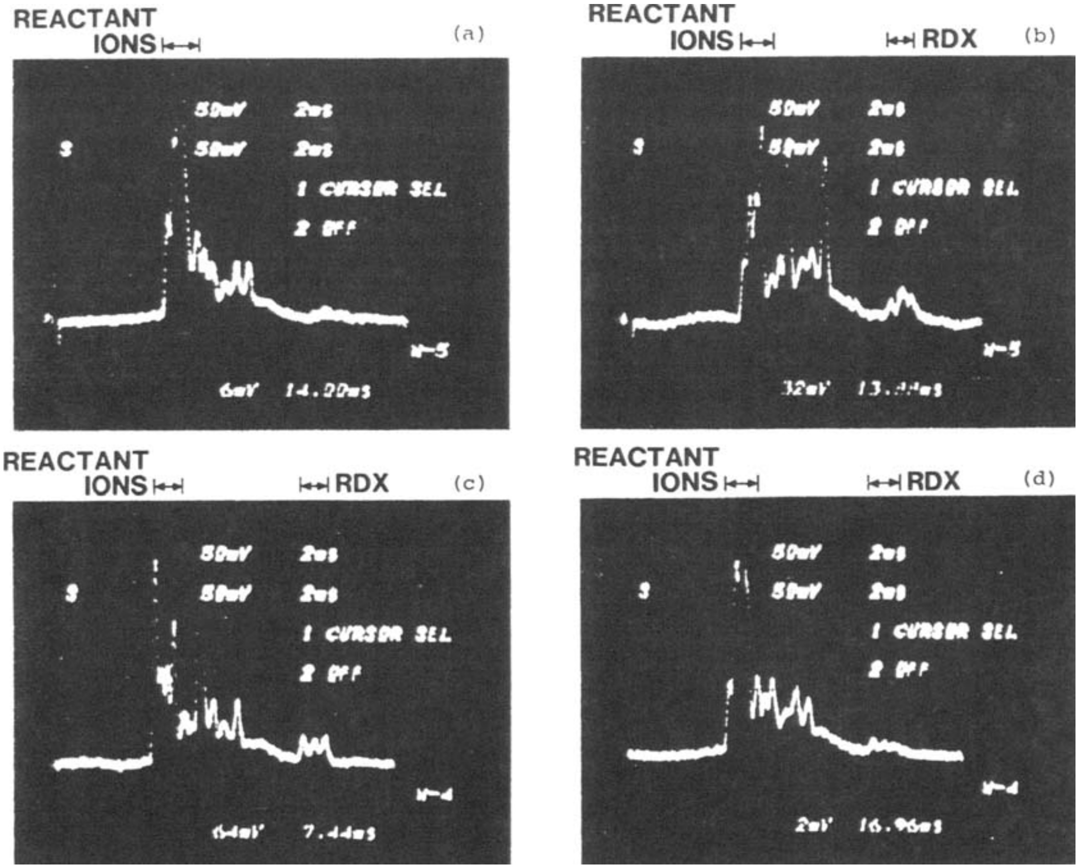

Figure 1. Ion mobility spectra. (a) environmental background; (b) pre-detonation sample taken above PBX-9404; (c) post-detonation sample taken 1-hr after detonation; (d) sample taken 30-hr after detonation. Note the peak-triad due to RDX in b-d.