

# Test method for vapor collection and ion mobility detection of explosives with low vapor pressure

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## Abstract

**Rationale:** IMS has been widely used for the on-site detection of explosives. Air sampling method is applicable only when the concentration of explosive vapor is considerably high in the air, but vapor pressures of common explosives such as TNT, RDX, and PETN are very low. A test method for analyzing the vapor detection efficiency of explosives with low vapor pressure via IMS was developed using artificial vapor and collection matrices. **Methods:** Artificial explosive vapor was produced by spraying an explosive solution in acetone. Fifteen collection matrices of various materials with woven or nonwoven structure were tested. Two arrangements of horizontal and vertical positions of the collection matrices were employed. Explosive vapor collected in the matrix was analyzed through IMS. **Results:** Only three collection matrices of stainless steel mesh (SSM), polytetrafluoroethylene sheet (PFS), and lens cleansing paper (LCP) showed the TNT and/or RDX ion peaks at explosive vapor concentration of 49 ng/L. There was no collection matrix to detect PETN vapor at lower than 49 ng/L. For the PFS, TNT and RDX were detected at 49 ng/L vapor concentration. For the LCP, TNT and RDX were detected at vapor concentrations of 14 and 49 ng/L, irrespectively. **Conclusions:** The difference in the explosive vapor detection efficiencies could be explained by the adsorption and desorption capabilities of the collection matrices. The proposed method can be used for evaluating the vapor detection efficiency of hazardous materials with low vapor pressure.

## Test method for vapor collection and ion mobility detection of explosives with low vapor pressure

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**Methods:** Artificial explosive vapor was produced by spraying an explosive solution in acetone. Fifteen collection matrices of various materials with woven or nonwoven structure were tested. Two arrangements of horizontal and vertical positions of the collection matrices were employed. Explosive vapor collected in the matrix was analyzed through IMS.

**Results:** Only three collection matrices of stainless steel mesh (SSM), polytetrafluoroethylene sheet (PFS), and lens cleansing paper (LCP) showed the TNT and/or RDX ion peaks at explosive vapor concentration of 49 ng/L. There was no collection matrix to detect PETN vapor at lower than 49 ng/L. For the PFS, TNT and RDX were detected at 49 ng/L vapor concentration. For the LCP, TNT and RDX were detected at vapor concentrations of 14 and 49 ng/L, irrespectively.

**Conclusions:** The difference in the explosive vapor detection efficiencies could be explained by the adsorption and desorption capabilities of the collection matrices. The proposed method can be used for evaluating the vapor detection efficiency of hazardous materials with low vapor pressure.

## 1 INTRODUCTION

Ion mobility spectrometry (IMS) has been widely used for the detection of hazardous materials such as explosives, drugs, chemical warfare agents, and polycyclic aromatic hydrocarbons (PAHs); it involves the use of large laboratory instruments, portable analyzers, or on-site detectors.<sup>1-17</sup> IMS is also one of the most widely used methods for detecting explosives in the field such as airport security checks. Various sampling methods for explosive detection via IMS have been reported.<sup>15,18-26</sup> For gas-phase sampling, a direct gas inlet, gas chromatograph, and semi-permeable membrane have been investigated.<sup>20-22,26</sup> The air sampling method can be conducted for the collection of explosive materials in the air by using a semi-permeable membrane upon air inhalation; however, it is applicable only when the concentration of explosive vapor is considerably high in the air. Vapor pressures of common explosives such as 2,4,6-trinitrotoluene (TNT), 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX), and pentaerythritol tetranitrate (PETN) are very low of  $5.50 \times 10^{-6}$ ,  $3.30 \times 10^{-9}$ , and  $1.16 \times 10^{-8}$  Torr at 25°C, respectively.<sup>27</sup>

Explosives with low vapor pressure can be vaporized by various methods including heating an explosive powder, nebulizing and heating an explosive solution, evaporating an explosive powder at room temperature for a long time, and using a vapor generator.<sup>28-32</sup> Mullen et al. studied explosive vapor transport efficiency using aqueous solutions of TNT and RDX by nebulizing and heating them at 130°C for the preparation of explosive vapor,<sup>28</sup> while Li et al. prepared explosive vapor by placing a solid-state explosive powder in a flask at 25°C for 48 h after sealing.<sup>31</sup> Vapor preparation by heating is not suitable for thermally labile chemicals; also, it is difficult to control the amount of vapor. Because vapor preparation at room temperature takes considerably long and the amount of vapor is low, it is not a suitable method for vaporizing explosives with low vapor pressure.

Explosive vapor prepared by heating can be detected through IMS.<sup>25,30</sup> Collection and thermal desorption of explosive vapors using quartz and packed tubes was reported.<sup>33</sup> However, these collection tubes need an additional thermal desorption device to evaporate the adsorbed explosives; moreover, this method suffers a risk of contamination when the tubes are reused. IMS has high explosive detection sensitivity and allows fast on-site detection of explosives. Hence, a simple and low-cost method for explosive vapor collection is required. Swab and smear matrices are typically used for collecting solid-state explosives for IMS detection.<sup>34-37</sup> Furthermore, they are simple and affordable.

In this study, vapors of common explosives (TNT, RDX, and PETN) with low vapor pressure were artificially generated by spraying their solutions in acetone. Explosive molecules in aerosols produced by spraying are isolated by solvent evaporation. Acetone quickly evaporates even at room temperature, and evaporation is accelerated by spraying the solution. This explosive vapor preparation method enables control of the amount of explosive vapor. Artificial vapor was collected using various collection matrices, and the collected vapor was analyzed through IMS. Fifteen collection matrices comprising various substances and having different structures were employed. The differences in the explosive vapor collection efficiencies depending on the collection matrices were investigated. The influence of the arrangements (horizontal and vertical positions) of the collection matrix on the detection efficiency was also examined. The experimental results were explained on the basis of the differences in the collection matrix structures and the interactions between the matrix and explosive molecule. We believe that the developed method can be useful for testing the vapor detection efficiency of hazardous materials with low vapor pressure.

## 2 METHODS

### 2.1 Materials

TNT, RDX, and PETN were supplied from Hanwha Co. (Republic of Korea). Acetone was purchased from Aldrich Chemical Co. (USA). Stainless steel mesh (SSM) and polytetrafluoroethylene (PTFE) sheet (PFS) were supplied from Newone S&T (Republic of Korea). Cotton fabric (COF) was purchased from Chungoa Co. (Republic of Korea), lens cleansing paper (LCP) was purchased from Sargent-Welch Scientific Co. (USA), polypropylene (PP) nonwoven (PPN) was purchased from Thesooop Co. (Republic of Korea), acrylate fabric (APF), poly(ethylene terephthalate) (PET) fabric (PTF), and polyamide (PA) fabric (PAF) were purchased from Dawon Co. (Republic of Korea), carbon nonwoven (CFN) was purchased from GNT filter Co. (Republic of Korea), carbon plain/twilled fabrics (CPF and CTF, respectively) and carbon fabrics (CF720 and CF730) (CF2 and CF3, respectively) were purchased from Hankuk Carbon Co. (Republic of Korea), filter paper (FPP) was purchased from Hyundai Micro Co. (Republic of Korea), and coffee filter (CFP) was purchased from Thomas & Green Co. (Singapore). Only SSM is made of metal and has mesh structure. Collection matrices with woven fabric structures are PFS, COF, APF, PTF, PAF, CPF, CTF, CF2, and CF3, while those with nonwoven structures are LCP, PPN, CFN, FPP, and CFP (Table S1 and Figure S1; Supplementary Information).

### 2.2 Preparation of artificial explosive vapor and vapor collection experiment

Each explosive was dissolved in a volatile solvent of acetone, and explosive solutions of 4.17  $\mu\text{g/mL}$  were prepared. Experiments were carried out using a DLH-010 fume hood (410 L) of Jeiotech Co. (Republic of Korea). The dimension of the collection matrix was  $5 \times 8 \text{ cm}^2$ . Explosive vapor was artificially produced by spraying the explosive solution. A total of 5, 10, and 20  $\mu\text{g}$  of the explosive were introduced into the hood by spraying 1.2, 2.4, and 4.8 mL of the explosive solution, respectively. These values correspond to the explosive vapor concentrations of 12, 24, and 49  $\text{ng/L}$ , respectively, in the hood. The experimental procedure was as follows: (1) two sets of the matrices were arranged at the bottom part of the hood, (2) the explosive solution was sprayed at the top part of the hood, (3) the explosive vapor was collected for 30 sec, and (4) IMS analysis was carried out with the collection matrix. The generation of artificial explosive vapor and the vapor deposition in the collection matrix are described in Figure 1. Aerosols were formed by spraying the explosive solution, which leads to the acceleration of acetone evaporation.

Two arrangement types of the horizontal and vertical positions of the collection matrices were employed as shown in Figures 2 and 3, respectively. The base side area of the hood was  $90 \times 64 \text{ cm}^2$ . For the horizontal arrangement, two sets of 15 collection matrices were placed at 12 cm from the wall. For the vertical arrangement, two sets of 15 collection matrices were placed at 14 and 15 cm from the wall. Two sets of collection matrices were located at different sites to avoid positional effects.

### 2.3 IMS analysis

Portable IMS equipped with corona discharge ionization source, IMS of Newone S&T (Republic of Korea), was used. The analysis conditions of IMS were as follows: temperature of the sample inlet part was  $150^\circ\text{C}$ , temperature of the drift tube was  $100^\circ\text{C}$ , the electric field was 200 V/cm, and the ion drift tube was 13.2 cm. The IMS analysis was performed in the negative ion mode. The same experiments were performed 5 times and it was determined to detect the explosive when detecting at least four of the five cases.

Detection limits of the solid-state explosives according to the collection matrices were analyzed. The explosive solutions of 0.1 - 500  $\text{ng}/\mu\text{L}$  were prepared. The explosive solution of 1.0  $\mu\text{L}$  was dropped on the collection matrix and the solvent was thoroughly evaporated to obtain solid-state explosive. The matrix was introduced into the sample inlet part of IMS and the IMS analysis was carried out.

## 3 Results and Discussion

### 3.1 Explosive vapor collection efficiency depending on the collection matrix

The experimental results are summarized in Table 1. Among the 15 collection matrices, only three matrices of the SSM, PFS, and LCP showed the TNT and/or RDX ion peaks in the IMS spectra at the explosive vapor concentration lower than 49 ng/L. There was no collection matrix to detect PETN at a vapor concentration lower than 49 ng/L. For the SSM, only TNT at 49 ng/L vapor concentration was detected for the horizontal position. For the PFS, TNT and RDX were detected at 49 ng/L vapor concentration irrespective of the arrangement types. For the LCP, TNT was detected at 24 ng/L vapor concentration and RDX was observed at 49 ng/L vapor concentration irrespective of the arrangements.

The base side area of the hood was  $90 \times 64 = 5760 \text{ cm}^2$ , and the size of the collection matrix was  $5 \times 8 = 40 \text{ cm}^2$ . Thus, for the horizontal position, each collection matrix covered 0.7% of the hood base. If 20  $\mu\text{g}$  artificial vapor completely and evenly spreads down to the hood base without any loss, the maximum amount adsorbed on each collection matrix will be 140 ng. However, considerable amount of explosive vapor cannot reach the hood base, because some explosive vapor will be adsorbed on the hood wall during the spraying of solution and spreading of vapor. Considering the adsorption of explosive vapor on the hood wall, a reasonable amount of explosive vapor adsorbed on each collection matrix should be much less than 140 ng. When 10  $\mu\text{g}$  vapor is introduced into the hood, the amount of explosive vapor adsorbed on each collection matrix should be much less than 70 ng. Considering this situation, the corrected detection limits of explosive vapors deposited on the collection matrices are summarized in Table 2.

### 3.2 Comparison of detection efficiencies of collected explosive vapor and solid-state explosive samples

The corrected detection limits of explosive vapors were compared to the detection limits of solid-state explosives. The solid-state explosive samples were prepared by dropping the explosive solution on the collection matrix and evaporating the solvent. The detection limits of solid-state explosives are listed in Table 3. The detection limits of solid-state explosives were significantly lower than those of the vapor samples. This is because of the difference in the distributions of the explosive samples in the matrix. For the solid-state explosives, the sample spot size is typically less than  $1 \text{ cm}^2$ , whereas for the collected explosive vapor the explosive molecules are evenly distributed over the entire matrix (Figure S2; Supplementary Information). Because the diameter of the inlet hole in the IMS instrument is less than 1 cm, a large amount of explosives adsorbed on the matrix cannot be sufficiently introduced into the ionization part. Thus, the inlet efficiency for the vapor-collected sample will be significantly lower than that for the solid-state explosive sample.

The LCP exhibited the best detection limit for the solid-state explosives, followed by the SSM. However, the detection limit of SSM for the explosive vapor was higher than that of PFS. This is because the SSM has a mesh structure, which limits the absolute area available to collect explosive vapor. Although the detection limits of solid-state TNT were less than 10 ng except for the PTF and CFN, the TNT vapor of 49 ng/L (the corrected amount  $< 140 \text{ ng}$ ) was not detected except for the SSM, PFS, and LCP. This can be explained by the thickness and bundle structure of the fine filaments. The matrices with woven fabric structures, such as the COF, APF, PTF, PAF, CFP, CF2, and CF3, are composed of bundles of fine filaments, while those with nonwoven structures, such as the PPN (0.33 mm), CFN (3.49 mm), FPP (0.14 mm), and CFP (0.11 mm), are relatively thick (Table S1 and Figure S1; Supplementary Information). For the woven fabric matrices, explosive vapor can penetrate into the inner part of the fine filament bundles, thereby reducing the desorption efficiency of the explosive molecules collected in the inner part. Although the PFS is a woven fabric, it is chemically inert and the filaments are very close to each other, so the explosive vapors may not deeply penetrate into the matrix. For the thick nonwoven matrices, explosive vapor can penetrate into the inner part of the matrix, thereby reducing the desorption efficiency.

### 3.3 Characteristics of IMS spectra of the collected explosive vapor samples

Figure 4 shows the IMS spectra of TNT vapors (24 ng/L) collected in the LCP. The TNT ion was detected for both the horizontal and vertical arrangements. The TNT ion peak is  $[\text{TNT} - \text{H}]^-$ .<sup>7,28-30</sup> For the horizontal arrangement, the TNT ion peak was more intensively observed at 5 – 6 sec after the sample inlet. For the vertical arrangement, the TNT ion peak was more intensively detected at 5 – 6 sec after the sample inlet

and it was observed until 10 sec. Detection sensitivity for the vertical arrangement was better than that for the horizontal arrangement, which was unexpected; however, it can be attributed to the flexibility and adsorption ability of the thin LCP (0.03 mm thickness). The LCP arranged with the horizontal position is fixed at the bottom and explosive vapor is adsorbed on the upper side, whereas for the vertical arrangement it is movable and explosive vapor is adsorbed on the both sides.

In the IMS spectra of TNT vapors (49 ng/L) adsorbed on the SSM, the TNT ion was detected at 36.3 ms for the horizontal arrangement, but it was not observed for the vertical arrangement (Figure S3; Supplementary Information). The TNT ion peak was more intensively observed at 5 – 6 sec after the sample inlet. In the IMS spectra of RDX vapors (24 ng/L) adsorbed on the PFS, the RDX ion was detected at approximately 38 ms for both the horizontal and vertical arrangements, but its intensity was weak (Figure S4; Supplementary Information). The intensity of the RDX ion peak was greater at longer delay times, which may be attributed to low volatility of RDX.

Figure 5 shows the IMS spectra of RDX vapors (49 ng/L) adsorbed on the LCP. For the horizontal arrangement, the RDX ion was detected at the delay time of 1 – 3 sec and two ion peaks were observed after 5 sec. The two RDX-related ions correspond to  $[\text{RDX} + \text{Cl}]^-$  and  $[\text{RDX} + \text{NO}_2]^-$ .<sup>28-31</sup> For the vertical arrangement, the two RDX-related ions were clearly detected at 37.3 and 39.5 ms after 5 sec. Similar to the TNT case, the detection sensitivity for the vertical arrangement of the LCP was greater than that for the horizontal arrangement, which is also because of the flexibility and adsorption ability of the LCP as discussed above.

### 3.4 Factors influencing the explosive vapor detection efficiency

The PETN vapor was not detected up to a vapor concentration of 49 ng/L for any of the collection matrices. This cannot be explained by the low vapor pressure of PETN because the vapor pressure of PETN is greater than that of RDX.<sup>27</sup> This can be attributed to the structural flexibility and the number of the nitrate groups of PETN molecule. The nitrite groups of TNT molecule are fixed in the rigid benzene ring, whereas those of RDX molecule are bonded to the six-membered ring of flexible methylene. The nitrate groups of PETN molecule are bonded to flexible alkyl chain. The nitrate group is more flexible than the nitrite group. The energy-minimized structures of TNT, RDX, and PETN molecules are shown in Figure 6. PETN contains four nitrate groups, while TNT and RDX contain three nitrite groups. Since the nitrate groups better interact freely and strongly with the polymers of the collection matrix than the nitrite ones, the desorption efficiency of the adsorbed explosives will be reduced.

Factors influencing the detection efficiency of explosive vapor can be divided into two categories of the adsorption and desorption capabilities. The factors affecting the adsorption capability of the collection matrix are area, material, and structure. All of the collection matrices have the same size of  $5 \times 8 \text{ cm}^2$ . However, the real adsorption area of SSM is much smaller than those of the others because of its mesh structure. The types of materials of the collection matrices can also influence the adsorption capability of explosive vapor. If a collection matrix is chemically more interactive with explosive vapor, the adsorption capability is expected to improve. Since the explosives are relatively polar, the collection matrix made of medium polar material may improve the adsorption capability.

The influencing factors related to the desorption capability of the collection matrix are chemical interactions, thermal conductivity, thickness, and structure. The desorption capability is compromised because of the increasing interactions between the explosive molecule and collection matrix. Since PETN might have stronger interactions with the collection matrix compared to the other explosives as discussed above, its desorption capability is expected to be poorer. The thermal conductivity of the collection matrix affects the desorption capability because the detection sensitivity depends on the amount of explosive molecules desorbed at a certain time. A collection matrix with good thermal conductivity can induce a more rapid and efficient evaporation of the explosives, thereby improving the detection sensitivity. Since explosive vapors can penetrate into the inner part of the collection matrix, a thicker matrix is less favorable for desorbing the explosive molecules compared to a thinner matrix. The bundle structure of fine filaments can improve the adsorption capability of explosive vapor, but will prevent thermal conduction. Thus, collection matrices

with a bundle structure would exhibit a poor detection efficiency.

## 4 CONCLUSIONS

A test method for vapor collection efficiency and IMS detection of explosives with low vapor pressure such as TNT, RDX, and PETN was developed using artificial explosive vapor and collection matrices. Explosive vapor was generated by spraying the explosive solution in acetone, and the collected vapor was detected using IMS. Of the 15 collection matrices, only the SSM, PFS, and LCP showed the TNT and/or RDX ion peaks in the IMS spectra at explosive vapor concentration of lower than 49 ng/L. PETN was not detected up to a vapor concentration of 49 ng/L because of the low desorption capability. For the SSM, only TNT at 49 ng/L of vapor concentration was detected for the horizontal arrangement. For the PFS, 49 ng/L of TNT and RDX vapors were observed in the IMS spectra. For the LCP, TNT was detected at 24 ng/L of vapor concentration and RDX was observed at 49 ng/L of vapor concentration. The detection limits of explosive vapors were significantly poorer than those for solid-state explosives owing to the difference in the introduction efficiencies. The adsorption and desorption capabilities could be factors that influence the explosive vapor detection efficiency. The factors affecting the adsorption capability of the collection matrix are area, material, and structure. The contributing factors related to the desorption capability are chemical interactions, thermal conductivity, thickness, and structure. The test method developed in this study can be used for evaluating vapor collection efficiency and IMS detection of hazardous materials with low vapor pressure and may be applied to on-site trace chemical vapor detection.

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**Table 1 Detection of explosive vapors collected in the collection matrices.**

| Explosive concentration (ng/L) | Collection matrix (Horizontal/Vertical) | Collection matrix (Horizontal/Vertical) | Collection matrix (Horizontal/Vertical) |
|--------------------------------|-----------------------------------------|-----------------------------------------|-----------------------------------------|
|                                | SSM                                     | PFS                                     | LCP                                     |
| TNT (12)                       | No/No                                   | No/No                                   | No/No                                   |
| TNT (24)                       | No/No                                   | No/No                                   | Yes/Yes                                 |
| TNT (49)                       | Yes/No                                  | Yes/Yes                                 | Yes/Yes                                 |
| RDX (24)                       | No/No                                   | No/No                                   | No/No                                   |
| RDX (49)                       | No/No                                   | Yes/Yes                                 | Yes/Yes                                 |
| PETN (49)                      | No/No                                   | No/No                                   | No/No                                   |

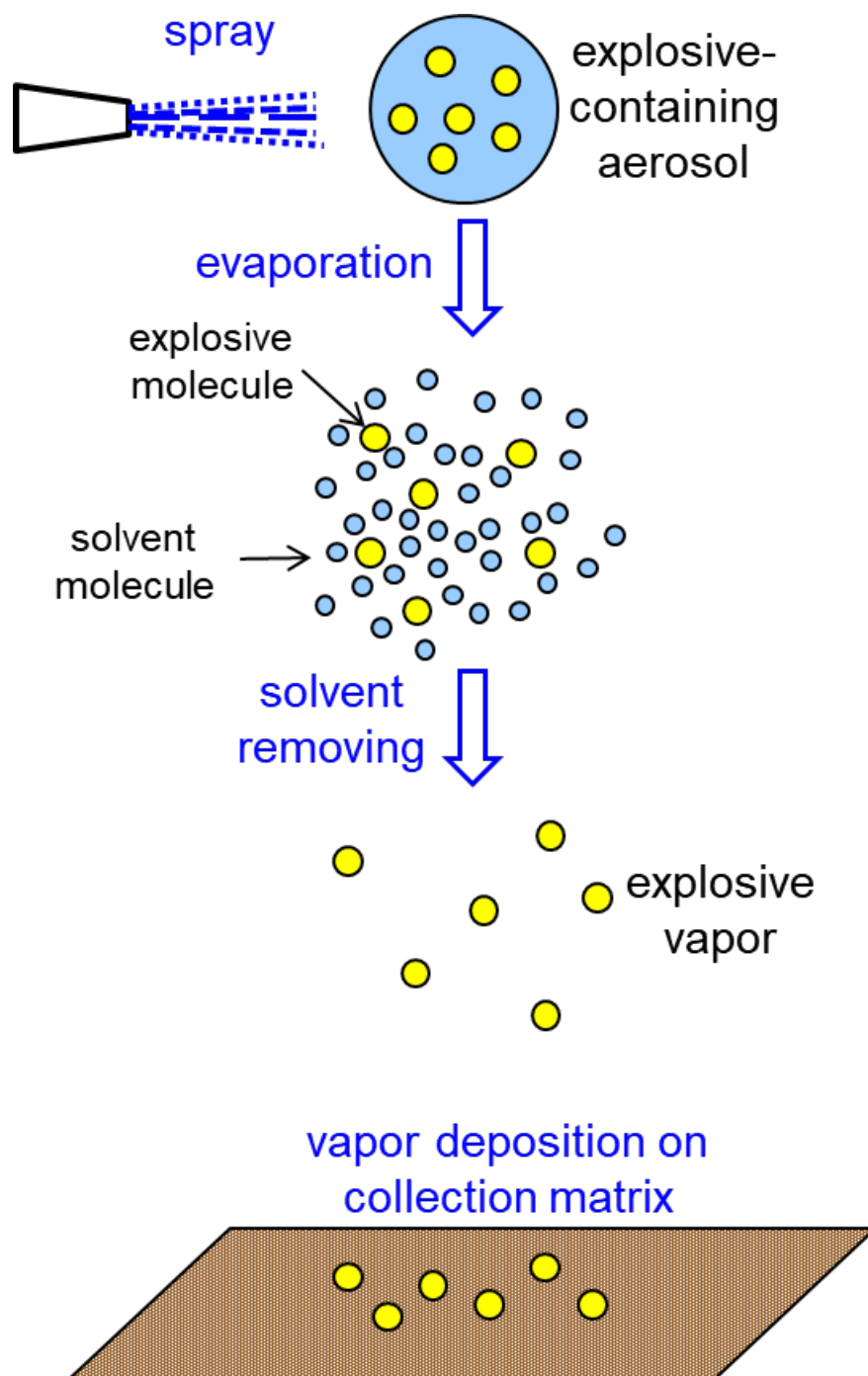
**Table 2 Corrected detection limits of the explosive vapors collected in the collection matrices (ng).**

| Explosive | Collection matrix   | Collection matrix   | Collection matrix   |
|-----------|---------------------|---------------------|---------------------|
|           | SSM                 | PFS                 | LCP                 |
|           | Horizontal position | Horizontal position | Horizontal position |
| TNT       | < 140               | < 140               | < 70                |
| RDX       | > 140               | < 140               | < 140               |
| PETN      | > 140               | > 140               | > 140               |
|           | Vertical position   | Vertical position   | Vertical position   |
| TNT       | > 140               | < 140               | < 70                |
| RDX       | > 140               | < 140               | < 140               |
| PETN      | > 140               | > 140               | > 140               |

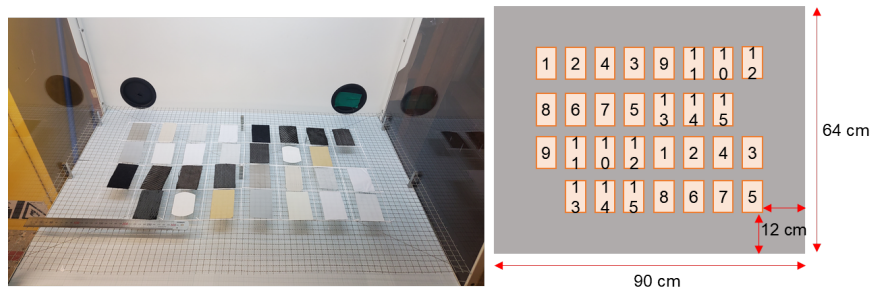
**Table 3 Detection limits of the solid-state explosives prepared by the solution spot according to the collection matrices (ng).**

| Collection matrix | TNT | RDX | PETN |
|-------------------|-----|-----|------|
| SSM               | 2   | 5   | 5    |
| PFS               | 5   | 20  | 20   |

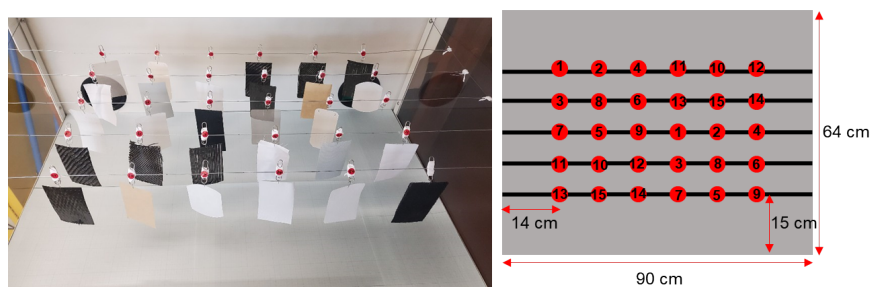
| Collection matrix | TNT | RDX   | PETN  |
|-------------------|-----|-------|-------|
| COF               | 5   | 20    | 20    |
| LCP               | 0.2 | 2     | 2     |
| PPN               | 5   | 10    | 20    |
| APF               | 7   | 70    | 70    |
| PTF               | 20  | 70    | 70    |
| PAF               | 5   | 50    | 50    |
| CFN               | 500 | > 500 | > 500 |
| CPF               | 7   | 50    | 50    |
| CTF               | 7   | 50    | 50    |
| CF2               | 7   | 50    | 50    |
| CF3               | 7   | 50    | 50    |
| FPP               | 5   | 20    | 20    |
| CFP               | 5   | 20    | 20    |



**FIGURE 1** Generation of artificial explosive vapor by spraying the explosive solution and the vapor deposition in a collection matrix.



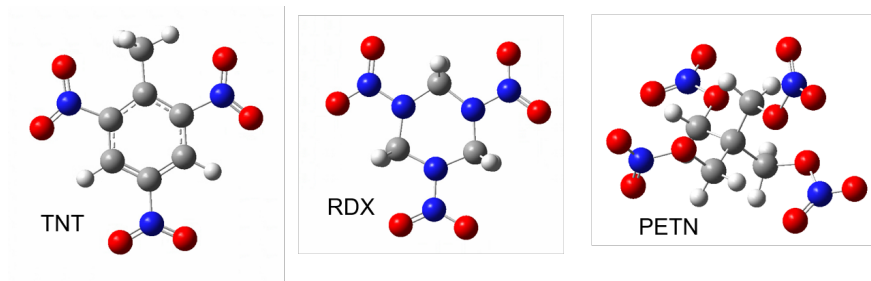
**FIGURE 2** Horizontal arrangement experiment of the collection matrices. The numbers are the sample codes marked in Figure 1.



**FIGURE 3** Vertical arrangement experiment of the collection matrices. The numbers are the sample codes marked in Figure 1.

**FIGURE 4** IMS spectra of the TNT vapors collected in the LCP matrix arranged with horizontal (a) vertical and (b) positions. The amount of explosive was 10  $\mu\text{g}$ .

**FIGURE 5** IMS spectra of the RDX vapors collected in the LCP matrix arranged with horizontal (a) vertical and (b) positions. The amount of explosive was 20  $\mu\text{g}$ .



**FIGURE 6**Energy-minimized structures of TNT, RDX, and PETN.