



## Thermal Desorption of Military Simulant: Linearity and Reproducibility

### Application Note Homeland Defense

This study details the analysis of the chemical weapon simulants Dimethyl Methyl Phosphonate (DMMP), 1,4-Oxathiane, and Triethyl Phosphate using thermal desorption. Linearity, reproducibility, and carry-over were examined.

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A three compound standard mixture was used (30ng/ $\mu$ l of each simulant in methanol). Tubes packed with Tenax were spiked with 2,4,6,8, or 10 $\mu$ l respectively of the standard mixture. These volumes were equal to 60,120,180,240, and 300 nanograms respectively. Each concentration was spiked in triplicate, and the tubes were thermally desorbed at 300°C/5min to a focussing trap. The focussing trap was then heated to 275°C/3min. The GC program was as follows: 60°C/1min, 12°C/min to 220°C.

The three areas of each simulant concentration were averaged and plotted (area/nanograms). The correlation coefficient of each graphed compound was 0.99 (see figures 1-3). Linearity is clearly established for these compounds up to the 300 nanogram range.

A series of eighteen Tenax tubes were spiked with a 4 $\mu$ l (120ng) of each simulant. They were thermally desorbed using the above thermal desorption parameters. Areas were averaged for each simulant and RSD's calculated. The 1,4-Oxathiane had an RSD of 11.9%, DMMP of 9.82% and TEP of 11.44%. Figures 4 and 5 show chromatograms of a duplicate run on the same tube. Figure 5 shows no observable carry over of compounds A (1,4 Ox) and B (DMMP). A negligible amount of C (TEP) is observed.

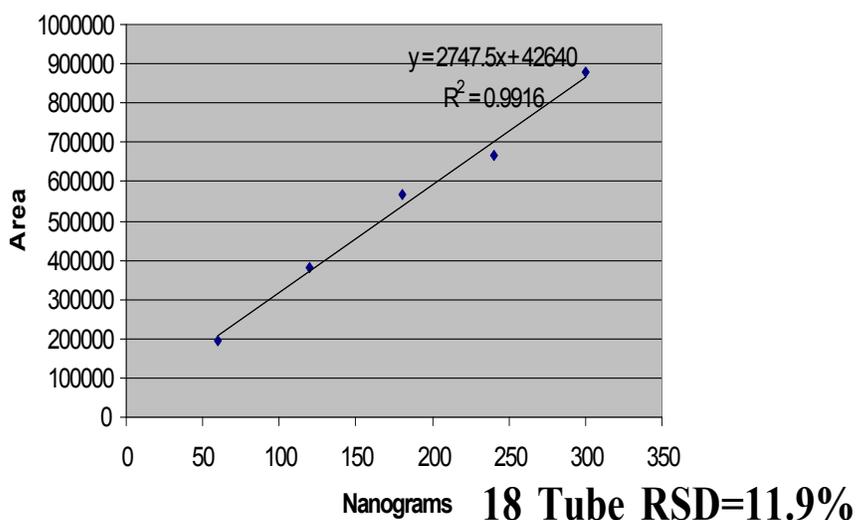


Figure 1. Linearity of 1, 4 Oxathiane

**Instrument Conditions**  
**Autosampler Dynatherm 9300**

Valve Oven: 250°C  
 Transfer Line: 275°C  
 Tube Heat: 300°C 5 minutes  
 Trap Heat: 300°C 3 minutes

**GC/MS**

Column: CP-Select 624  
 (30m x 0.25mm x 1.4µm)  
 Carrier: Helium, 50:1 split  
 Injector: 300°C  
 Oven: 60°C for 1 minutes  
 12°C/min to 220°C  
 Mass Range: 35-500

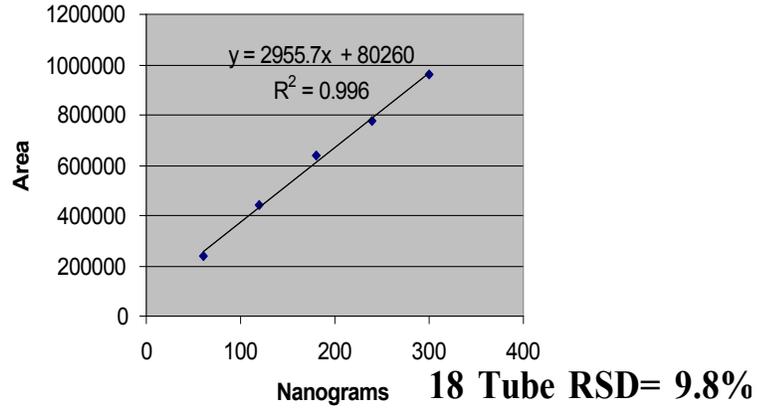


Figure 2. Linearity of DMMP

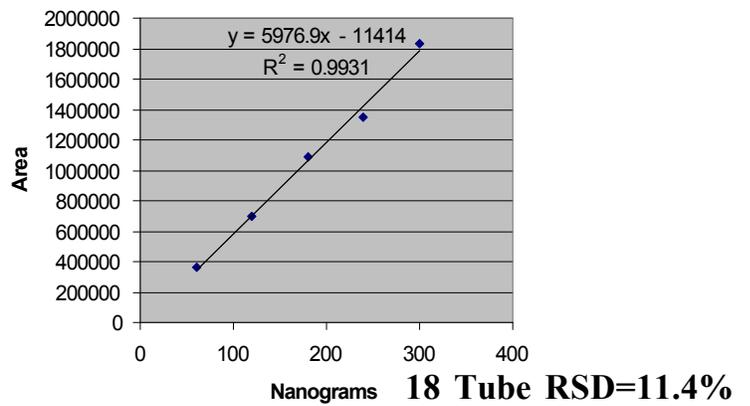


Figure 3. Linearity of Triethyl Phosphate

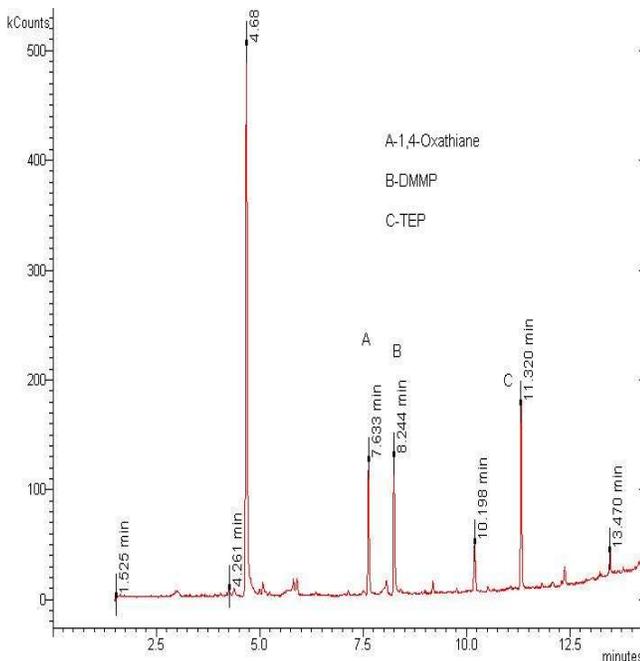


Figure 4. 1st run of tube

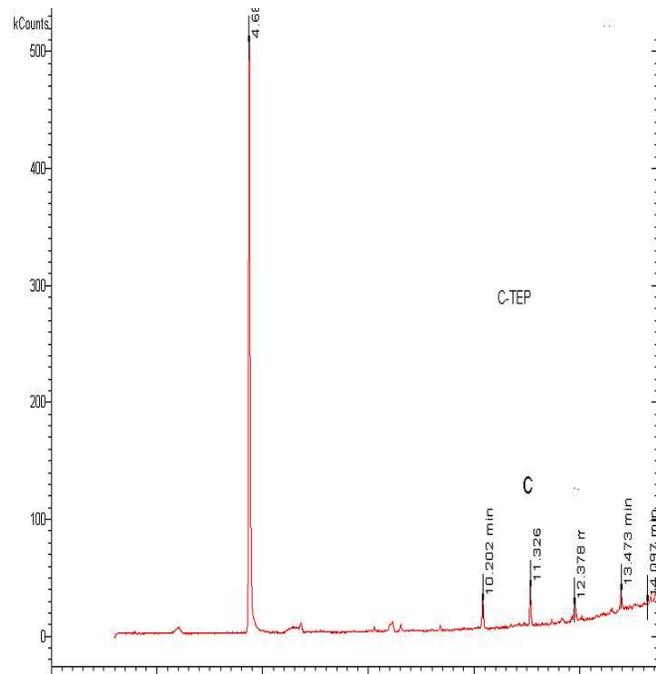


Figure 5. 2nd run of tube