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## Migration of PBX 9501 Constituents

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### Introduction

The nominal composition of PBX 9501 is 94.9% HMX, 2.5% Estane 5703, 2.5% bis-2,2-dinitropropyl acetal/formal (nitroplasticizer, NP), and 0.1% stabilizer (diphenylamine, DPA or Irganox 1010). In addition to the stabilizer added to the PBX formulation, the NP eutectic liquid contains 0.1% of the stabilizer phenyl-beta-naphthylamine (PBNA). For PBX 9501 containing weapons, it is known that NP migrates from the charge into the shield material, causing a concentration gradient within the HE.<sup>1</sup> It is thought that the shield polymer, an ethylene-vinyl acetate-vinyl alcohol terpolymer, becomes saturated over time with NP and that migration is then stopped. Experiments have been performed showing the saturation concentration of the shield material to be 8.8 weight percent.<sup>2</sup>

Prior to this work, analyses were performed on weapon components from a W76 unit that had been in the stockpile for 172 months.<sup>3</sup> The HE, stress cushions, and shields were analyzed for NP and for possible products of NP decomposition. Although no evidence of NP decomposition was found, it was discovered that the PBX stabilizer and the HMX impurity, RDX, were also moving into the shields. This paper will summarize the analytical data obtained from a number of weapons of various ages. Quantitation of NP, DPA, Irganox, RDX, and PBNA has been performed on shields from six different W76 units.

### Experimental

The solvent used for extraction of the shields was 1,2-dichloroethane (DCE). A 25 gram sample of the shield material was cut into approximately 0.5-inch square pieces, and mixed with 50 milliliters of solvent. The samples were then placed in a cooled (20°C) ultrasonic bath for 18 hours.

The extracts were analyzed by high performance liquid chromatography (HPLC) using a C-18 column and an ultraviolet absorbance detector set at 230 nm. An eluent gradient starting at 60/40 methanol/water and ending at 100% methanol was used to elute all analytes in a 35 minute run. The HPLC sample was prepared by diluting the DCE extract with methanol, 4 parts methanol to 1 part DCE.

### Results & Discussion

Table 1 lists the W76 unit numbers, age of the units, shield part numbers, and the lot number of PBX 9501 that each weapon contained.

Table 1. W76 Unit Information for Shields Analyzed.

| Unit No. | Stockpile Age (mo) | Shield No.   | HE Lot No. |
|----------|--------------------|--------------|------------|
| 770158   | 188                | BBN-1075-E78 | 685-001    |
| 770158   | 188                | BBN-1076-E78 | 685-001    |
| 361848   | 182                | BBN-1515-C79 | 685-002    |
| 361848   | 182                | BBN-1678-C79 | 685-002    |
| 931065   | 181                | BBN-1716-E79 | 685-002    |
| 931065   | 181                | BBN-1966-F79 | 685-004    |
| 883901   | 176                | BBN-2220-J79 | 685-005    |
| 775852   | 175                | BBN-2408-K79 | 685-005    |
| 775852   | 175                | BBN-2297-I79 | 685-005    |
| 854535   | 100                | BBN-7620-I85 | 730-006    |
| 854535   | 100                | BBN-7343-H85 | 730-006    |

Both forward and aft shields were analyzed from all weapons except for unit # 883901, for which only the forward part was available. In the case of unit # 931065, different lots of PBX 9501 were used for

the forward and aft charges. Of the six units studied, only one contained Irganox as the PBX stabilizer.

The results obtained from the HPLC analyses are summarized in Table 2, below. Regardless of the age of the unit, it appears that the NP content of the shield levels off at approximately five weight percent. In fact, the older units showed lower NP concentration in the shields than did the youngest ones analyzed. Recent analyses of library samples of the HE lots used in these units shows the oldest lots to contain significantly less NP than the newer lots, although most are still within the material specification requirements.

Table 2. Analytical Results from HPLC Analysis of Shields

| Shield No. | NP Wt% | BDNPA/F Ratio | Stabil. Wt% | PBNA Wt% | RDX Wt% |
|------------|--------|---------------|-------------|----------|---------|
| 1075       | 4.374  | 1.134         | 0.0981      | 0.0078   | 0.0559  |
| 1076       | 4.374  | 1.132         | 0.1099      | 0.0052   | 0.0602  |
| 1515       | 4.388  | 1.137         | 0.0756      | 0.0060   | 0.0584  |
| 1678       | 4.442  | 1.150         | 0.1141      | 0.0088   | 0.0559  |
| 1716       | 3.780  | 1.139         | 0.0928      | 0.0057   | 0.0500  |
| 1966       | 4.679  | 1.138         | 0.1264      | 0.0086   | 0.0577  |
| 2220       | 5.539  | 1.120         | 0.1355      | 0.0148   | 0.0066  |
| 2408       | 4.939  | 1.124         | 0.1304      | 0.0141   | 0.0061  |
| 2297       | 5.064  | 1.122         | 0.1286      | 0.0136   | 0.0058  |
| 7620       | 4.968  | 1.095         | 0.1077      | 0.0013   | 0.0025  |
| 7343       | 4.944  | 1.098         | 0.1128      | 0.0006   | 0.0024  |

It is assumed that the presence of DPA, Irganox, PBNA, and RDX in the shield material is due to solubility of these species in the NP eutectic liquid. Concentrations of these chemicals in the shield will be dependent on their solubilities in NP, on the age of the unit, and on the amounts that the HE formulation contained.

### Conclusions

Assuming a nominal concentration of 2.5% NP in the PBX, the 5% level found in the shield would lower the concentration in the HE to 2.4%. The material specification for PBX 9501 allows a NP concentration as low as 2.3%. Similarly, assuming a nominal stabilizer concentration of 0.1%, the migration into the shield will only lower the stabilizer content in the HE to 0.098%. The concentration of PBNA found in the shields from the unit that had Irganox-stabilized HE, was significantly lower than for the DPA containing units. This may indicate that PBNA is consumed when the HE has Irganox as stabilizer. The RDX concentration found in the shields tracks the concentration in the HE when the HMX has very low levels of RDX contamination. For PBX lots that had relatively high amounts of RDX, the shield concentration appears to level off at approximately 0.06%. This is likely due to saturation of the NP with RDX.

### References

1. Fletcher, M. A., Buntain, G. A., Rivera, T., "W-76 High Explosive Surveillance", LACP-94-177.
2. Mortensen, G. F., Smith, R. E., LANL Internal Memoranda/Reports, 1989.
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