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CHARACTERIZATION OF MOCK HIGH-EXPLOSIVE POWDER

C. R. Schmitt
G. F. Dorsey

March 1979

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OAK RIDGE Y-12 PLANT
OAK RIDGE, TENNESSEE

*prepared for the U.S. DEPARTMENT OF ENERGY under
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C. R. Schmitt
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Chemical Processes Department
Y-12 Development Division

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Oak Ridge Y-12 Plant

P. O. Box Y, Oak Ridge, Tennessee 37830

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ABSTRACT

Analytical characterization and explosibility tests were made on a simulative high-explosive powder consisting of cyanuric acid, melamine, nitrocellulose, and tris-(β -chloroethyl)-phosphate. Tests indicated that the powder presents no unusual safety or health hazards in isostatic-pressing and dry-machining operations.

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SUMMARY

Analytical verification and characterization analyses were made on some mock high-explosive powder that was to be isostatically pressed and dry machined at the Oak Ridge Y-12 Plant.^(a) A sequential extraction and filtration procedure, using methylene chloride, hot water, and acetone, was used to verify the four constituents in the formulation which analyzed 62.8% cyanuric acid, 30.5% melamine, 2.9% nitrocellulose, and 3.8% tris-(β -chloroethyl)phosphate.

The explosive limits of the powder were also determined and were found to be well within a safe range (> 1.63 g per liter of air). No unusually hazardous gaseous evolution products were observed by thermogravimetric/quadrupole mass spectrographic analysis from 25 to 150° C.

(a) Operated by the Union Carbide Corporation's Nuclear Division for the Department of Energy.

INTRODUCTION

The purpose of this study was to verify the identity of mock high-explosive (Mock HE 90503) powders and to characterize the material with regard to the hazards involved in their handling at Y-12. Mock HE is a nondetonating material with properties selected to closely approximate those of a given explosive. Two lots of Mock 90503 were received at Y-12 for processing into finished parts by isostatic pressing and dry machining. Since this was the first time Y-12 had been involved with processing such material, and because of the association of the material with high explosives, a study of this type was warranted.

Mock 90503 is prepared by the Mason and Hanger - Silas Mason Company, Inc, Pantex Plant, and simulates the atomic compositions of two high explosives—PBX-9404 and LX-10. Mock 90503 has four major constituents, with the following nominal compositions by weight: ¹ 60% cyanuric acid, 32% melamine, 4% nitrocellulose, and 4% tris-(β -chloroethyl)-phosphate. Table 1 lists information concerning these constituents.

Cyanuric acid, $C_3H_3N_3O_3$, is a high-melting solid that has the structural formula:

and is formed by the trimerization of isocyanic acid, HNCO. The chief concern in handling cyanuric acid is the possibility of its thermal decomposition to isocyanic acid, hydrogen cyanide, and cyanogen, all of which are highly toxic. No data were found on the toxicity of cyanuric acid itself, although it has been described as highly toxic. ² This description is probably due to its general association with cyanide and cyanate chemistry.

Thermal decomposition occurs at temperatures much higher than expected in a machining operation. At temperatures above 300° C, cyanuric acid decomposes to isocyanic acid gas; ^{1,3} above 500° C the pyrolysis products include hydrogen cyanide and cyanogen. ¹ In the presence of moisture, isocyanic acid hydrolyzes rapidly to carbon dioxide and ammonia; however, in the absence of moisture, as in an inert-gas glove box used for machining, hydrolysis does not occur. In this case, care must be taken to control the effects of the toxic gases if, indeed, they are produced during machining of the mock HE.

Table 1
 INFORMATION ON CONSTITUENTS OF MOCK HIGH-EXPLOSIVE POWDER
 (HE 90503)

Item of Information	Constituent			
	Cyanuric Acid	Melamine	Nitrocellulose	Tris-(β -chloroethyl)phosphate
Synonyms	1,3,5-triazine-2,4,6-triol s-triazine-2,4,6-triol s-2,4,6-triazinetriol	2,4,6-triamino-s-triazine Cyanuramide Cyanuro triamide Cyanuro Triamine	Cellulose Nitrate ⁽¹⁾ (a) Celluloid Pyroxylin (b) Soluble Pyroxylin Colloid Cotton Dynamite Cotton (c) Guncotton, mixtures of	Chloroethyl Phosphate, CEF; 2-Chloroethanol Phosphate
Formula	$C_3H_3N_3O_3$	$C_3H_6N_6$	Mono - $(C_6H_9NO_7)_x$ Di - $(C_6H_8N_2O_9)_x$ Tri - $(C_6H_7N_3O_{11})_x$	$C_6H_{12}Cl_3O_4P$
Molecular Weight	129.08	126.12	Mono - 414.28x Di - 504.28x Tri - 594.27x	285.49
Chemical Weight	108805	108781		115968
Physical Properties:				
Melting Point ($^{\circ}$ C)	> 360	> 300	-	-
Density (g/cm ³)	2.50	1.57	-	-
Solubility				
Water	1 g/200 ml	Slightly Soluble	Insoluble	-
Hot Water	Very Soluble	Slightly Soluble	-	-
Methylene Chloride	Insoluble	Insoluble	-	Soluble
Acetone	Insoluble	Insoluble	Soluble	-
Toxicity	Highly Toxic ⁽²⁾	Oral-Mouse LD ₅₀ : 1600 mg/kg ⁽³⁾	No Specific Data; May Decompose to NO ₂	Oral-Rat LD ₅₀ : 521 mg/kg ⁽⁴⁾

(1) Nitrogen contents: (a) 10.5 - 11% N; (b) 11.5 - 12.3% N; (c) 12.5 - 13.5% N.

(2) From Sax.²

(3) From *The Toxic Substances List*, Entry OS 07000, p 466.⁵

(4) From *The Toxic Substances List*, Entry KK 24500, p 336.⁸

Besides the toxic effect of the evolved gases, there is the possibility of an explosion involving condensed isocyanic acid.³ At 0° C, isocyanic acid in the gaseous form can condense to a liquid (eg, this condition might occur in a cold trap). When the condensate is warmed to room temperature, the liquid isocyanic acid has been reported³ to spontaneously and explosively form cyanuric acid and cyamelide $[(\text{NHCO})_x]$, a linear polymer]. No cold traps or other condensation points were expected in the processing operations here at Y-12.

Melamine, $\text{C}_3\text{H}_6\text{N}_6$, the cyclic trimer of cyanamide, has the following structural formula:

Melamine is a high-melting solid whose common use is in the preparation of melamine resins. The material has been described⁴ as having little or no toxicity. The reported toxic dose (LD_{50} , oral-mouse) is 1600 mg/kg.⁵

Nitrocellulose is manufactured chiefly in three forms:⁶ (1) celluloid pyroxylin - 10.5 to 11% nitrogen; (2) soluble pyroxylin (colloid cotton, or dynamite cotton) - 11.5 to 12.3% nitrogen, and (3) guncotton - 12.5 to 13.5% nitrogen.

All three types of nitrocellulose are soluble in acetone and all are mixtures rather than pure compounds since cellulose mono, di, and trinitrates should contain 6.76, 11.11, and 14.14 wt % N, respectively. Nitrocellulose decomposes when kept in well-closed containers and exposed to light; thus, it can be shipped safely only when wet with 25 - 30% water.⁷

Tris-(β -chloroethyl)phosphate, $(\text{ClCH}_2\text{CH}_2\text{O})_3\text{PO}$ (CEF), is used commercially as a plasticizer. The reported toxic dose (LD_{50} , oral-rat) is 521 mg/kg.⁸ There is a family resemblance between this compound and the fire retardant tris-(2,3-dibromopropyl)-phosphate, a suspected carcinogen, but no data were found to indicate that CEF is carcinogenic.

Verification analyses of the nominal composition of the mock HE samples combined with additional analytical characterization were needed to ascertain the safety and health aspects of this material for production processing operations. Additional characterizations needed were: (1) a determination of the explosive limits of the samples, and (2) identification of any gaseous evolution products of the heated material. Temperatures from 25 to 150° C for the gaseous-evolution study were expected to give a large safety factor in interpretation of the data. Weight-loss data at 65° C, which approximates the surface temperatures expected in the dry-machining operation, and at 150° C were also needed.

CHARACTERIZATION OF MOCK HE POWDER

EXPERIMENTAL RESULTS

Verification analyses, determination of the explosive characteristics, identification of the gaseous evolution products, and powder-characterization analyses required for processing operations were carried out on the mock HE powders. Verification analysis of Mock 90503 was accomplished by using a published sequential extraction procedure.⁹ Explosive characteristics studied were the minimum energy and the lower explosion limit; weight losses at 65 and 150° C were determined by thermogravimetric analysis (TGA). Identification of the evolved gases was made by thermogravimetric/quadrupole mass spectrographic analyses at various temperatures from 25 to 150° C. Other analyses included water solubility, surface area (krypton), density (pycnometer), free-flow density, particle-size distribution, and infrared analysis.

The sequential-extraction scheme, which allows quantitative separation and determination of the Mock HE 90503 components, is outlined in Figure 1. Analytical results on two separate lots of the material received at Y-12 are presented in Table 2. The verification procedure consists of first determining the tris-(β -chloroethyl)phosphate (CEF) content by extracting with methylene chloride; the remaining material was then digested with hot water which converts an amount of cyanuric acid equivalent to the melamine present to the melamine cyanurate complex. Excess cyanuric acid was then removed by filtration. Finally, the nitrocellulose was extracted with acetone, leaving a residue of melamine cyanurate.

A study of the explosive characteristics of the mock HE powder, particularly dust resulting from the dry-machining operations, was also needed. These results, together with other powder-characterization analyses required for isostatic pressing, handling, and other processing operations involved with the powder, are presented in Table 3.

Figure 1. STEPS IN THE QUANTITATIVE SEPARATION OF MOCK HIGH-EXPLOSIVE COMPONENTS.

Table 2
COMPOSITION-VERIFICATION ANALYSES OF
MOCK HIGH-EXPLOSIVE POWDER
(All Values are in Percent)

Component	Lot 1	Lot 2	Machine Dust	Nominal Composition ⁽¹⁾
Cyanuric Acid ⁽²⁾	62.8	55.3	62.3	60
Melamine	30.48	36.8 ⁽³⁾	30.20	32
	30.53		29.08	
Average	30.5		29.6	
Nitrocellulose	3.21	3.57	3.55	4
	2.65	3.40	3.60	
Average	2.9	3.5	3.6	
Tris-(β -chloroethyl)phosphate	3.79	4.11	4.24	4
	3.66	4.61	4.71	
Average	3.8	4.4	4.5	

(1) From *The Merck Index*, p 896.⁷

(2) Obtained by subtracting the sum of the other three constituents from 100%.

(3) Results of a second analytical determination were abnormally high and were discarded.

The minimum energy value (Table 3) serves as an indicator of the powder's ignition sensitivity to relatively weak igniting sources, such as electrostatically generated sparks. The fact that neither the sample of mock HE powder nor the machining dust sample from parts made from this powder ignited at the maximum energy available for the minimum-energy tests (ie, 12.8 J) indicates that there is no hazard from such ignition sources.

The lower explosion limit also shown in Table 3 establishes the smallest dispersed dust concentration that will, by the arbitrary definition, be considered as explosive upon the application of a strong igniting force. The lower-explosion-limit value of $> 1.63 \text{ g/dm}^3$ (representing the upper limit of the amount of powder dispersed in the test apparatus) for mock HE and the machining dust indicates that there is no explosive hazard for these two materials.

As indicated in Table 3 the weight losses by TGA at 65 and 150° C were 1.1 and 2.4%, respectively. These values are not high enough to indicate gross decomposition. These losses were indicated, by subsequent analyses discussed later (infrared and thermogravimetric/quadrupole mass spectrographic analysis), to be primarily from water and CEF.

Thermogravimetric/quadrupole mass spectrographic analyses were used to identify the gases evolved from the heated samples. Gases of primary concern were isocyanic acid, hydrogen cyanide, and cyanogen. It was estimated that the maximum temperature involved in the processing of the mock HE would be 65° C; but, as a safety factor, analyses were continued to 150° C. Results of the thermogravimetric/quadrupole mass spectrographic analyses are

reported in Figure 2. A chemical identification of the probable gaseous decomposition species and products evolved by heating mock HE from 25 to 150° C is given in Table 4. Isocyanic acid, hydrogen cyanide, and cyanogen were not observed. The peak at $m/e = 18$, assigned to water, gave the highest ion intensities in the study.

The bulk powder was too opaque to allow study by standard infrared (IR) spectroscopy. However, IR analysis of the volatiles from mock HE permitted a qualitative determination of the presence of CEF. The liquid condensate from a heated sample of the as-received powder was analyzed by IR analysis (Figure 3) and that spectrum compared favorably with published scans of tris-(β -chloroethyl)phosphate (Figure 4). The similarity of the spectra was taken as evidence of the presence of CEF in the mock HE.

DISCUSSION

A mock high explosive is a nonexplosive equivalent of a particular high-explosive compound or a formulation that duplicates certain properties or characteristics of the real high explosive, but lacks its explosive nature. For laboratory test purposes it is convenient and much safer to be able to conduct tests on such materials that duplicate certain properties of the high-explosive formulation. Some typical properties of interest in high explosives that are usually mock formulated are presented in Table 5;¹⁰ some typical chemical formulations of mock HE, including the Mock 90503 formulation used in this study, are shown in Table 6.¹⁰

Mock high explosives are not necessarily inert. "They may be toxic, combustible, or even radioactive. All that can be said is that they will not detonate."¹⁰ For these reasons, suitable protective respiratory equipment must be worn if dust is created, and the possibility of static-ignition dust explosions and health-physics toxicity problems must be evaluated. Isostatic pressing, dry machining, and handling operations that were to be made with the

Table 3
CHARACTERIZATION ANALYSES OF
MOCK HIGH-EXPLOSIVE POWDER

Color	Pink
Water Solubility, at 25° C (g/dm ³)	8.6
Surface Area, Krypton (m ² /g)	0.34
Density, Pycnometer (g/cm ³)	1.658
Free-Flow Density (g/ml)	0.926
Tap Density (g/ml)	1.16
Explosibility	
Minimum Energy ⁽¹⁾ (J)	> 12.8
Lower Explosion Limit ⁽²⁾ (g/dm ³)	> 1.63
Particle Size Distribution (screen)	
US Sieve ⁽³⁾	Percent
+ 4	8.1
- 4 + 6	2.0
- 6 + 10	1.4
- 10 + 16	12.7
- 16 + 20	16.9
- 20 + 30	16.4
- 30 + 40	10.7
- 40 + 60	6.6
- 60 + 100	5.5
- 100 + 140	10.0
- 140 + 200	3.8
- 200 + 325	4.0
- 325 +	1.9
Thermogravimetric Analysis	
Atmosphere	Helium
Gas Flow Rate (dm ³ /hr)	5.07
Heating Rate (° C/min)	4
Weight Loss, at 65° C (%)	1.1
Weight Loss, at 150° C (%)	2.4

- (1) The smallest capacitor discharge required to produce flame propagation four inches or longer in a dust cloud of optimum concentration.
- (2) The smallest sample weight which may be ignited by an induction spark to produce a low-ordered explosion of an established magnitude within an enclosed volume.
- (3) Plus (+) signifies "retained on" and minus (-) signifies "passed through" the screen size shown.

Figure 2. THERMOGRAVIMETRIC/QUADRUPOLE MASS SPECTROGRAPHIC ANALYSES OF MOCK HIGH EXPLOSIVE. (Mass-to-Charge Ratios are Shown by Numbers)

Figure 3. INFRARED SPECTRUM OF LIQUID CONDENSATE FROM A HEATED SAMPLE OF MOCK HIGH-EXPLOSIVE POWDER.

mock HE material would result in the generation of considerable dusts and fine particulates which could present a potential problem of ignition and detonation by static electricity. It was estimated that the dry-machining operations on isostatically pressed mock HE billets might result in a surface temperature of 65° C, making knowledge of any toxic decomposition gases or products formed at this temperature of interest from the standpoint of industrial health and hygiene.

Mock HE powder (Mock 90503) is an inert material that is prepared by Mason and Hanger - Silas Mason Co, Inc, Pantex Plant, which simulates the atomic composition of Explosives PBX-9404 and LX-10. Before any

work with the mock HE powder could begin at Y-12, verification analyses of the four constituents in the formulation were needed to ensure that the material was indeed mock HE and not the real thing, and that it had been formulated properly. An error in formulation such as making up the 4% nitrocellulose constituent of the material to the nominal 60% level of the cyanuric acid or the 32% level of the melamine constituent could have caused a drastic effect on the explosibility and general safety characteristics of the powder blend. The analyses were at least a quality control device to monitor slight changes in formulation or the substitution of an alternate mock HE or other material.

Table 4

ANALYSIS OF THE MASS SPECTRUM OF GASES EVOLVED FROM MOCK HIGH-EXPLOSIVE POWDER AT 25 - 150° C

Atomic Mass Unit(1)	Probable Chemical Identification(2)	Corresponding Chemical Formula
2	Hydrogen	H ₂
18	Water	H ₂ O
28	Nitrogen (or carbon monoxide)	N ₂ (or CO)
30	Nitric Oxide	NO
31	Nitrogen/Hydroxide Fragment	N ₂ OH
32	Oxygen	O ₂
43	Methyl Ethyl Ketone Fragment	CH ₃ CO
44	Carbon Dioxide	CO ₂
63	Nitric Acid	HNO ₃
72	Methyl Ethyl Ketone	CH ₃ COC ₂ H ₅

(1) Mass-to-charge ratio observed in the quadrupole mass spectrometer.

(2) Parent or fragment ion of gas evolved from mock HE during thermogravimetric analysis at 25 - 150° C.

Figure 4. PUBLISHED INFRARED SPECTRUM OF TRIS-(β-CHLOROETHYL)PHOSPHATE. (Source: Sadtler Research Laboratories, Inc, Number E2331)

A study of the explosive characteristics of the mock HE powder, particularly the dust from the dry-machining operations, indicated that no hazard was expected. Characterization was made with respect to minimum energy and the lower explosion limit. Minimum energy is defined as the smallest capacitor discharge required to produce flame propagation four inches or longer in a dust cloud of optimum concentration. Lower explosion limit is defined as the smallest weight which may be ignited by an induction spark to produce a low-ordered explosion of an established magnitude within an enclosed volume. The mock HE samples did not explode in the tests. Values of $>12.8 \text{ J}$ and $>1.63 \text{ g/dm}^3$ for the respective tests represent limiting values for the test equipment and indicate that the 90503 mock HE and machine dusts do not constitute an explosion hazard.

Although mock HE does not represent a hazard from the standpoint of being an explosive, there was the possibility that toxic gases might be evolved from the processed parts. The most critical situation was localized heating during the

Table 5
PROPERTIES AND CHARACTERISTICS OF A MOCK
HIGH-EXPLOSIVE FORMULATION THAT
ARE OF USUAL INTEREST FOR
LABORATORY TESTING

Atomic Composition
Density
Thermal Properties
Thermal Conductivity
Specific Heat
Coefficient of Thermal Expansion
Glass Transition Temperatures
Mechanical Properties
Compressive Stress/Strain Curves at Various Strain Rates
Longitudinal Modulus versus Temperature
Tension Creep Data
Coefficient of Friction versus Sliding Velocity
Hugonot Data (sound velocity)
Machinability

Table 6
FORMULATIONS OF SOME TYPICAL MOCK HIGH-EXPLOSIVE POWDER

Mock Type	Explosive Properties that are Mocked	Composition ⁽¹⁾ (wt %)	Empirical Formula ⁽²⁾
00010	PBX-9404: Mechanical Properties	Pentaerythritol 48.0 Ba(NO ₃) ₂ 46.0 NC 2.8 CEF 3.2	C _{1.89} H _{4.44} N _{0.38} O _{2.62} Ba _{0.18} Cl _{0.03} P _{0.01}
90503	PBX-9404 and LX-10: Atomic Composition	Cyanuric Acid 60 Melamine 32 NC 4 CEF 4	C _{2.32} H _{3.18} N _{2.96} O _{1.60} Cl _{0.04} P _{0.01}
LM-04-0	LX-04: Atomic Composition ⁽³⁾	Cyanuric Acid 59.7 Melamine 23.5 Viton A 16.8	C _{2.34} H _{2.66} N _{2.51} O _{1.39} F _{0.63}
RM-04-BG	LX-04: Mechanical Properties—Static and Dynamic	Cyanuric Acid 70.5 Ba(NO ₃) ₂ 14.5 Viton A 15	C _{2.02} H _{1.86} N _{1.75} O _{1.97} F _{0.54} Ba _{0.06}

(1) Approximately 0.05% of a red pigment is also added to these formulations.

(2) Molecular weights of these mixtures are arbitrarily taken as 100.

(3) Although designed as an atomic-composition mock, LM-04-0 can also be used as an approximate mock of the mechanical properties of LX-04-1 at ambient conditions.

machining operations. Of primary concern was the possible liberation of the gases (isocyanic acid, hydrogen cyanide, and cyanogen).

Thermogravimetric/quadrupole mass spectrographic analyses indicated that the three possible toxic gases were not evolved from the mock HE. Since the machining operation did not exceed 65^o C, analyses from 25 to 150^o C represented a large safety factor. No peaks of mass-to-charge ratio (*m/e*) at 27 (HCN) and at 52 (C₂N₂) were found. The peak at *m/e* = 43, which would be consistent with an HNCO parent ion, was assigned to a methyl ethyl ketone fragment (CH₃CO)⁺. As noted in Figure 2, the ion intensity of the *m/e* = 43 peak tracks that of the *m/e* = 72 peak [methyl ethyl ketone parent ion, (CH₃COC₂H₅)⁺] as a function of temperature.

The type of nitrocellulose involved with the mock HE will determine the degree of hazard involved. The higher the nitrogen content, the higher the detonation potential. Calculations, assuming the worst cases—13.5% nitrogen (guncotton)—and the nitrogen contents of the other components (cyanuric acid and melamine), give an overall nitrogen content that is consistent with the published^{1,10} empirical formula (Table 6). Therefore, isolation of this material, as during the extraction procedure, would indicate the need for the degree of handling that is required for guncotton.

Mock 90503 was too opaque to permit a successful analysis by transmission infrared spectroscopy. Reflectance infrared techniques, which would have been an ideal first analysis on the as-received material, were not attempted. Instrumentation such as the Fourier transform [(FT)-IR] which can apply the reflectance techniques was not available at the time of this study.

Alternatively, FT ¹³C nuclear magnetic resonance, which provides both qualitative and quantitative analysis on many organic materials, might form the basis for a nonseparative analytical procedure for the mock HE.

NMR analysis for ¹³C is indicated since the two major constituents of Mock 90503—cyanuric acid and melamine—are without the C-H bonding which is useful for proton NMR analysis. However, the carbon atoms in the skeletal structures of the mock HE components are sufficiently different to be amenable to analysis by ¹³C-NMR. Future evaluations of mock HE should involve this technique.

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