

EXPLOSIVE EVALUATION OF COORDINATION COMPOUNDS

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INTRODUCTION

An investigation of "low power" explosives was undertaken as a cooperative effort between the Sandia Corporation and the Universal Match Corporation. The primary objective of this program was the investigation of homogeneous chemical compounds expected to yield detonation pressures of less than 100 kilobars. Secondary objectives included the attainment of adequate thermal stability, suitable impact sensitivity and high density. The wide range of properties found in coordination compounds caused efforts to be concentrated in this area.

In general, a limited number of tests were performed in order to screen out unsuitable compounds. Those compounds which appeared promising were then subjected to further testing. The initial evaluation of explosive output was obtained from the standard sand bomb test. This test was abandoned when it became apparent that the consolidation density of the explosive was an important factor. Later testing utilized the plate dent test and a limited amount of streak camera data.

The explosive properties of the coordination compounds tested varied over a wide range, and depended on several factors. The consolidation density was important. The oxygen balance (to carbon monoxide) was also significant. The insertion of a heavy ion into the explosive (for example, iodate or thallos) lowered the detonation velocity but the increased density of the total molecule tended to keep the detonation pressure high.

EXPERIMENTAL

Detonation pressures were estimated by the plate dent technique. Figure 1 shows the plot of detonation pressure versus depth of dent in the steel plate (hardness in Rockwell, 88-90, B scale). Detonation pressures for those cases where the streak camera technique was utilized were calculated from the approximation:

$$p \doteq 0.010 \rho \frac{D^2}{4}$$

where:

p = detonation pressure in bars
 ρ = density in grams per cubic centimeter
 D = detonation velocity in meters per second

The other tests conducted were 40-hour vacuum stability at 100°C, impact sensitivity by the Bureau of Mines two-kilogram drop test apparatus, density, melting point, and autoignition temperature. Not all tests were conducted on each compound, and unsuitable compounds were eliminated.

All compounds were prepared and purified by standard methods to be found in the literature, and analyzed by conventional techniques.

Table I summarizes the data collected during this investigation.

DISCUSSION

Cobalt - The oxygen balance of the cobalt complexes was varied by varying both the ligands and the oxidizing anion. The iodate anion was chosen for most of the compounds because of its high density, ability to cause propagation in small diameters, and low oxygen equivalent as compared to IO_4^- and ClO_4^- . The data collected on two cobalt compounds are shown in Figure 2.

Several interesting facts should be pointed out. (1) The compounds containing Cl^- , such as $\text{Co}(\text{NH}_3)_5\text{Cl}(\text{IO}_3)_2$, even though having a favorable oxygen balance, failed to sustain detonation. (2) The outputs of the compounds are variable over a wide range, for instance: $\text{Co}(\text{NH}_3)_6(\text{IO}_3)_2 \cdot \frac{1}{2}\text{H}_2\text{O}$ gave a pressure of 15 kilobars at a density of 1.51 g/cc (49.5 percent crystal density) and 215 kilobars at 2.70 g/cc (88.8 percent crystal density). Another example is $\text{Co}(\text{en})_2(\text{IO}_3)_2$: 55 kilobars at 1.9 g/cc (69.1 percent crystal density) and 165 kilobars at 2.48 g/cc (90.1 percent crystal density) (See Figure 2).

Copper, Zn and Other Metal Complexes - The coordination compounds of copper, platinum, zinc, nickel, mercury, and cadmium were similar to those of cobalt in explosive properties. The metal ion does not appear to effect the output. The nickel ion, with its valence of two and possible coordination number of six, was interesting because of the low oxygen balances which could be obtained. None of the nickel compounds sustained detonation in a 0.5 inch diameter column. With $\text{Cu}(\text{en})_2(\text{IO}_3)_2$ and $\text{Zn}(\text{en})_2(\text{IO}_3)_2$, we see the production of low detonation pressure at high densities. Data on these two compounds are given in Table II and Figure 2.

Table II

| Compound | Density (g/cc) | Percent Crystal Density | Estimated Detonation Pressure (kilobars) |
|---|-------------------|----------------------------|--|
| $\text{Cu}(\text{en})_2(\text{IO}_3)_2$ | 1.89 | 69.1 | 40 |
| | 2.38 | 87.2 | 155 |
| $\text{Zn}(\text{en})_2(\text{IO}_3)_2$ | 1.73 | 69.8 | 27 |
| | 2.43 | 97.8 | 145 |

It is to be pointed out that the explosive outputs of the two compounds are similar at equal actual densities rather than equal percent crystal densities. This phenomenon was shown by several other explosive complex salts.

Another interesting situation is the different behavior of two isomers $\text{Cu}(\text{tmen})_2(\text{IO}_3)_2$ and $\text{Cu}(\text{pn})_2(\text{IO}_3)_2$. In a 1/2 inch diameter by 1.37 inches long configuration, the tmen complex sustained detonation (See Figure 3) while the pn complex did not. The tmen complex gave 125 kilobars at a density of 2.30 g/cc (89.7 percent crystal density).

However, in a 1 1/4 inch diameter by 5.1 inches long configuration, the mn salt did sustain giving an estimated detonation pressure of 105 kilobars at a density of 2.18 g/cc.

SUMMARY

It appears that oxygen balances of 20-30 percent (to carbon monoxide) are necessary to obtain low pressures at densities approaching crystal density. This requirement probably necessitates the use of larger column diameters or more sensitive classes of compounds such as chlorates to obtain steady detonation.

One of the properties of these coordination compounds is the apparent low detonation pressure produced at relatively high densities. Figure 4 shows the relationship of detonation pressure to density for hexamminocobalt iodate hemihydrate and TNT. The coordination compound yields the same detonation pressure at a density of 2.7 g/cc that TNT exhibits at 1.6 g/cc. The coordination compounds, regardless of oxygen balance, ligand, or central ion, all appear to possess a similar relationship between output and density.

ACKNOWLEDGMENT

This work was performed under the auspices of the United States Atomic Energy Commission. Special appreciation is extended Dr. Herbert Ellern for his technical guidance and assistance.

TABLE I

| Compound | Oxygen Balance (%) | Impact Value (cm) | Crystal Density (g/cc) | Sand Crush (g) | Detonation Velocity (m/sec) at density | Detonation Pressure (kilobars) at density |
|---|--------------------|-------------------|------------------------|----------------|--|---|
| $\text{Co}(\text{NH}_3)_6(\text{IO}_4)_3$ | 115 | 22 | - - - | 23 | - - - | 220 (2.24) |
| $[\text{Co}(\text{NH}_3)_5(\text{NO}_3)](\text{NO}_3)_2$ | 100 | 47 | 1.846 | 37.6 | - - - | - - - |
| $\text{Co}(\text{NH}_3)_6(\text{IO}_3)_3 \cdot \frac{1}{2}\text{H}_2\text{O}$ | 86 | 17 | 3.04 | 18 | 2750 (2.0) | 15 (1.51) 90 (2.06) 210 (2.70) |
| $\text{Co}(\text{NH}_3)_3(\text{NO}_2)_3$ | 100 | 12 | 2.024 | 35.1 | 6100 (1.8) | - - - |
| $[\text{Co}(\text{en})_2\text{Cl}_2]\text{IO}_3 \cdot \text{HIO}_3$ (trans) | 50 | 35 | 2.658 | 12 | - - - | - - - |
| $\text{Co}(\text{NH}_3)_6(\text{NO}_3)_3$ | 86 | 40 | 1.804 | 32.3 | - - - | - - - |
| $\text{Co}(\text{en})_3(\text{IO}_3)_3$ | 46 | 34 | 2.760 | 16.1 | 4610 (2.21) | 54 (1.91) 96 (2.19) 170 (2.40) |
| $[\text{Co}(\text{NH}_3)_5\text{NCS}](\text{ClO}_4)_2$ | 73 | 26 | 1.906 | 44.5 | 6500 (1.70) | - - - |
| $[\text{Co}(\text{NH}_3)_5\text{Cl}](\text{IO}_3)_2$ | 71 | >104 | - - - | 0 | - - - | - - - |
| $[\text{Co}(\text{en})_2\text{Cl}_2]\text{IO}_4$ (trans) | 32 | 34 | - - - | 12.2 | - - - | - - - |
| $[\text{Co}(\text{en})_2\text{Cl}_2] \cdot \text{ClO}_4$ (cis) | 33 | 57 | 1.872 | 0 | - - - | - - - |
| $[\text{Co}(\text{en})_2\text{Cl}_2] \cdot \text{ClO}_4$ (trans) | 33 | 81 | 1.844 | 0 | - - - | - - - |
| $[\text{Co}(\text{NH}_3)_4(\text{NCS})_2] \cdot \text{ClO}_4$ | 31 | 49 | 1.65 | 0 | - - - | - - - |
| $\text{Cu}(\text{en})_2(\text{IO}_3)_2$ | 46 | 37 | 2.720 | 17.6 | - - - | 40 (1.89) 160 (2.28) |
| $\text{Cu}(\text{pn})_2(\text{IO}_3)_2$ | 35 | 19 | - - - | 12.1 | - - - | - - - |
| $\text{Cu}(\text{tmen})_2(\text{IO}_3)_2$ | 35 | 54 | 2.594 | - - - | - - - | 11 (1.52) 25 (1.72) 125 (2.20) |

TABLE I (continued)

| Compound | Oxygen Balance (%) | Impact Value (cm) | Crystal Density (g/cc) | Sand Crush (g) | Detonation Velocity (m/sec) at density | Detonation Pressure (kilobars) at density |
|--|--------------------|-------------------|------------------------|----------------|--|---|
| Pt(NH ₃) ₄ (IO ₃) ₂ | 100 | - - - | - - - | 17.0 | - - - | - - - |
| Zn(pn) ₂ (IO ₃) ₂ | 35 | - - - | - - - | 6.8 | - - - | - - - |
| Zn(en) ₂ (IO ₃) ₂ · 1½ H ₂ O | 46 | 24 | 2.48 | 12.4 | - - - | 25 (1.73) 60 (2.00) 145 (2.43) |
| Ni(en) ₃ (IO ₃) ₂ | 32 | 51 | - - - | 0 | - - - | - - - |
| Ni(pn) ₃ (IO ₃) ₂ | 24 | 24 | - - - | 0 | - - - | - - - |
| Hg(en)(IO ₃) ₂ · H ₂ O | 100 | >100 | - - - | 17.0 | - - - | - - - |
| Cd(en) ₂ (IO ₃) ₂ | 46 | 31 | - - - | 16.2 | - - - | - - - |

NOTES: en = ethylenediamine

pn = propylenediamine

tmen = trimethylenediamine

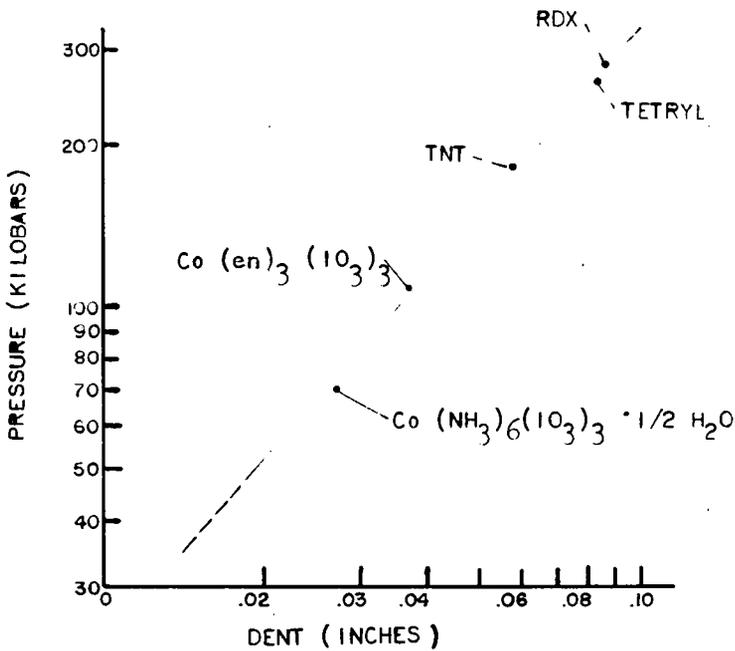


FIGURE 1

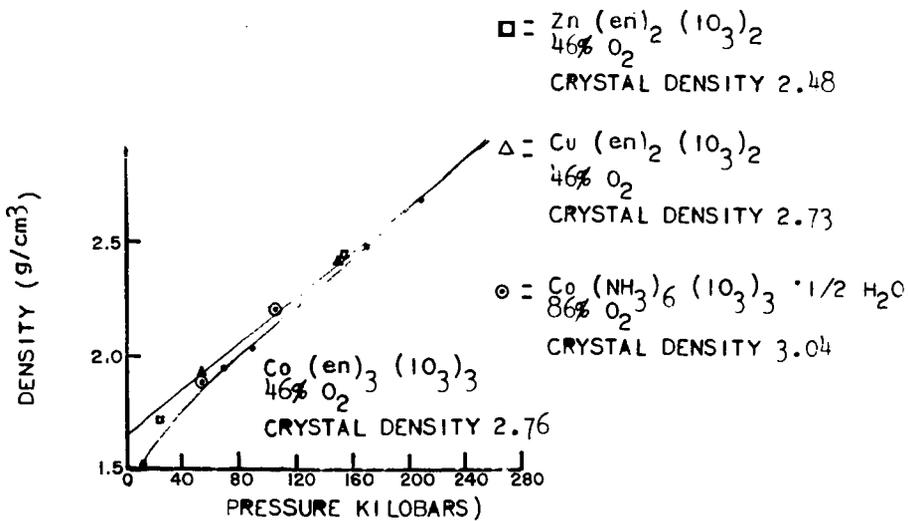


FIGURE 2

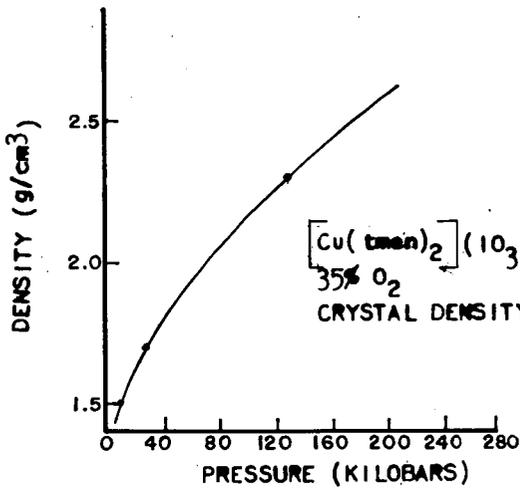


FIGURE 3

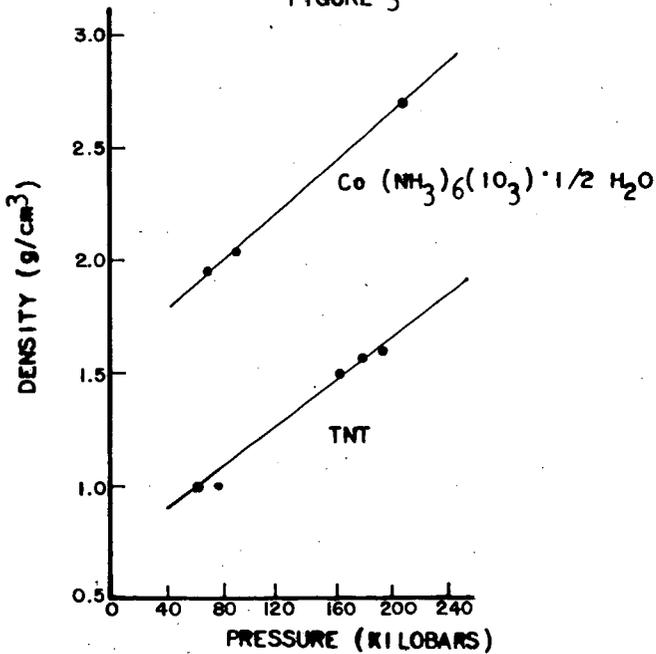


FIGURE 4