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Calculation of the Explosive Power of Mixtures of Chlorine Trifluoride and Ammonia (Both Liquid)

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SUBJECT: Calculation of the Explosive Power of Mixtures of Chlorine Trifluoride and Ammonia (Both Liquid)

TO: The Chief of Ordnance
Department of the Army
Washington 25, D.C.

Attn: ORDGU-IN

1. Reference - None


3. Abstract of the Report is as follows:

The explosive power of mixtures of liquid NH₃ and ClF₃ within the range of ratios of 1.4 to 2.3 moles of NH₃ per mole ClF₃ are calculated. Calculations are based on the correlation of the Berthelot Product for the mixtures to its value for Picric Acid under normal condition in the explosive calorimeter. The optimum mixture of 2.8 parts by weight of ClF₃ with 1 part of NH₃ gave a calculated value of 188 which is theoretically about equivalent to Methyl Nitrate (185) and somewhat better than RDX (183). These calculations assume intimate mixture and complete reaction which would be very difficult to achieve in practice.

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by

G.H.S. Young

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1. INTRODUCTION.

The explosive effectiveness of a given substance relative to that of the accepted standard, picric acid, as measured for example by the Trautzl Block or the Ballistic Mortar methods, is found to be fairly well correlated with the relative value of the "Borthclot Product". The latter is proportional to Q, where Q is the heat (per gm) which would be liberated by the chemical change which actually takes place in the explosion, if it could take place in the same way at ambient temperature (300°K.), while n is the number of gram molecules of gaseous products obtained in the explosion from one gram of the substance. The Explosive Power (Pr) is therefore defined as one hundred times the ratio of the value of this Borthclot Product for the given substance under stated conditions to its value for Picric Acid under normal conditions in the explosive calorimeter.

2. SYSTEM CONSIDERED.

Assuming approximate thermodynamic equilibrium the principal reaction within the range of mixture ratios studied (1.4 to 2.3 moles of NH₃ per mole of CIF₃) is as follows:

\[ \text{CIF}_3 + x \text{NH}_3 = 3\text{HF} + \text{HCl} + \frac{x}{2} \text{N}_2 + \frac{3x}{2} \text{H}_2 \]

As x approaches the boundary value \( \frac{4}{3} \), the temperature of the adiabatic constant volume flame rises steeply (see Fig.2) and the dissociation products, atomic chlorine and atomic fluorine become appreciable in amount (3-4%), the amounts of the molecular forms, Cl₂ and F₂, being somewhat less while the dissociation of hydrogen and nitrogen remains effectively small at the high pressures involved.

The main reaction alters in two stages as x is still further diminished; the hydrogen virtually disappears and atomic chlorine and (ultimately) fluorine appear as main products.

The necessary thermodynamic data for calculating the flame temperature and explosive power at these lower values of x can only be estimated rather imperfectly, but fortunately the optimum mixture ratio, as regards explosive power, appears to lie within the higher range of x as indicated by the graph (Fig.1). It was therefore not necessary to investigate the lower range of x in detail.

The heat of formation of gaseous CIF₃, about which there has been some variation of opinion, was taken to be 28 k.cal. per mole (H.V. v. Wartenberg, Z.anorg.Chem., 1919, 268, 356) and the latent heat of vaporization as 5 k.cal. per mole. The remaining thermodynamic data was obtained from Pike's tables and from the compilation of the American Bureau of Standards.

The volume of the system was taken to be the sum of the volumes of the liquid components CIF₃ and NH₃ at 300°K. (assumed to be under suitable pressures).

/3. RESULTS.
3. RESULTS.

The essential results of the calculations are as follows:

<table>
<thead>
<tr>
<th>Temperature °K.</th>
<th>x</th>
<th>Pr.</th>
</tr>
</thead>
<tbody>
<tr>
<td>3870</td>
<td>2.24</td>
<td>186.55</td>
</tr>
<tr>
<td>4065</td>
<td>2.07</td>
<td>187.7</td>
</tr>
<tr>
<td>4355</td>
<td>1.85</td>
<td>187.76</td>
</tr>
<tr>
<td>4455</td>
<td>1.78</td>
<td>187.65</td>
</tr>
<tr>
<td>4645</td>
<td>1.65</td>
<td>187.3</td>
</tr>
<tr>
<td>4840</td>
<td>1.51</td>
<td>186.2</td>
</tr>
<tr>
<td>4935</td>
<td>1.42</td>
<td>184.6</td>
</tr>
</tbody>
</table>

The decimal places in the value of Pr are of little significance except in showing the smooth trend of the calculated values, with a definite maximum of about 188 at $x = 1.95$.

This maximum figure, 188, for a mixture of 2.8 parts by weight of CIF$_3$ with 1 part of NH$_3$, can be compared with:

<table>
<thead>
<tr>
<th>Explosive</th>
<th>Pr.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Picric Acid</td>
<td>100</td>
</tr>
<tr>
<td>T.N.T.</td>
<td>108</td>
</tr>
<tr>
<td>R.D.X.</td>
<td>168</td>
</tr>
<tr>
<td>Methyl Nitrate</td>
<td>185</td>
</tr>
<tr>
<td>Nitromethane</td>
<td>154</td>
</tr>
</tbody>
</table>

Thus the optimum mixture is theoretically about equivalent to methyl nitrate in explosive power and somewhat better than R.D.X.

It seems apparent from these calculations that liquid fluorine would give a higher explosive power with liquid ammonia, because the energy per unit mass is greater, and there would be no heat of formation term to be taken into account.

The calculations assume that it would be possible to get an intimate mixture, and complete reaction. In practice this would be very difficult to achieve, and explosion rather than detonation, might occur.

4. ACKNOWLEDGEMENTS.

The calculations on which this note is based were carried out by Dr. B.M. Cavanagh and Miss M.A. Hooper.
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**FLAME TEMP. (°K)**

VERSUS

**NO. OF MOLS. OF NH₃ PER MOL. OF ClF₅.**

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**FIG. 2.**

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