DNGU: Synthesis, Formulation and Testing of an Affordable, Less-Sensitive Energetic Material

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DNGU-Background

- DNGU has been known for years and has been studied by Chinese and French researchers.
- It was evaluated in the 1980s as a potential high performance explosive to replace HMX.
  - However, its measured performance did not match the predicted performance and was subsequently abandoned.
- Its actual properties may better lend itself to be used as an IM ingredient, being slightly less powerful than RDX and NTO, and as a potential replacement for NQ or TATB in some formulations.
- It also has the advantage of being a very affordable explosive ingredient, with a projected cost between RDX and HMX.
**DNGU-Properties**

- DNGU may be comparable to TATB in terms of sensitivity and superior in performance.
- Although VoD may be somewhat low, high density of DNGU boosts performance.
- Data from multiple sources is contradictory at times
  - It was decided that DNGU needed to be evaluated in-house in an effort to resolve discrepancies and determine the potential applications of DNGU.
- DNGU has been shown to have a faster burn rate (1.2x) than HMX.

<table>
<thead>
<tr>
<th></th>
<th>RDX</th>
<th>NQ</th>
<th>DNGU</th>
<th>TATB</th>
<th>NTO</th>
</tr>
</thead>
<tbody>
<tr>
<td>m.w. (g)</td>
<td>222.1</td>
<td>104.1</td>
<td>232.1</td>
<td>258.2</td>
<td>130.1</td>
</tr>
<tr>
<td>Oxygen Balance (%)</td>
<td>-21.6</td>
<td>-30.7</td>
<td>-27.6</td>
<td>-55.8</td>
<td>-21.6</td>
</tr>
<tr>
<td>Nitrogen Content(%)</td>
<td>37.84</td>
<td>53.83</td>
<td>36.21</td>
<td>32.55</td>
<td>43.07</td>
</tr>
<tr>
<td>Vol. Explosive gases (l/kg)</td>
<td>903</td>
<td>1042</td>
<td>*</td>
<td>*</td>
<td>855</td>
</tr>
<tr>
<td>Heat of Explosion (kJ/kg)</td>
<td>6322</td>
<td>2730</td>
<td>*</td>
<td>3062</td>
<td>2993</td>
</tr>
<tr>
<td>Density (g/cc)</td>
<td>1.82</td>
<td>1.71</td>
<td>1.94</td>
<td>1.97</td>
<td>1.93</td>
</tr>
<tr>
<td>lead block test (cc/10g)</td>
<td>480</td>
<td>305</td>
<td>*</td>
<td>175</td>
<td>*</td>
</tr>
<tr>
<td>VOD (m/s)</td>
<td>8750</td>
<td>8200</td>
<td>7580</td>
<td>8450</td>
<td>7350</td>
</tr>
<tr>
<td>Impact Sensitivity (Nm)</td>
<td>7.5</td>
<td>49</td>
<td>5</td>
<td>(questionable)</td>
<td>1200</td>
</tr>
<tr>
<td>Friction Sensitivity (N)</td>
<td>120</td>
<td>353</td>
<td>200-300</td>
<td>353</td>
<td>353</td>
</tr>
<tr>
<td>Impact Sensitivity (cm)</td>
<td>30</td>
<td>&gt;177, 73</td>
<td>88-124</td>
<td>&gt;177</td>
<td>292</td>
</tr>
<tr>
<td>Impact Sensitivity (J)</td>
<td>5.5</td>
<td>*</td>
<td>8</td>
<td>*</td>
<td>8</td>
</tr>
<tr>
<td>Julius Peters</td>
<td>2.5</td>
<td>*</td>
<td>&gt;4</td>
<td>&gt;4</td>
<td>*</td>
</tr>
<tr>
<td>30 kg shock drop height on 100g (meters)</td>
<td>*</td>
<td>*</td>
<td>210</td>
<td>190</td>
<td></td>
</tr>
<tr>
<td>Card gap test (cards)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SSJGT</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pressure CJ (GPa)</td>
<td>34.6</td>
<td>27.4</td>
<td>34.2</td>
<td>31</td>
<td>~28</td>
</tr>
<tr>
<td>DSC (onset of exotherm)</td>
<td>220</td>
<td>210</td>
<td>210-234, 240-250</td>
<td>350</td>
<td>270</td>
</tr>
</tbody>
</table>
DNGU-Synthesis

- DNGU is produced from a simple nitration of glycoluril (inexpensive)
  - Glycoluril produced from very inexpensive materials (urea and glyoxal)
    - Glycoluril is commercially available and can be made at HSAAP
- Cost of DNGU estimated to be between RDX and HMX
- OSI R&D has made over 40 pounds of DNGU.
- Currently optimizing synthesis process
  - Original DNGU product particle size was ~15-20 microns
  - New route can provide much larger material (200-300 microns)
  - Yields typically 90-95% with purities >99%
# DNGU-Reaction Calorimetry

<table>
<thead>
<tr>
<th>Batch</th>
<th>Enthalpy per Mole Glycoluril</th>
<th>ΔT(ad)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1106-17</td>
<td>-97.6 kJ/mol</td>
<td>65.0 °C</td>
</tr>
<tr>
<td>1106-19</td>
<td>-101.8 kJ/mol</td>
<td>75.8 °C</td>
</tr>
</tbody>
</table>

- Reaction calorimetry (RC1) performed to quantify exotherms and assess scale-up safety
  - Batch 1106-17: 0.5 lb batch
  - Batch 1106-19: 1.0 lb batch
- Exothermicity of reaction appears relatively mild (especially for a nitration)
- Reaction deemed safe for scale-up within R&D

*•Mild, straight-forward, easily-controlled synthesis*
DNGU-Thermal Analysis

- DNGU has no melting point before decomposition.
- DNGU has sharp exothermic transition at 245-250°C
  - Between RDX (200-250°C) and NTO (270-280°C)
  - DNGU seems to have a faster decomposition rate than RDX.
- VTS: 0.41 cc/g
- Future planned work includes TGA and ARC (accelerated rate calorimetry)
DNGU-Analytical

- Impact Sensitivity: 80-100 cm (Holston apparatus)
  - RDX: 17 cm
- Friction Sensitivity: >360 N
  - RDX: 164 N
- Surface Area (BET): 1.3-1.4 g/m²
- Particle Size (typical below):

![Particle Size Distribution Graph](image-url)
DNGU-SEM Analysis

• DNGU material from early in development program has rough “coral reef” appearance and looks like agglomerates of small particles.
  ➢ Probably not good for formulating

• However, there appear to be large crystals hiding in some of the “agglomerates”…..
DNGU SEM Analysis

- DNGU produced after optimization efforts has more defined and larger crystal shapes
DNGU Formulations

- Purpose: Prepare coated DNGU and RDX for pellet pressing and performance/sensitivity evaluations.
- No optimization performed at this time.
- DNGU is compatible with:
  - RDX, HMX, C-4 binder, TNT, Aluminum, DNAN, Viton

- DNGU was coated with 5% Viton through a standard Holston slurry coating process.
- 2.5 lb batch size
- RDX was processed same as DNGU.

Impact: 70 cm
Impact: 200 cm

DNGU molding powder

RDX molding powder
DNGU Molding Powder

- Over 150 pellets of each formulation were pressed
- Average press densities
  - DNGU: 1.65-1.66 (84% TMD)
  - RDX: 1.65-1.66 (91% TMD)
DNGU-Cheetah Calculations

- DNGU coated with 5% Viton compared against RDX (class 1) coated with 5% Viton and TATB (PBX-9502).

<table>
<thead>
<tr>
<th></th>
<th>%TMD</th>
<th>Density</th>
<th>VoD (m/s)</th>
<th>Pressure (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DNGU</td>
<td>98</td>
<td>1.93</td>
<td>8400</td>
<td>31.0</td>
</tr>
<tr>
<td>RDX</td>
<td>98</td>
<td>1.78</td>
<td>8444</td>
<td>31.8</td>
</tr>
<tr>
<td>TATB</td>
<td>98</td>
<td>1.89</td>
<td>8015</td>
<td>27.0</td>
</tr>
<tr>
<td>DNGU</td>
<td>84</td>
<td>1.65</td>
<td>7200</td>
<td>21.7</td>
</tr>
<tr>
<td>RDX</td>
<td>91</td>
<td>1.65</td>
<td>8000</td>
<td>27.2</td>
</tr>
<tr>
<td>TATB</td>
<td>86</td>
<td>1.65</td>
<td>7300</td>
<td>20.8</td>
</tr>
</tbody>
</table>

- At high TMD, DNGU comparable to RDX. At low TMD, DNGU comparable to TATB
DNGU Testing—Performance

- VoD and Blast pressure measured together (unconfined)
- Pressure measured at 5, 10, and 15 feet intervals.
- DNGU pressure: ~73% of RDX
  - (TATB: PBX—9502 (95% TATB) has a pressure of ~ 76% of RDX/Viton-calculated at similar TMD)
- RDX/Viton VoD: ~8000 m/s
- DNGU/Viton VoD: ~7600 m/s
  - (TATB: PBX—9502 (5% KelF) has a VoD of ~7600 m/s)
    - Reported value
- All data is preliminary.

• Data indicates DNGU has TATB-like performance
DNGU Testing - LSGT

- DNGU coated with 5% Viton compared against RDX (class 1) coated with 5% Viton
- DNGU: 130 cards
- RDX: 301 cards
- (TATB: PBX—9502 (5% KelF) has a card gap of approximately 70 cards (50% point at 97% TMD))

• DNGU is much less shock-sensitive than RDX
Conclusions

- DNGU is an affordable, insensitive energetic material that may find use in explosives and propellants
- DNGU shows promise as:
  - An alternative to TATB (better on cost)
  - An alternative to NTO (no water solubility)
  - A way to reduce use of RDX in energetic formulations
Path Forward

• Further development (synthesis and recrystallization) needed to optimize particle shape and size.
• Evaluate DNGU as a TATB alternative in pressable formulations such as PBXN-7 and PBXW-14.
• Evaluate DNGU as an NTO alternative in melt-pour formulations such as IMX-101 and IMX-104.
• Use these formulations to generate more performance (VoD, pressure) and sensitivity (LSGT) data for DNGU
• Evaluate DNGU for propellant applications.
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